Convergence of Evolution Strategies with Covariance Matrix Adaptation (CMA-ES)

Armand Gissler

Tuesday 26th September, 2023

CMAP, École polytechnique & Inria
(with Anne Auger & Nikolaus Hansen)

Black-box optimisation and Evolution strategies

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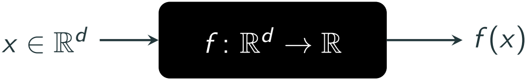

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CMA-ES approximates the minimum x^* of f by a multivariate normal distribution $\mathcal{N}(m, C)$ **by adapting** the mean $m \in \mathbb{R}^d$ **and the covariance matrix** $C \in \mathcal{S}^d_{++}$.

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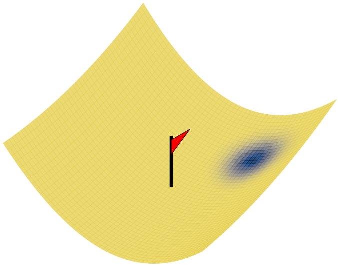

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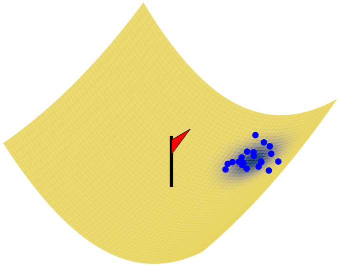

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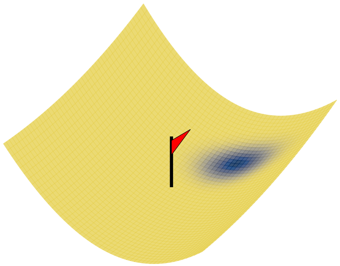

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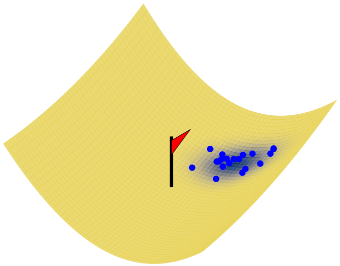

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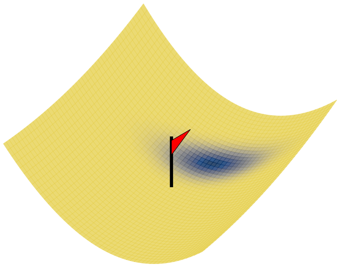

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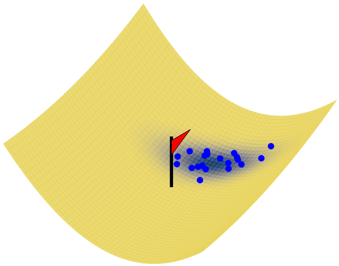

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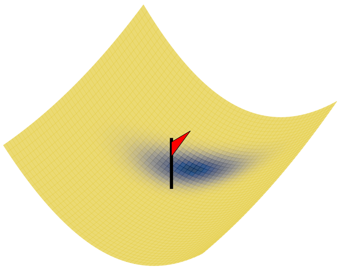

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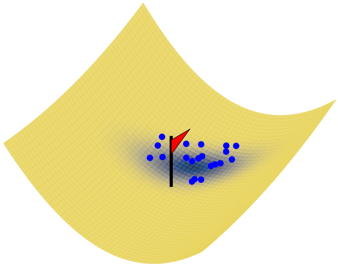

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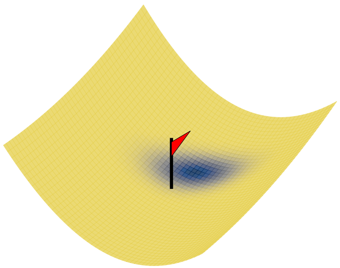

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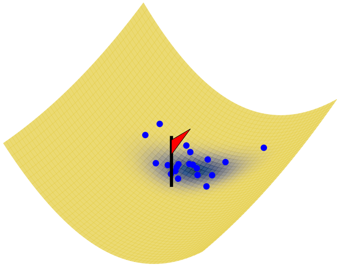

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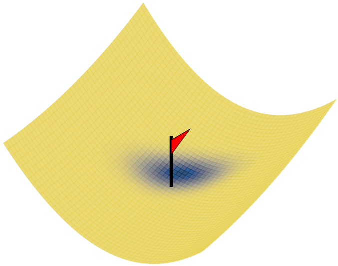

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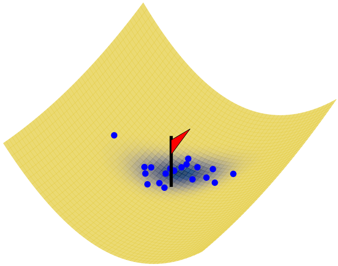

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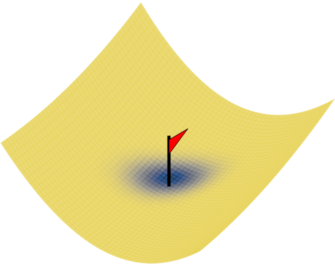

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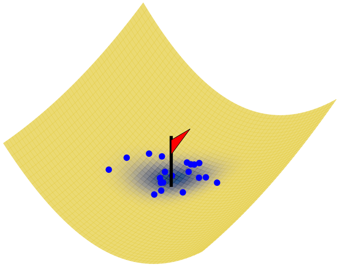

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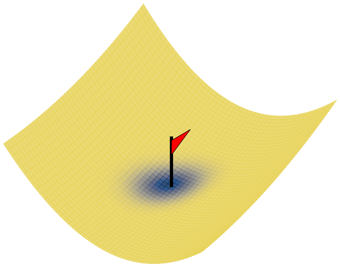

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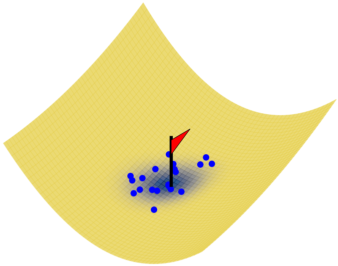

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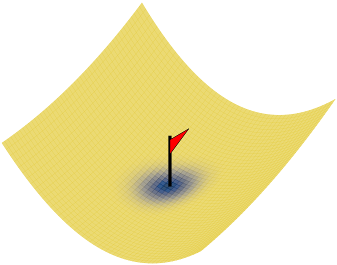

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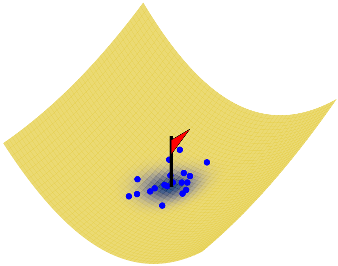

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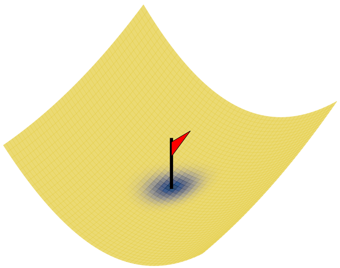

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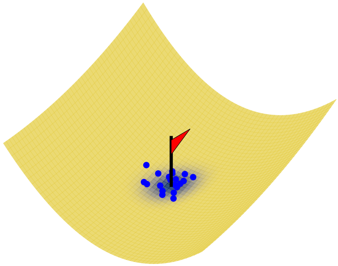

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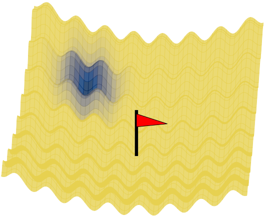

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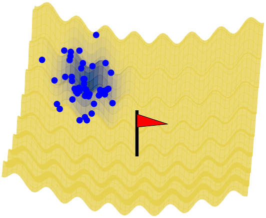

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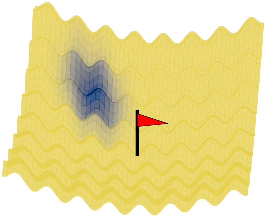

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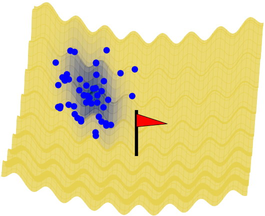

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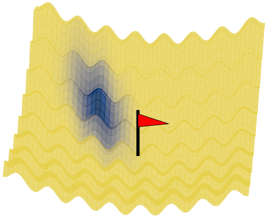

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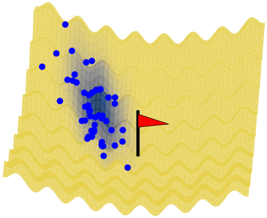

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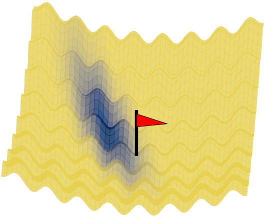

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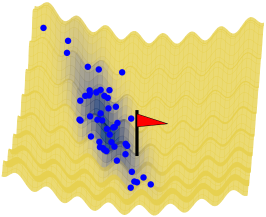

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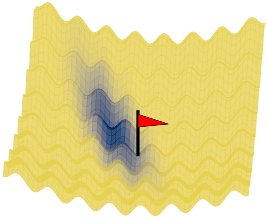

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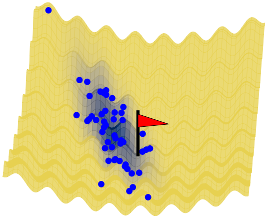

