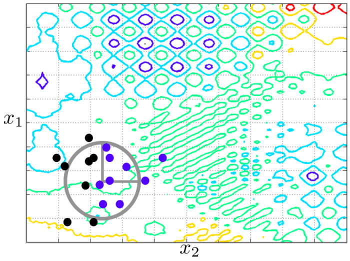
Optimization in Machine Learning

Evolutionary Algorithms
CMA-ES Wrap Up



Learning goals

- Advantages & Limitations
- IPOP-CMA-ES
- Benchmark

CMA-ES: WRAP UP

Algorithm CMA-ES

Input: $m \in \mathbb{R}^d$, $\sigma \in \mathbb{R}_+$, λ (problem-dependent)

Initialize: $\boldsymbol{C} = \mathbb{I}$, $\boldsymbol{p_c} = \boldsymbol{0}$, $\boldsymbol{p}_\sigma = \boldsymbol{0}$

Set: $c_{\boldsymbol{C}} \approx 4/d$, $c_\sigma \approx 4/d$, $c_1 \approx 2/d^2$, $c_\mu \approx \mu_w/d^2$, $c_1 + c_\mu \leq 1$, $d_\sigma \approx 1 + \sqrt{\mu_w/d}$ and $w_{i=1,\dots,\mu}$ such that $\mu_w = \frac{1}{\sum_{i=1}^{\mu} w_i^2} \approx 0.3\lambda$

while not terminate **do**

- $\boldsymbol{x}^{(i)} = \boldsymbol{m} + \sigma\mathcal{N}(\boldsymbol{0}, \boldsymbol{C}) \quad$ for $i = 1, \dots, \lambda$ — *Sampling*
- $\boldsymbol{y}_w = \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}$, where $\boldsymbol{y}_{i:\lambda} = (\boldsymbol{x}_{i:\lambda} - \boldsymbol{m})/\sigma$ — *Selection/Recombination*
- $\boldsymbol{m} \leftarrow \boldsymbol{m} + \sigma \boldsymbol{y}_w$ — *Update* $\boldsymbol{m}$
- $\boldsymbol{p_C} \leftarrow (1 - c_{\boldsymbol{C}})\boldsymbol{p_C} + \sqrt{c_{\boldsymbol{C}}(2 - c_{\boldsymbol{C}})\mu_w}\,\boldsymbol{y}_w$ — *Cumulation of* $\boldsymbol{C}$
- $\boldsymbol{p}_\sigma \leftarrow (1 - c_\sigma)\boldsymbol{p}_\sigma + \sqrt{c_\sigma(2 - c_\sigma)\mu_w}\,\boldsymbol{C}^{-1/2}\boldsymbol{y}_w$ — *Cumulation of* σ
- $\boldsymbol{C} \leftarrow (1 - c_1 - c_\mu \sum w_j)\boldsymbol{C} + c_1 \boldsymbol{p_C}\boldsymbol{p_C}^\top + c_\mu \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}\boldsymbol{y}_{i:\lambda}^\top$ — *Update* $\boldsymbol{C}$
- $\sigma \leftarrow \sigma \times \exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{||\boldsymbol{p}_\sigma||}{\mathbb{E}||\mathcal{N}(\boldsymbol{0}, \mathbb{I})||} - 1\right)\right)$ — *Update* σ

end while

CMA-ES: WRAP UP - DEFAULT VALUES

Related to selection and recombination:

- $\boldsymbol{\lambda}$: offspring number, population size $\quad 4 + \lfloor 3 \ln d \rfloor$
- $\boldsymbol{\mu}$: parent number, solutions involved in mean update $\quad \lfloor \lambda / 2 \rfloor$
- $\boldsymbol{w_i}$: recombination weights (preliminary convex shape)
  $\ln \frac{\lambda+1}{2} - \ln i, \;\text{for } i = 1, \ldots, \lambda$

Related to $\boldsymbol{C}$-update:

- $\mathbf{1} - \boldsymbol{c_C}$: decay rate for evolution path, cumulation factor $\quad 1 - \frac{4+\mu_w/d}{d+4+2\mu_w/d}$
- $\boldsymbol{c_1}$: learning rate for rank-one update of $\boldsymbol{C}$ $\quad \frac{2}{(d+1.3)^2+\mu_w}$
- $\boldsymbol{c_\mu}$: learning rate for rank-μ update of $\boldsymbol{C}$ $\quad \min\left(1 - c_1, 2 \cdot \frac{\mu_w - 2 + 1/\mu_w}{(d+2)^2+\mu_w}\right)$

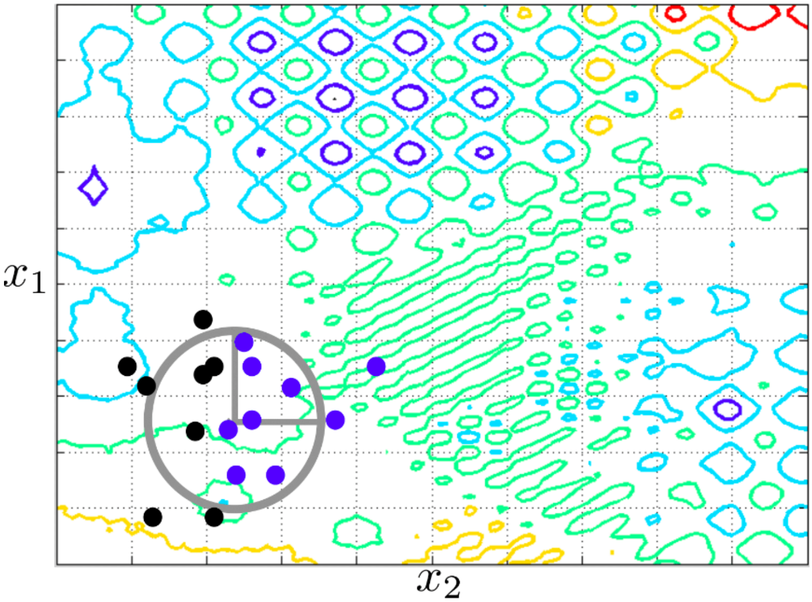
Related to σ-update:

- $\mathbf{1} - \boldsymbol{c_\sigma}$: decay rate for evolution path $\quad 1 - \frac{\mu_w+2}{d+\mu_w+5}$
- $\boldsymbol{d_\sigma}$: damping for σ-change $\quad 1 + 2\max\left(0, \sqrt{\frac{\mu_w-1}{d+1}} - 1\right) + c_\sigma$

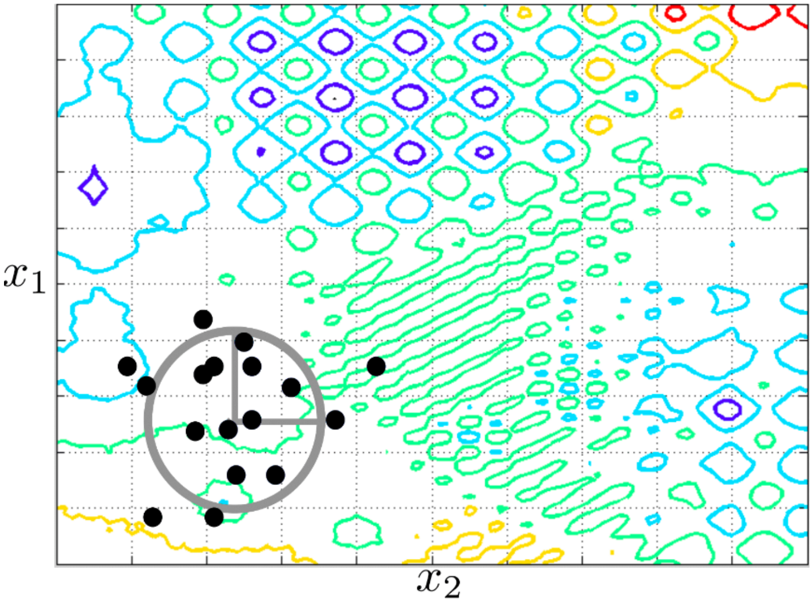
with $\mu_w = \left(\frac{||\boldsymbol{w}||_1}{||\boldsymbol{w}||_2}\right) = \frac{(\sum_{i=1}^{\mu} |w_i|)^2}{\sum_{i=1}^{\mu} w_i^2} = \frac{1}{\sum_{i=1}^{\mu} w_i^2}$ and typical default parameter values.