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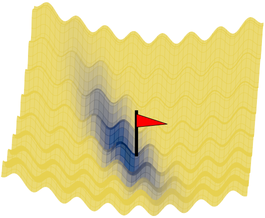

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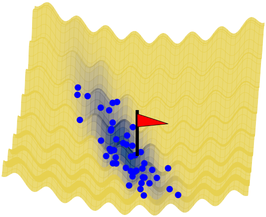

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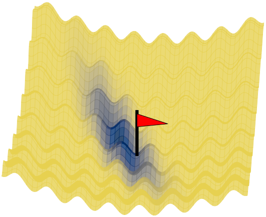

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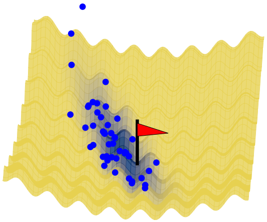

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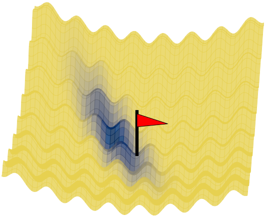

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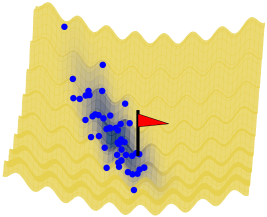

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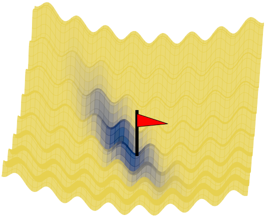

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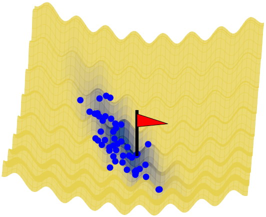

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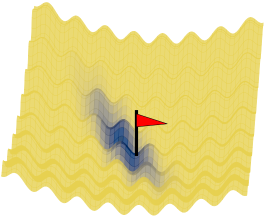

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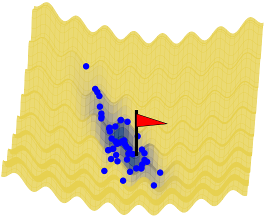

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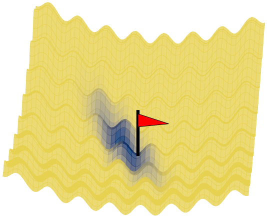

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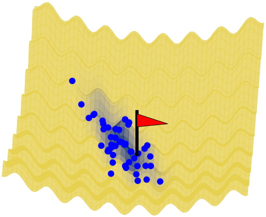

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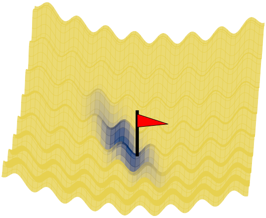

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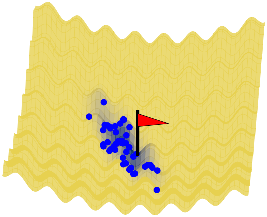

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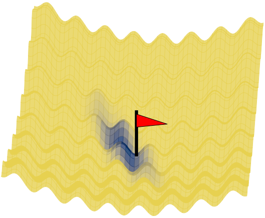

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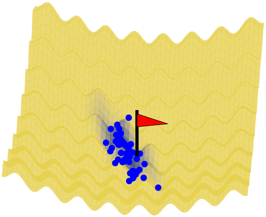

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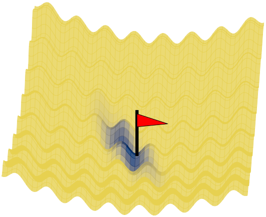

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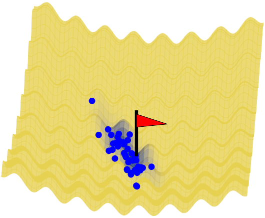

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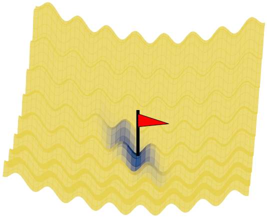

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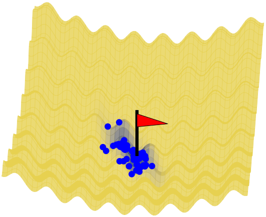

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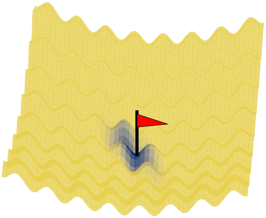

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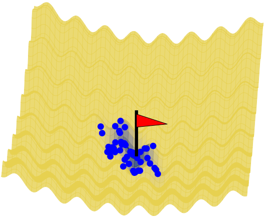

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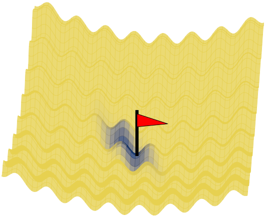

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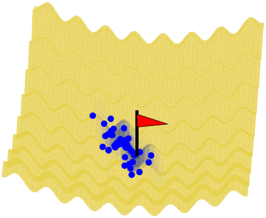

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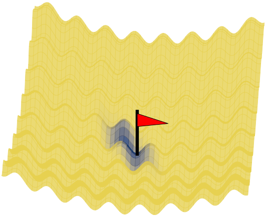

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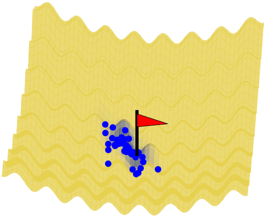

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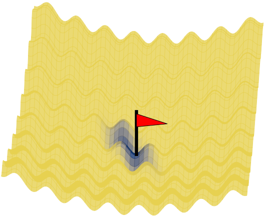

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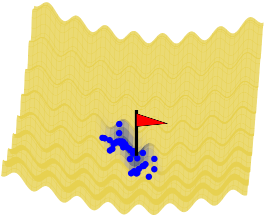

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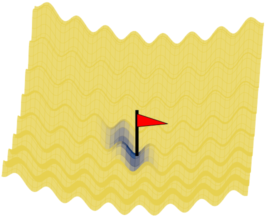

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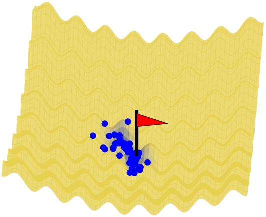
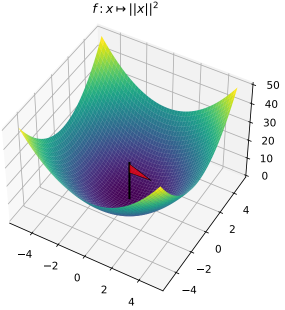
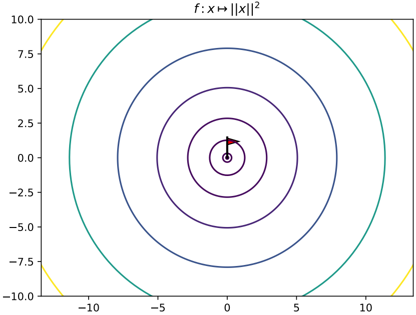


CMA-ES: algorithm presentation

Level sets representation





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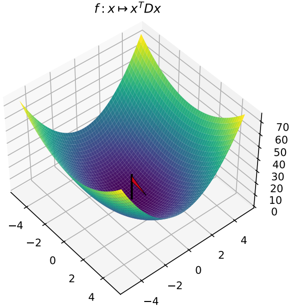

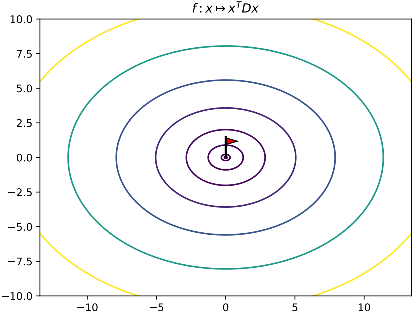

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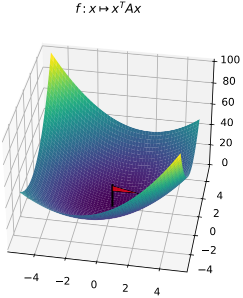
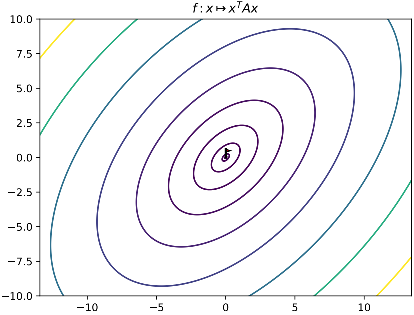
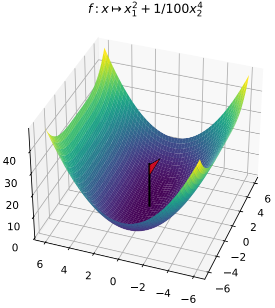
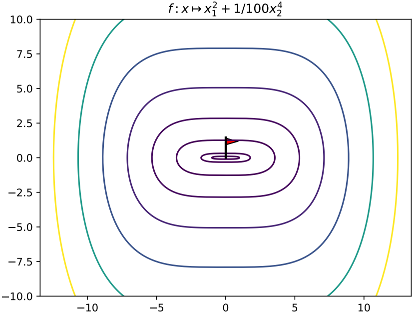


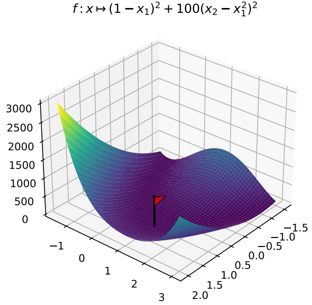


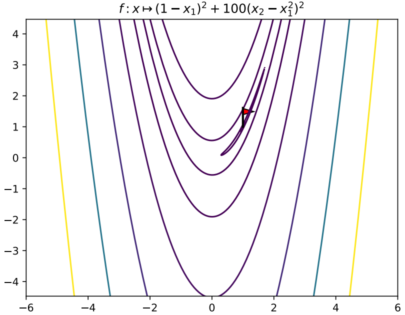
Level sets representation





Level sets representation





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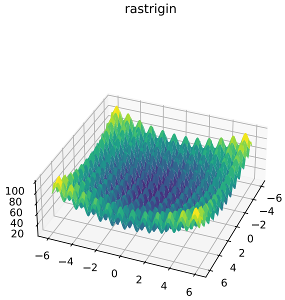
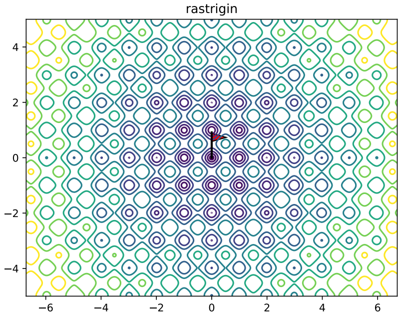
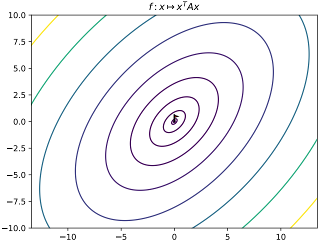




Presentation of the algorithm

Algorithm 1 CMA-ES

Goal: $\min_{x \in \mathbb{R}^d} f(x)$



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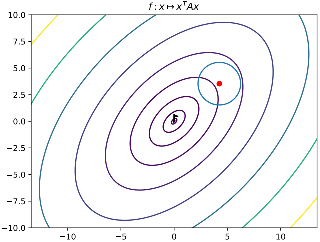
Given: $m_0 \in \mathbb{R}^d$, $C_0 \in \mathcal{S}^d_{++}$



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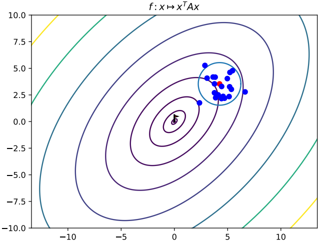

λ population size

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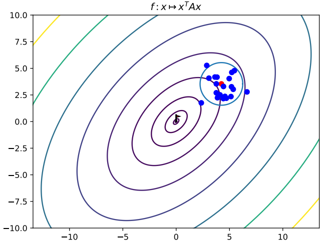

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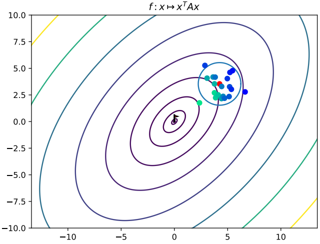

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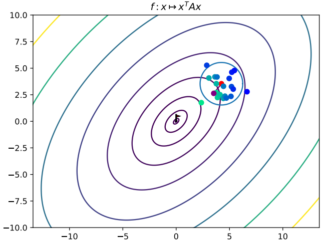

λ population size

μ parent number

Presentation of the algorithm

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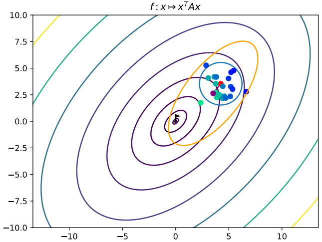
4. $C_{t+1} = (1-c)C_t + c \sum_{i=1}^{\mu} w_i \left[x^{i:\lambda}_{t+1} - m_t\right] \left[x^{i:\lambda}_{t+1} - m_t\right]^T$

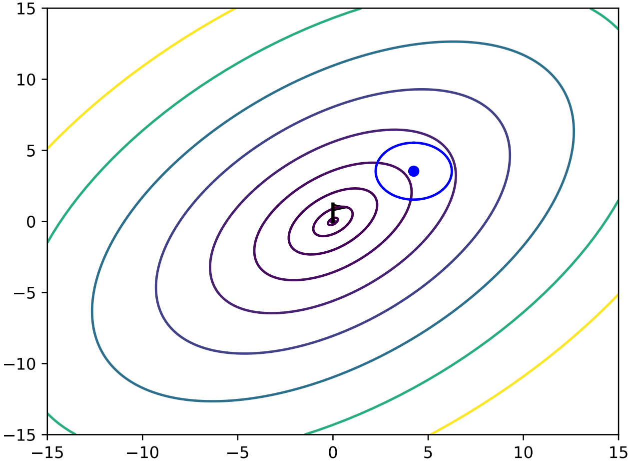


λ population size

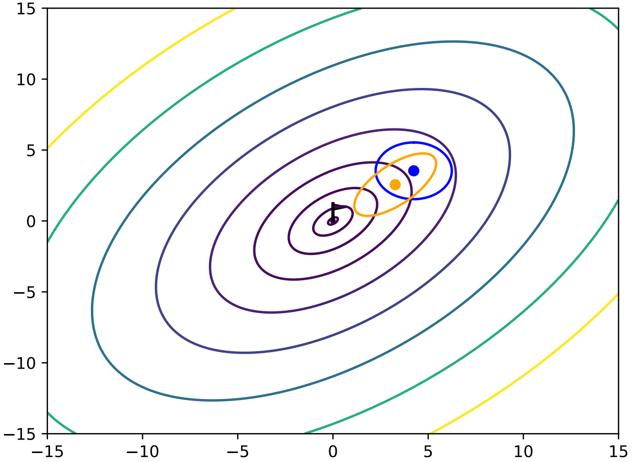
μ parent number

Linear convergence

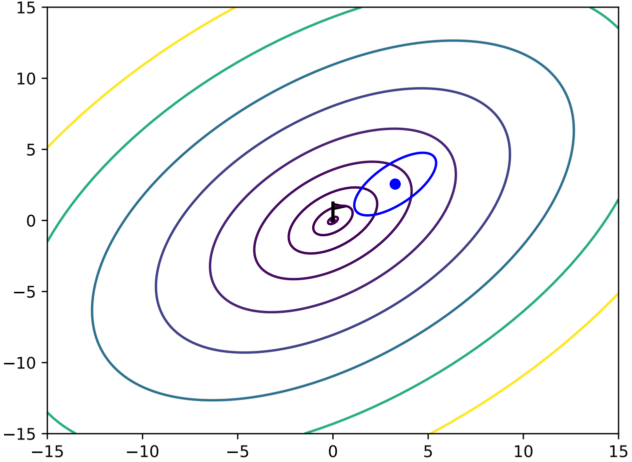
Convergence



Convergence



Convergence



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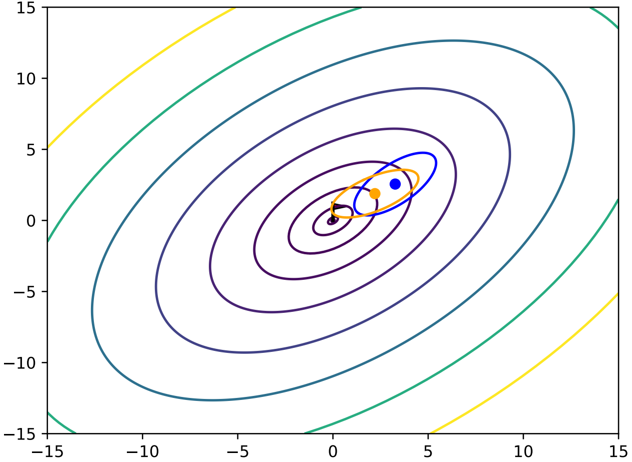

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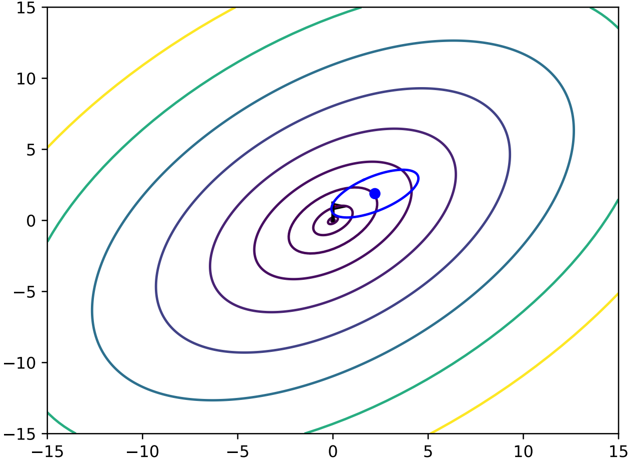
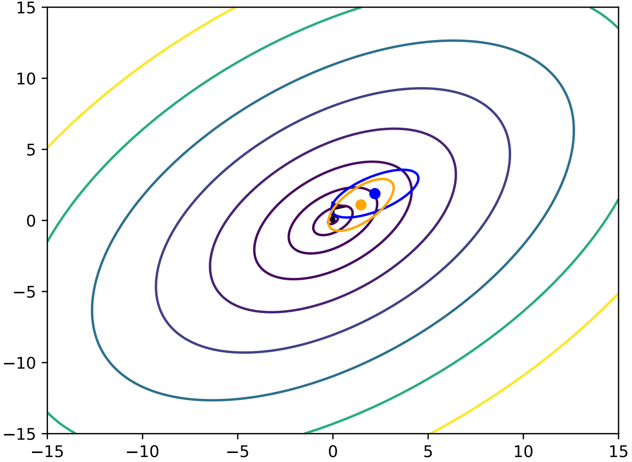