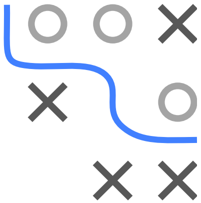
- μ_w can be extended to λ instead of μ weights, allowing negative weights for the remaining $\lambda - \mu$ points (“active covariance adaptation”).

CMA-ES: WRAP UP

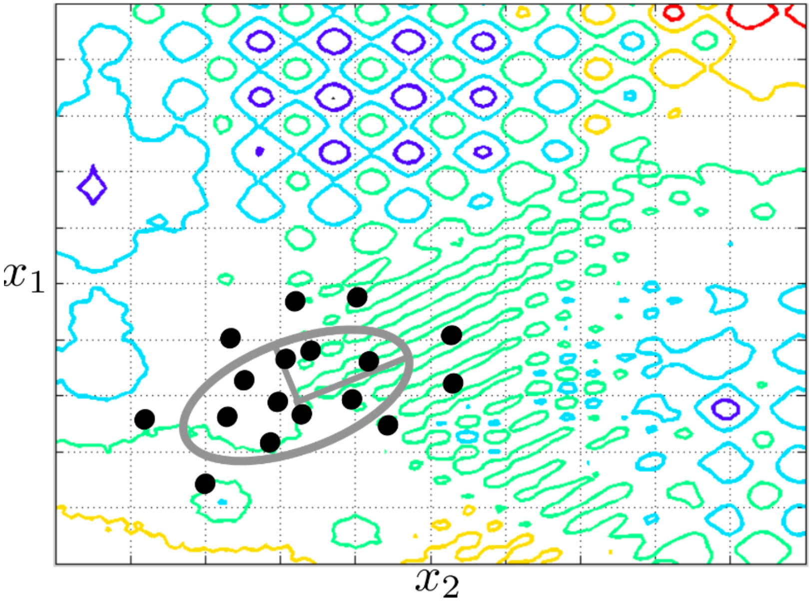


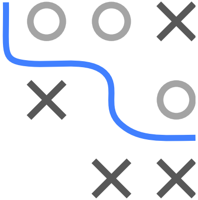
CMA-ES: WRAP UP



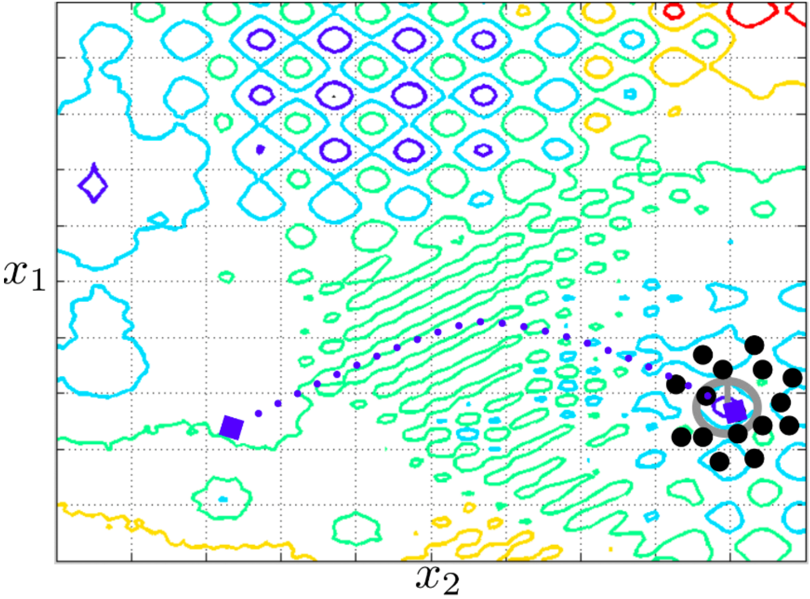


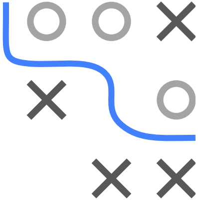
CMA-ES: WRAP UP





CMA-ES: WRAP UP





CMA-ES: WRAP UP - ADVANTAGES

- CMA-ES can outperform other strategies in following cases:
- Non-separable problems (parameters of the objective function are dependent)
- Derivative of the objective function is not available
- High-dimensional problems (large d)
- Very large search space
- Useful in case “classical” search methods like quasi-Newton methods (BFGS) or conjugate gradient methods fail due to a non-convex or rugged search landscape (e.g. outliers, noise, local optima, sharp bends).