Convergence



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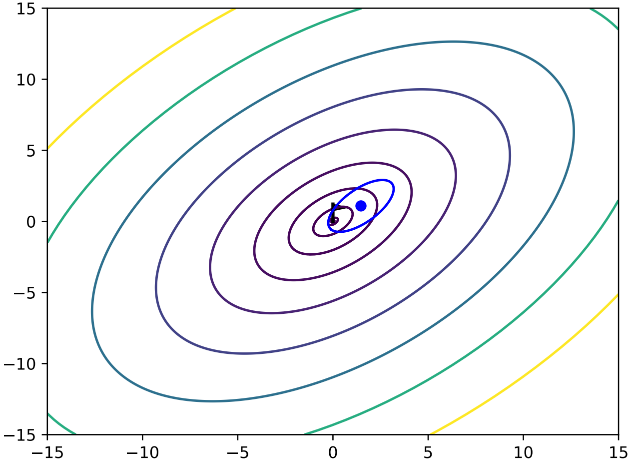

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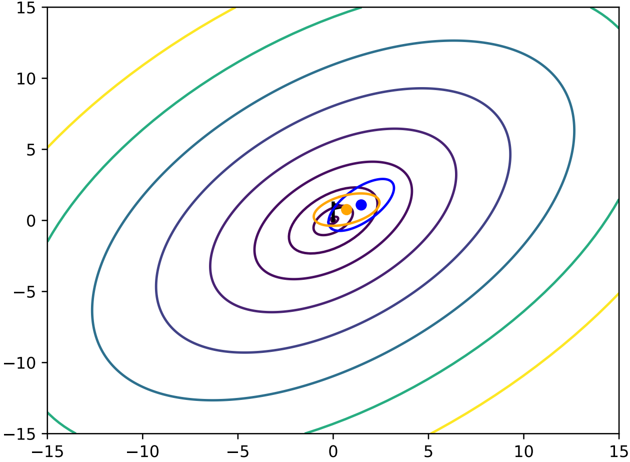

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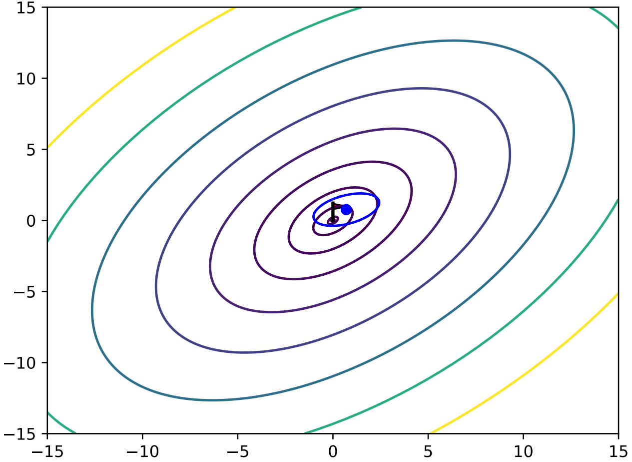

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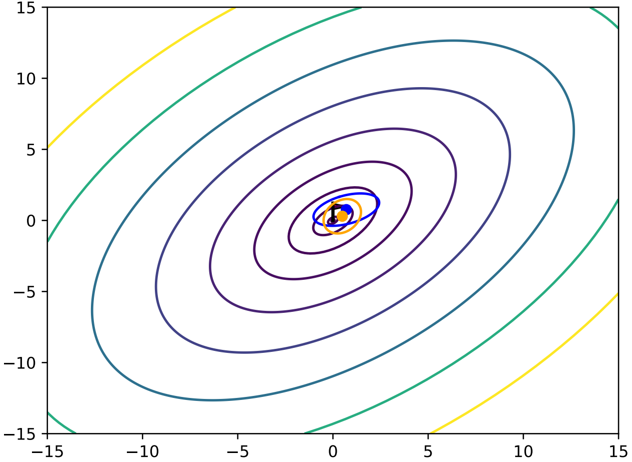

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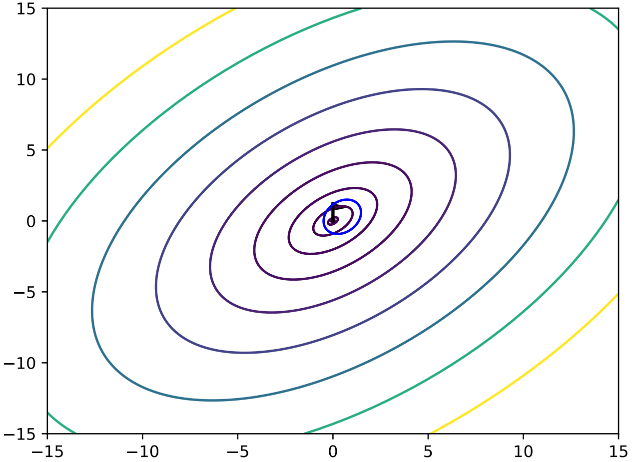

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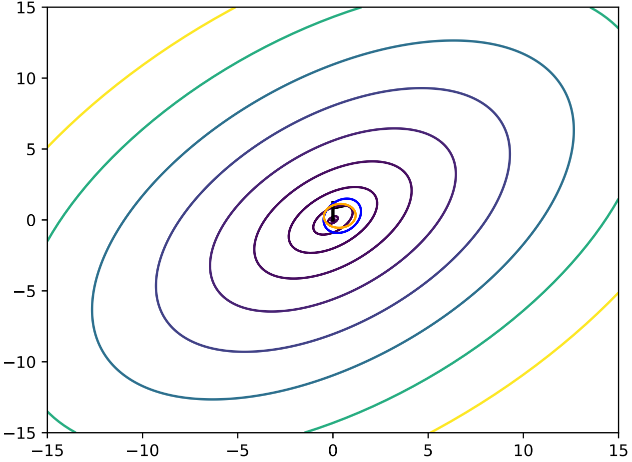

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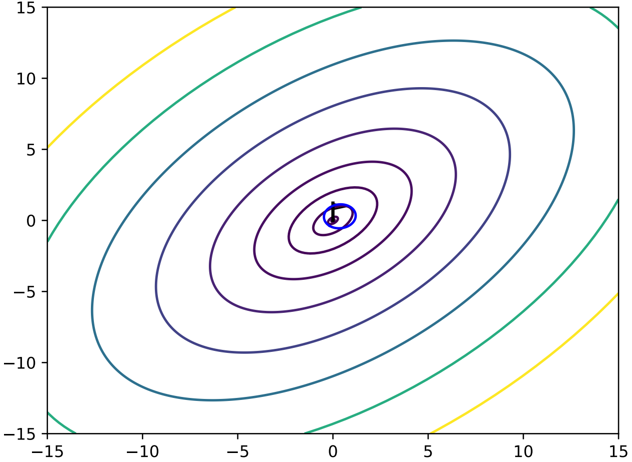

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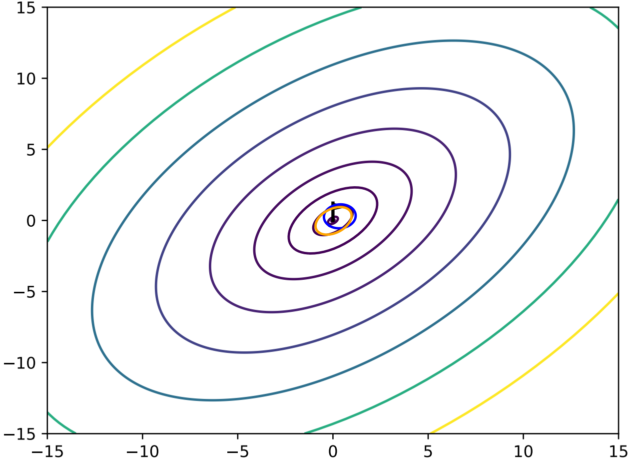

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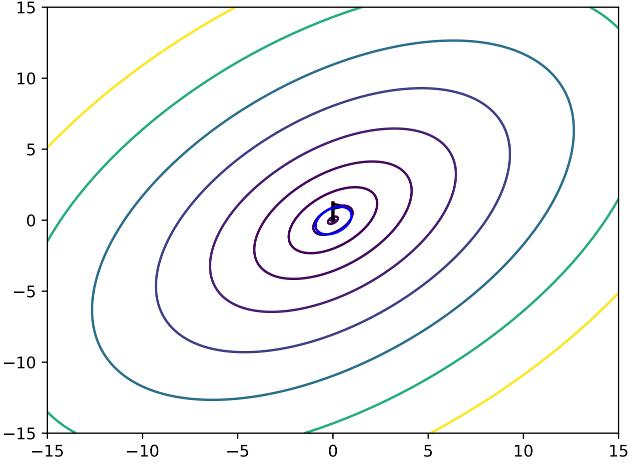

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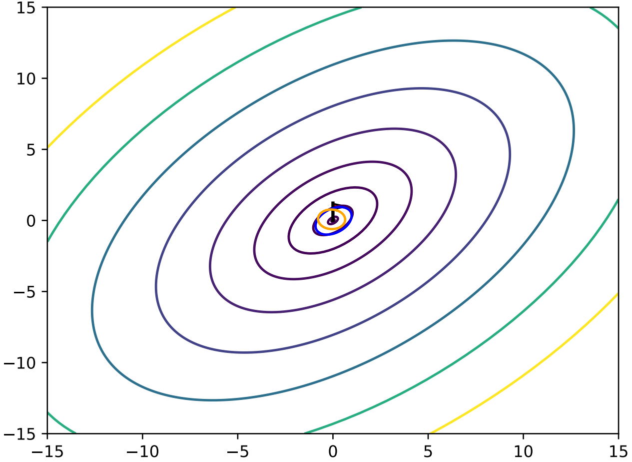

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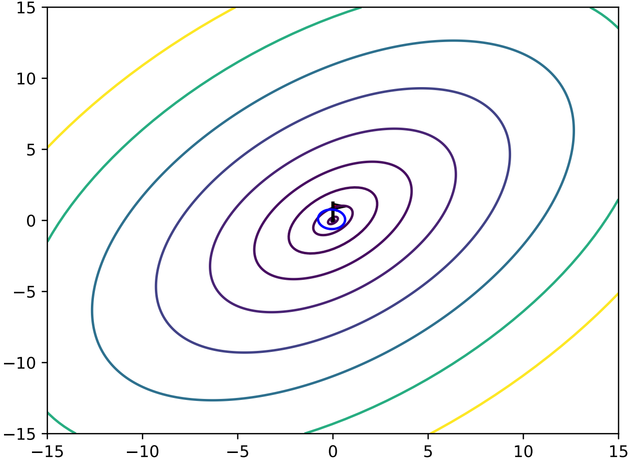

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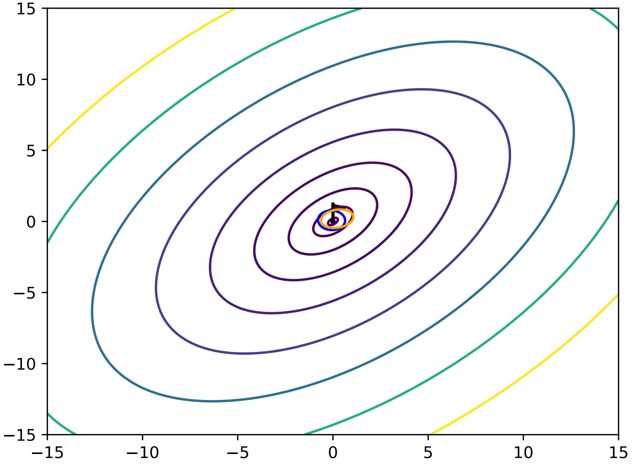

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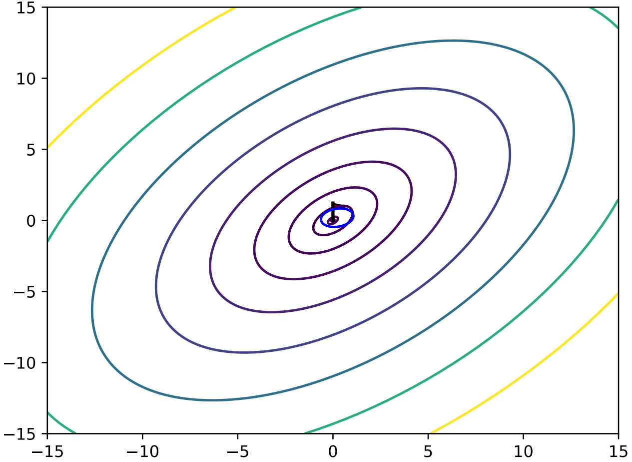

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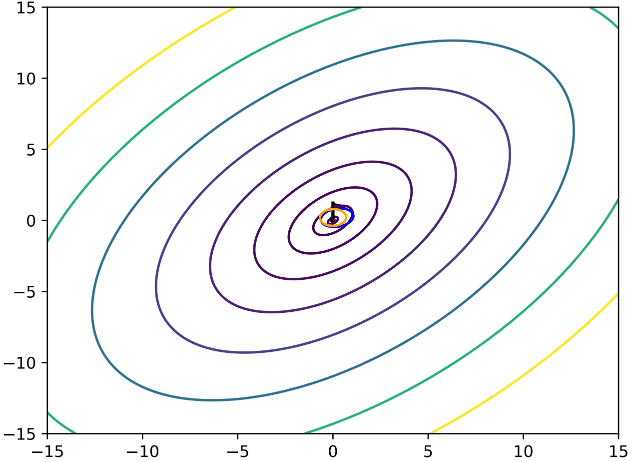

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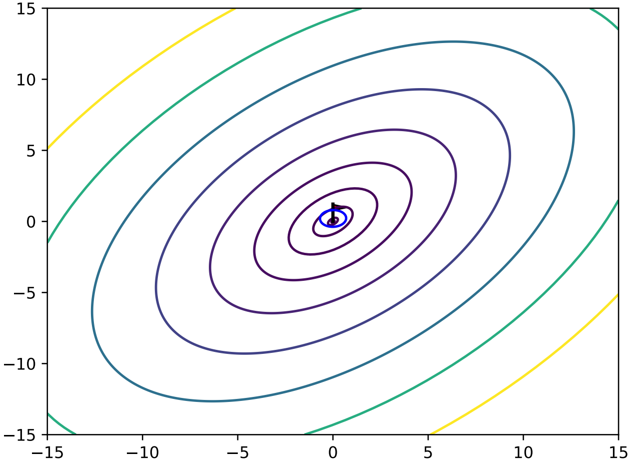

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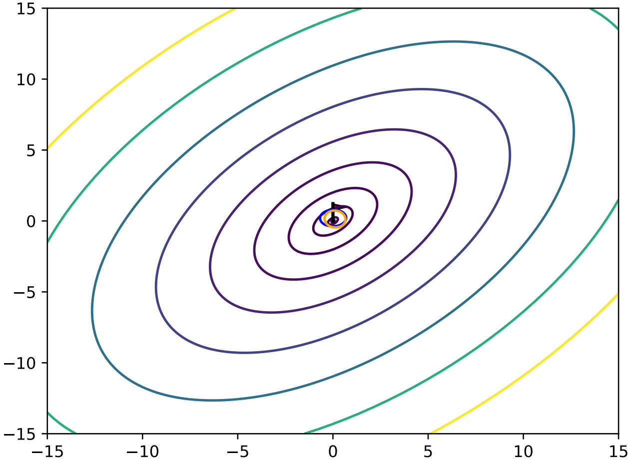

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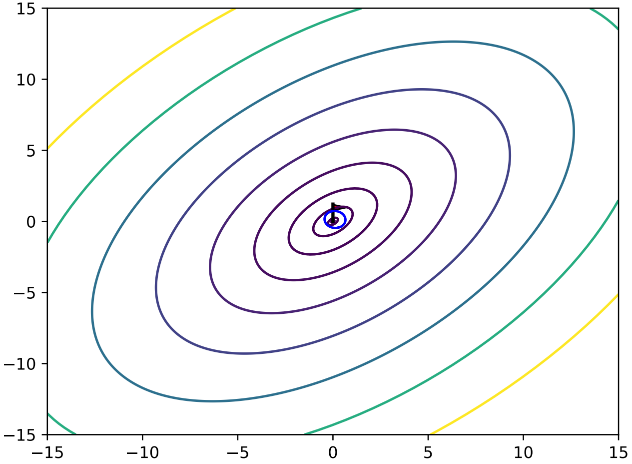

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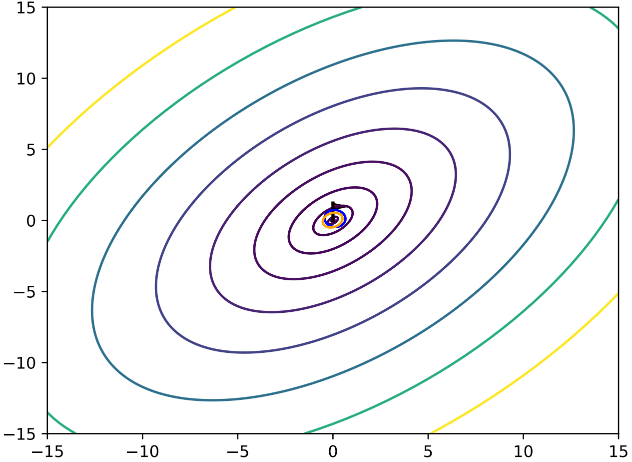