CMA-ES: WRAP UP - LIMITATIONS

- CMA-ES can be outperformed by other strategies in following cases:
- Partly separable problems (i.e. optimization of n-dimensional objective function can be divided into a series of d optimizations of every single parameter)
- Derivative of the objective function is easily available $\rightarrow$ Gradient Descent / Ascent
- Low dimensional problems (small d)
- Problems that can be solved by using a relatively small number of function evaluations (e.g. $< 10d$ evaluations)

CMA-ES: IPOP

- Many special forms and extensions of the “basic” CMA-ES exist
- CMA-ES efficiently minimizes unimodal objective functions and is in particular superior on ill-conditioned, non-separable problems
- Default population size $\lambda_{default}$ has been tuned for unimodal functions and however can get stuck in local optima on multi-modal functions, such that convergence to global optima is not guaranteed
- It could be shown that increasing the population size improves the performance of the CMA-ES on multi-modal functions
- **IPOP-CMA-ES** is a special form of restart-CMA-ES, where the *population size is increased for each restart* (IPOP)
- By increasing the population size the search characteristic becomes more global after each restart
- For the restart strategy CMA-ES is stopped whenever some stopping criterion is met, and an independent restart is launched with the population size increased by a factor of 2 (values between 1.5 and 5 are reasonable).

CMA-ES: WRAP UP - BENCHMARK EAS

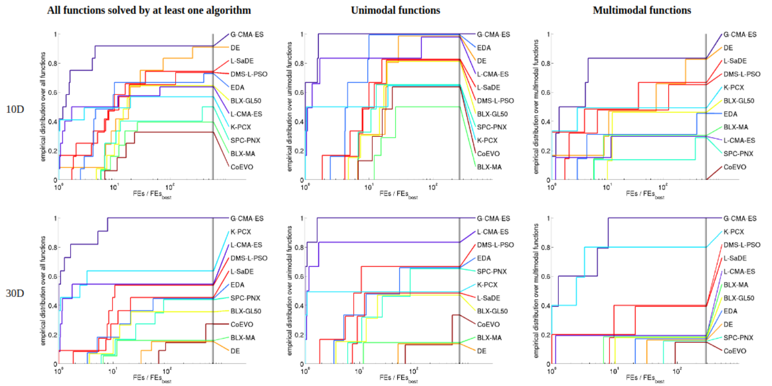
- **Example:** Black-box optimization of 25 benchmark functions under thoroughly defined experimental and recording conditions for the 2005 IEEE Congress on Evolutionary Computation: Session on Real-Parameter Optimization.
  ▸ Suganthan et al. 2005

  17 papers were submitted, 11 were accepted, thereunder hybrid methods.
  Two of the Algorithms:

- L-CMA-ES: A CMA evolution strategy with small population size and small initial step-size to emphasize on local search characteristics. Independent restarts are conducted until the target function value is reached or the maximum number of function evaluations is exceeded. ▸ Auger and Hansen 2005b

- G-CMA-ES: A CMA evolution strategy restarted with increasing population size (IPOP). Independent restarts are conducted with increasing population size until the target function value is reached or the maximum number of function evaluations is exceeded. With the initial small population size the algorithm converges fast, with the succeeding larger population sizes the global search performance is emphasized in subsequent restarts. ▸ Auger and Hansen 2005a

CMA-ES: WRAP UP - BENCHMARK EAS



- Comparison of performance results from 11 algorithms for search space dimension 10 and 30 on different function subsets
- Expected number of function evaluations (FEs) to reach the target function value is normalized by the value of the best algorithm on the respective function FEs_{best}
- Calculation of the empirical cumulative distribution function of FEs / FEs_{best} for each algorithm over different sets of functions in 10 and 30D
- Small values for FEs / FEs_{best} and therefore large values of the graphs are preferable.