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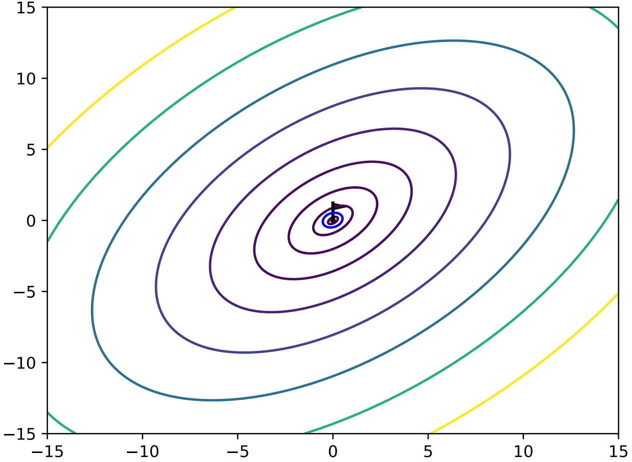

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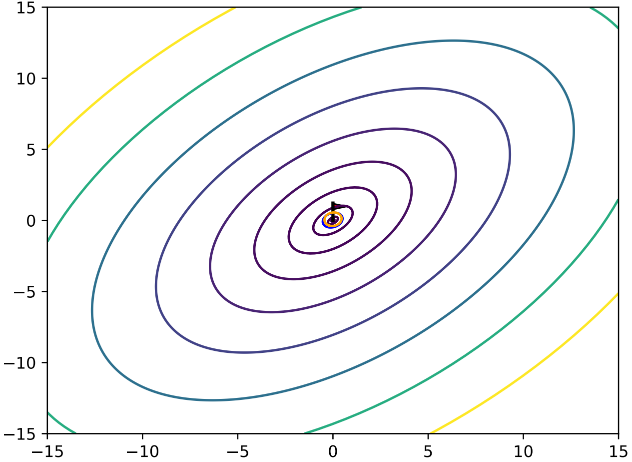

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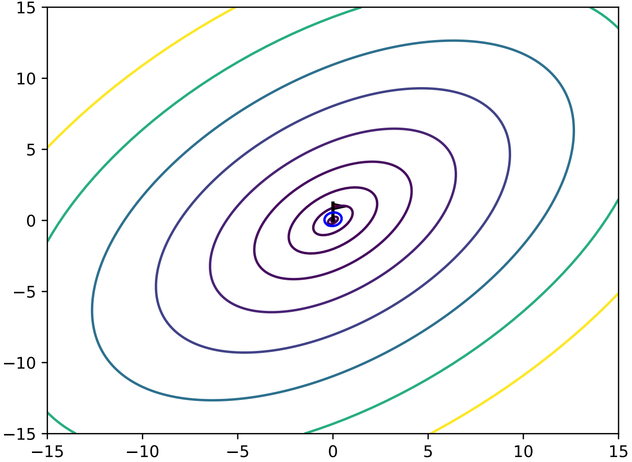

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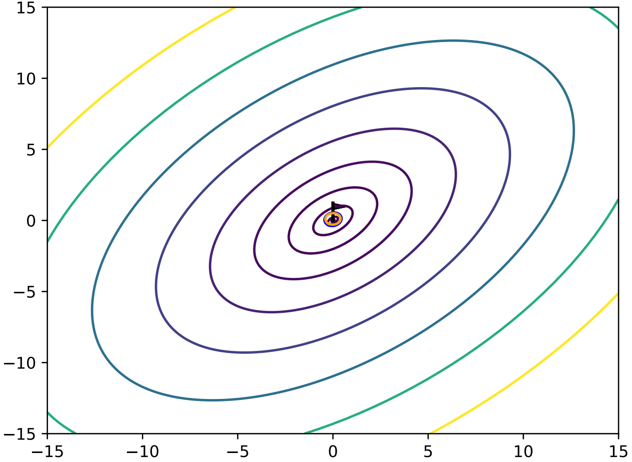

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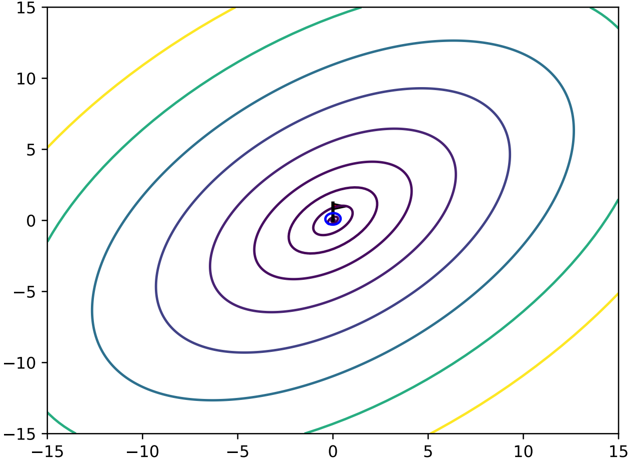

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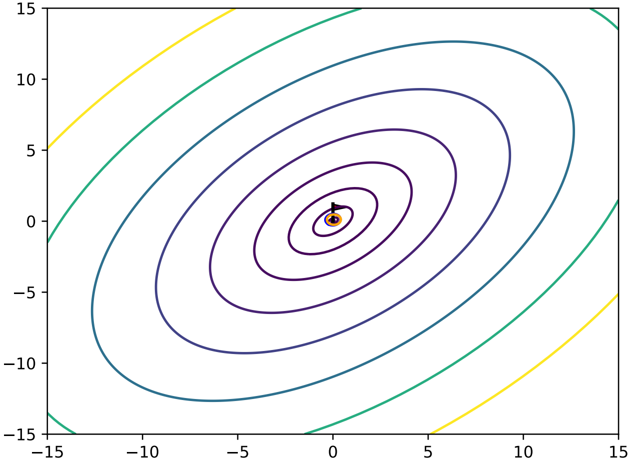

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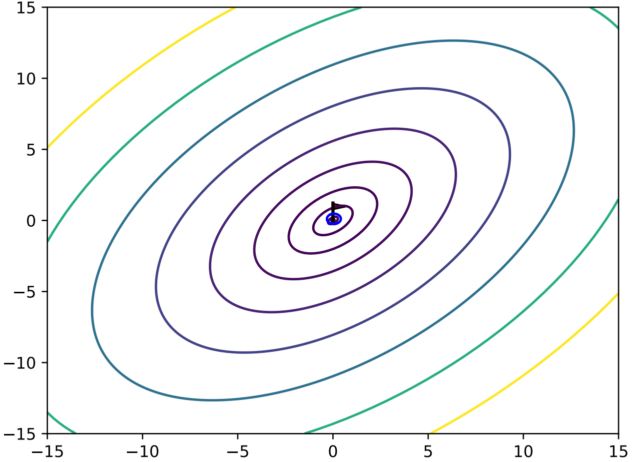

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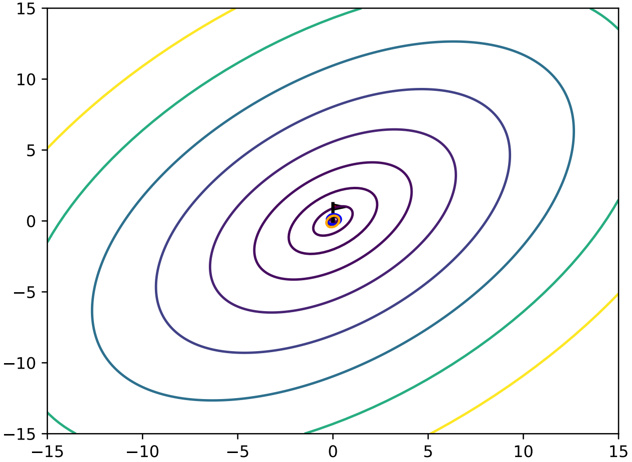

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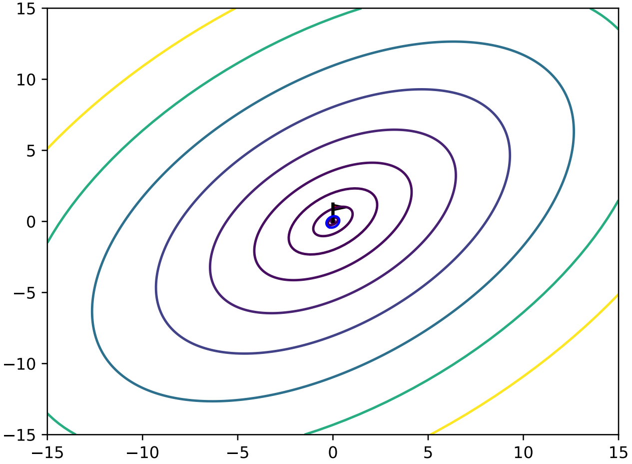

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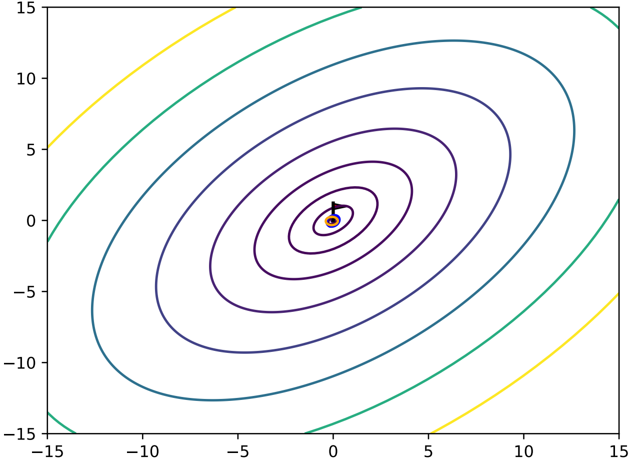

Convergence

We observe

$$m_t \underset{t \to \infty}{\longrightarrow} x^* \in \arg\min f$$

and

$$C_t \underset{t \to \infty}{\longrightarrow} H^{-1}$$

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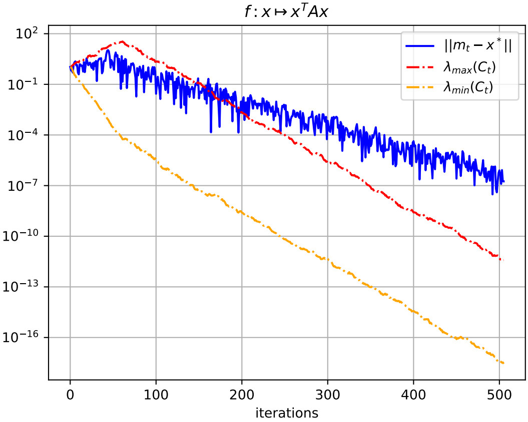
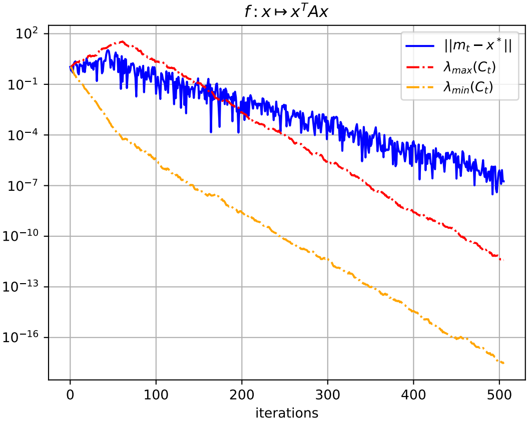
Linear convergence



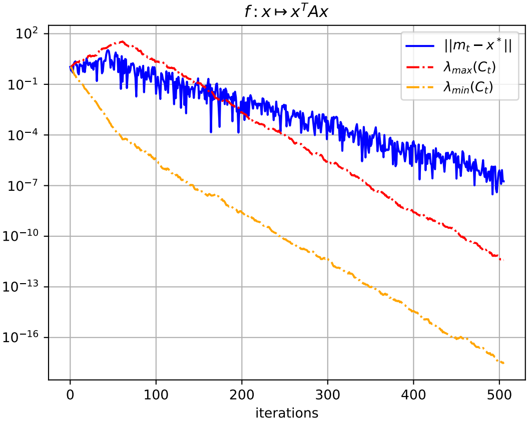
$$\frac{||m_t - x^*||}{||m_0 - x^*||}$$

Linear convergence



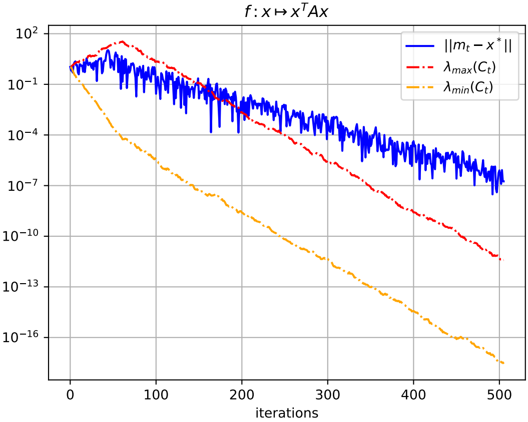
$$\log \frac{\|m_t - x^*\|}{\|m_0 - x^*\|}$$

Linear convergence



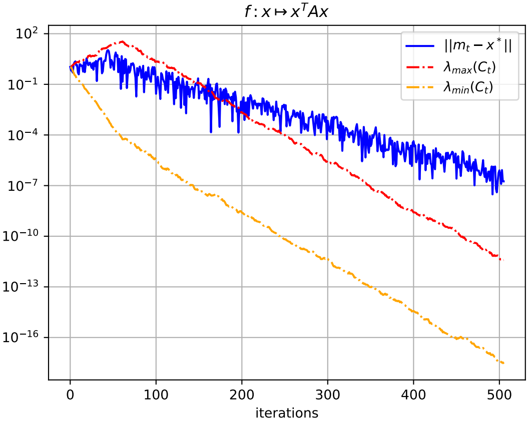
$$\log \frac{\|m_t - x^*\|}{\|m_0 - x^*\|} = -\mathrm{CR} \times t$$

Linear convergence



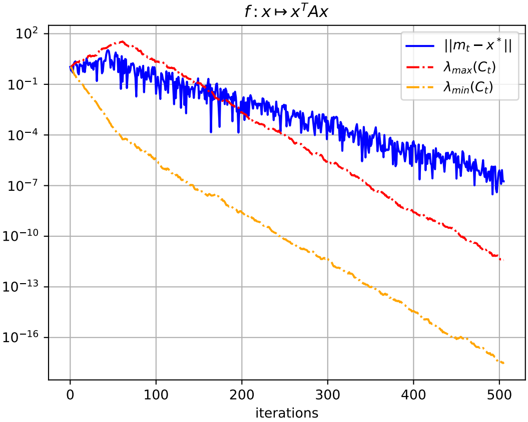
$$\frac{1}{t} \log \frac{\|m_t - x^*\|}{\|m_0 - x^*\|} = -\mathrm{CR}$$

Linear convergence



$$\lim_{t \to \infty} \frac{1}{t} \log \frac{\|m_t - x^*\|}{\|m_0 - x^*\|} = -\mathrm{CR}$$

Linear convergence



$$\lim_{t\to\infty} \frac{1}{t} \log \frac{\|m_t - x^*\|}{\|m_0 - x^*\|} = -\mathrm{CR}$$

Convergence analysis via Markov chains

Markov chains

A **Markov chain** is a random sequence $(\theta_t)_{t\in\mathbb{N}}$ such that

$$\text{Distribution}\left(\theta_{t+1} \mid \theta_0, \ldots, \theta_t\right) = \text{Distribution}\left(\theta_{t+1} \mid \theta_t\right)$$

Presentation of the algorithm

Algorithm 1 CMA-ES

Goal: $\min_{x \in \mathbb{R}^d} f(x)$

Given: $m_0 \in \mathbb{R}^d$, $C_0 \in \mathcal{S}^d_{++}$

For $t = 0, 1, 2, \dots$:

1. $x^1_{t+1}, \dots, x^\lambda_{t+1} \sim \mathcal{N}(m_t, C_t)$
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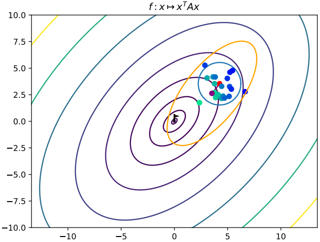

λ population size

μ parent number

Markov chains

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- The Markov chain $(\theta_t)_{t\in\mathbb{N}}$ is **irreducible** if any state is reachable in finite time with positive probability.

Irreducibility of CMA-ES

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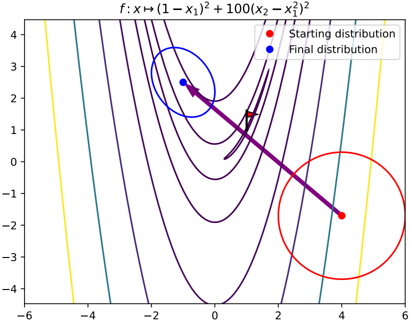

Markov chains

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- The Markov chain $(\theta_t)_{t\in\mathbb{N}}$ is **irreducible** if any state is reachable in finite time with positive probability.
- Then, it admits a **period** $P \geqslant 1$. When $P = 1$, $(\theta_t)_{t\in\mathbb{N}}$ is **aperiodic**.

Markov chains

A **Markov chain** is a random sequence $(\theta_t)_{t \in \mathbb{N}}$ such that

$$\mathrm{Distribution}\left(\theta_{t+1} \mid \theta_0, \ldots, \theta_t\right) = \mathrm{Distribution}\left(\theta_{t+1} \mid \theta_t\right)$$

- The Markov chain $(\theta_t)_{t \in \mathbb{N}}$ is **positive recurrent** if there exists a unique **invariant** probability measure π, i.e.,

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  (π is a fixed point for $(\theta_t)_{t\in\mathbb{N}}$)
- If the chain is irreducible, aperiodic, positive recurrent, then a **Law of Large Numbers** (LLN) holds

  $$\lim_{T\to\infty} \frac{1}{T} \sum_{t=0}^{T-1} f\left(\theta_t\right) = \int f(\theta)\, d\pi(\theta).$$

CMA-ES as a Markov chain

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Question: Could we use the **LLN** for Markov chains to prove the **linear convergence** of CMA-ES?

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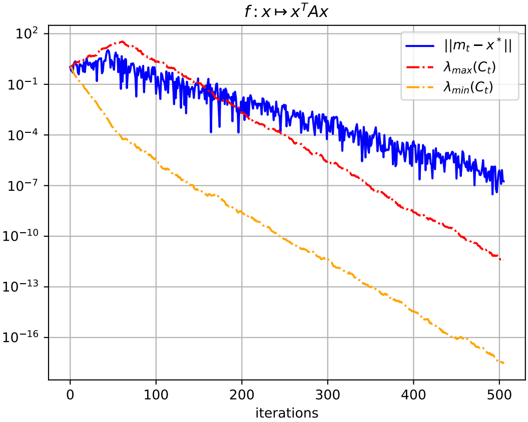
If π is an invariant measure of $(m_t, C_t)_{t\in\mathbb{N}}$

$$(m_t, C_t) \sim \pi \Rightarrow (m_{t+1}, C_{t+1}) \sim \pi$$

Not possible if $m_t \to x^*$ and $C_t \to 0$.

Linear convergence



$$\lim_{t \to \infty} \frac{1}{t} \log \frac{\|m_t - x^*\|}{\|m_0 - x^*\|} = -\mathrm{CR}$$

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$\|m_t - x^*\|$ and $\lambda_{\min}(C_t) \to 0$

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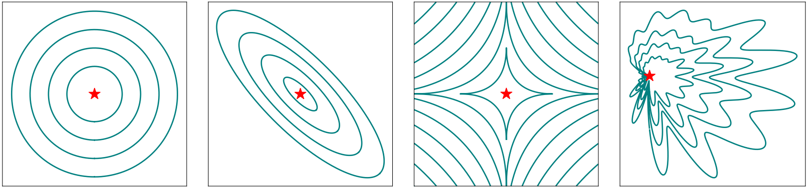
is a Markov chain. (if f is **scaling-invariant***)*

Scaling-invariant functions



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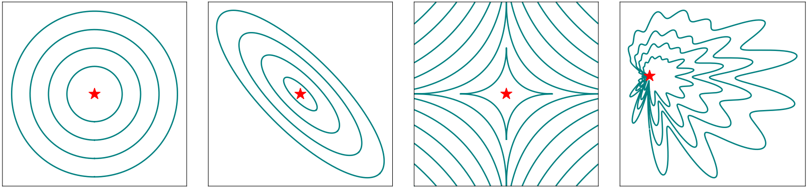


$$f\left(x_{t+1}^{1:\lambda}\right) \leqslant \cdots \leqslant f\left(x_{t+1}^{\lambda:\lambda}\right) \Leftrightarrow f\left(z_{t+1}^{1:\lambda}\right) \leqslant \cdots \leqslant f\left(z_{t+1}^{\lambda:\lambda}\right)$$

Algorithm

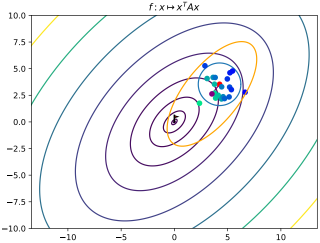
Algorithm 1 CMA-ES

Goal: $\min_{x \in \mathbb{R}^d} f(x)$

Given: $m_0 \in \mathbb{R}^d$, $C_0 \in \mathcal{S}^d_{++}$

For $t = 0, 1, 2, \ldots$:

1. $x^1_{t+1}, \ldots, x^\lambda_{t+1} \sim \mathcal{N}(m_t, C_t)$
2. $\text{sort } f(x^i_{t+1})$:
   $f\left(x^{1:\lambda}_{t+1}\right) \leqslant \cdots \leqslant f\left(x^{\lambda:\lambda}_{t+1}\right)$
3. $m_{t+1} = \sum_{i=1}^{\mu} w_i x^{i:\lambda}_{t+1}$
4. $C_{t+1} = (1-c)C_t + c\sum_{i=1}^{\mu} w_i \left[x^{i:\lambda}_{t+1} - m_t\right]\left[m^{i:\lambda}_{t+1} - m_t\right]^T$



λ population size

μ parent number

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Algorithm 1 normalized CMA-ES

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Given: $z_0 \in \mathbb{R}^d$, $\Sigma_0 \in \mathcal{S}^d_{++}$

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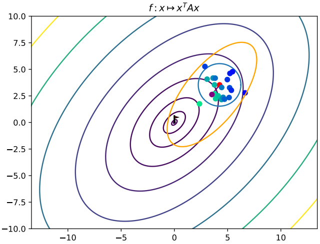

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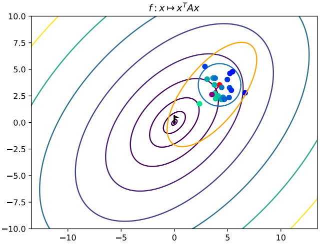

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$$\frac{1}{T}\log\frac{\|m_T - x^*\|}{\|m_0 - x^*\|} = \frac{1}{T}\sum_{t=0}^{T-1}\log\frac{\|z_{t+1}\|}{\|z_t\|} - \frac{1}{2}\log\lambda_{\min}(\tilde{\Sigma}_{t+1})$$

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Corollary

Then

$$(z_t, \Sigma_t)_{t\in\mathbb{N}}$$

is **irreducible** *and* **aperiodic**.

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$$\mathbb{E}_t \left[V \left(z_{t+1}, \Sigma_{t+1} \right) \right] \leqslant (1 - \varepsilon) V \left(z_t, \Sigma_t \right)$$

outside of a compact $\mathcal{K} \subset \Theta$.

Drift condition

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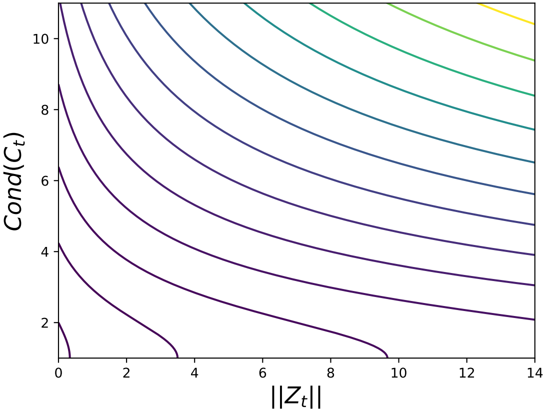

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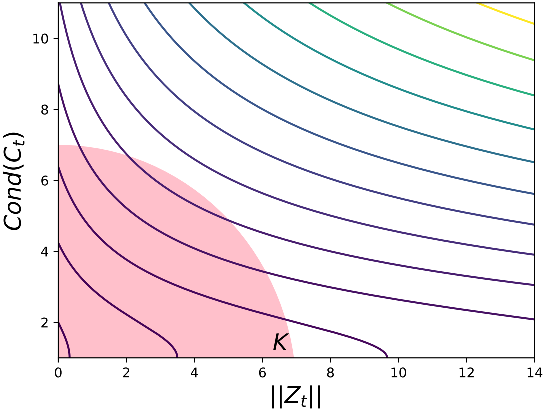

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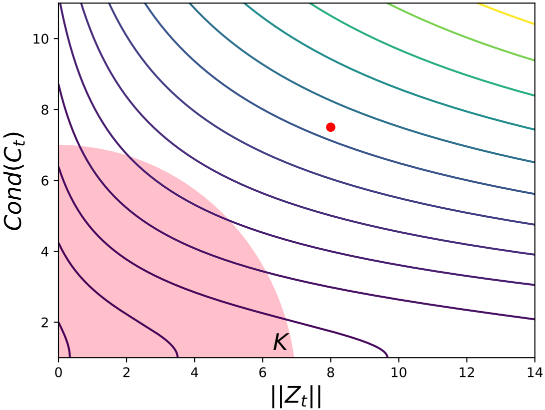

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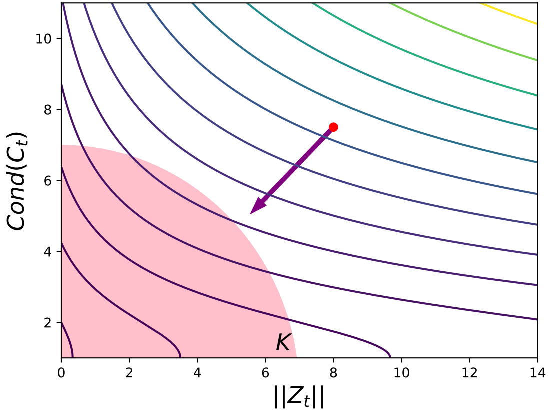

Theorem (Drift condition for the normalized chain)

When minimizing a **spherical** *function* $f : x \mapsto g\left(x^T x\right)$ *then* $(z_t, \Sigma_t)_{t\in\mathbb{N}}$ *satisfies a drift condition with*

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This can be generalized to **ellipsoid** functions $f(x) = g(x^T H x)$ using the **affine-invariance** of CMA-ES.

Affine-Invariance

$$
\begin{array}{ccc}
(m_0, C_0) & \xrightarrow{\min f(x)} & (m_1, C_1) \\
\Psi \big\downarrow & & \big\uparrow \Psi^{-1} \\
(m_0', C_0') & \xrightarrow{\min f(Bx + b)} & (m_1', C_1')
\end{array}
$$

Convergence

Theorem

When $f = g(x^T Hx)$, *then*

$$\lim_{T\to\infty} \frac{1}{T} \log \frac{\|m_T - x^*\|}{\|m_0 - x^*\|} = \lim_{t\to\infty} \mathbb{E}\left[\log \frac{\|m_{t+1} - x^*\|}{\|m_t - x^*\|}\right] = -\mathrm{CR}$$

and

$$\lim_{t\to\infty} \mathbb{E}\left[\frac{C_t}{\det C_t}\right] \propto H^{-1}.$$

Thank you!