

Convergence analysis of evolution strategies with covariance matrix adaptation

PhD students seminar

Armand Gissler

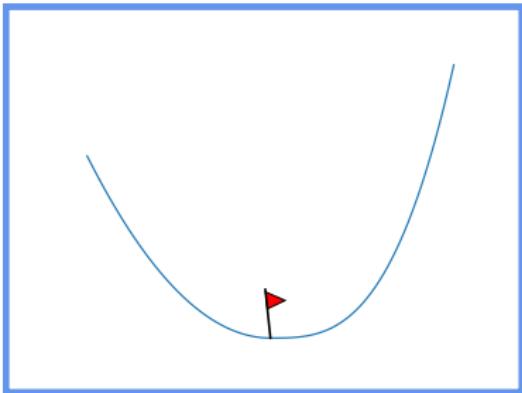
Wednesday 10th April, 2024

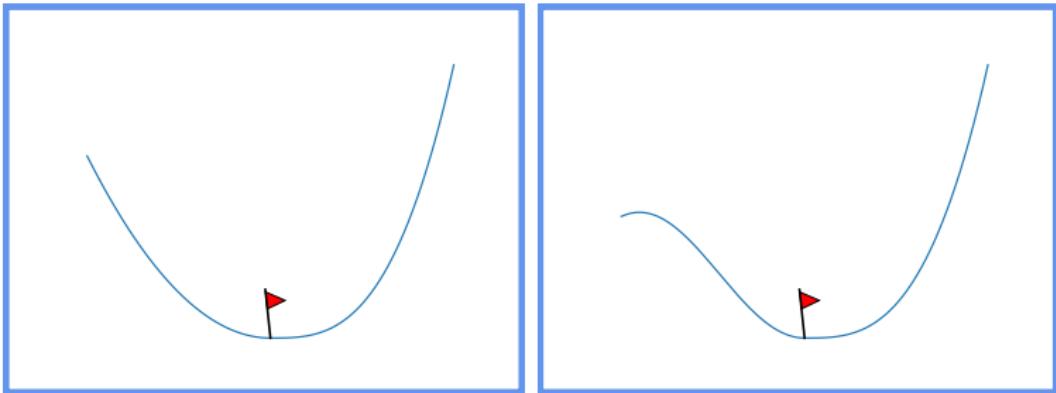
RandOpt team, Inria & École
polytechnique

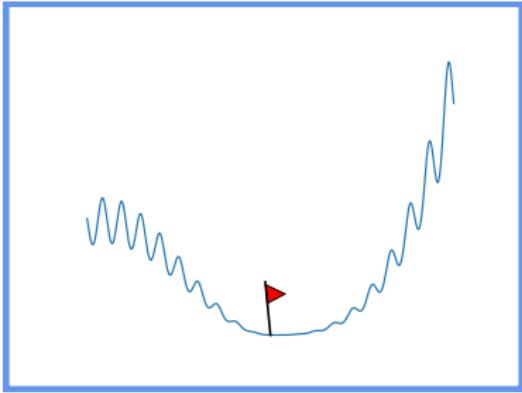
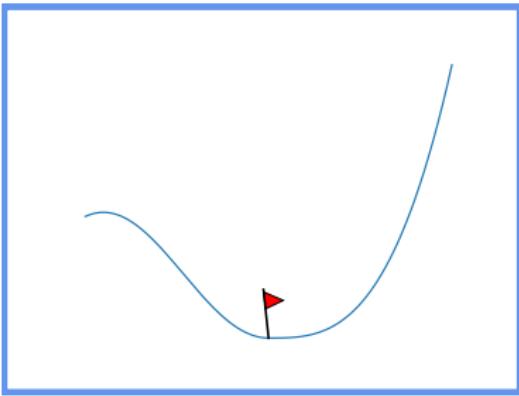
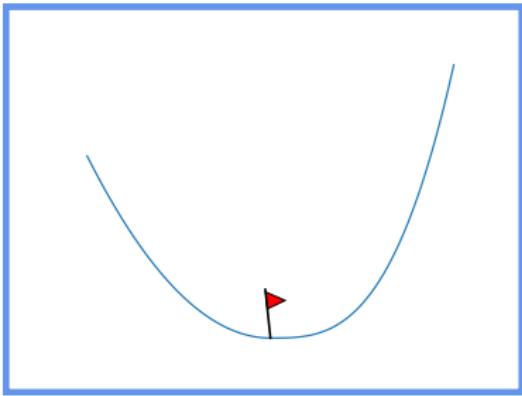
Advisors: Anne Auger & Nikolaus Hansen

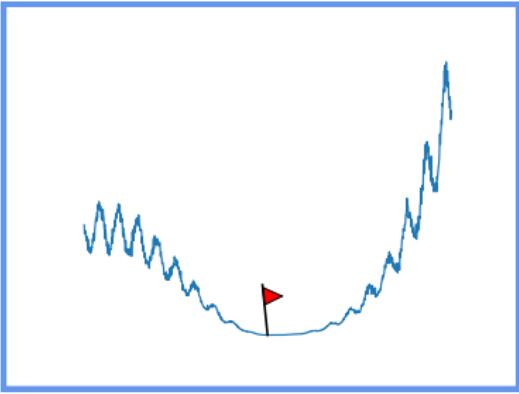
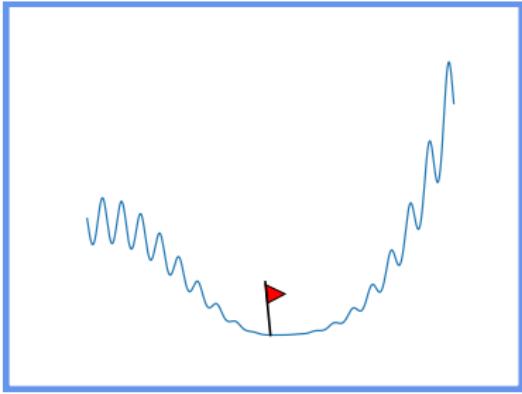
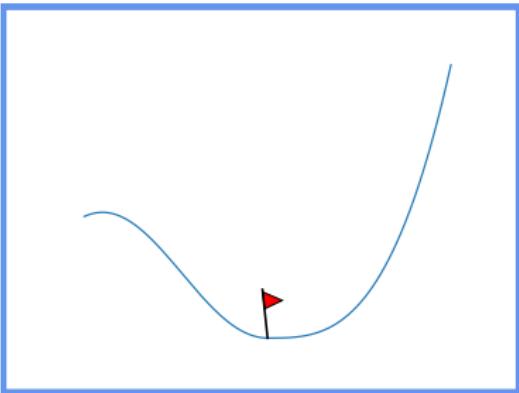
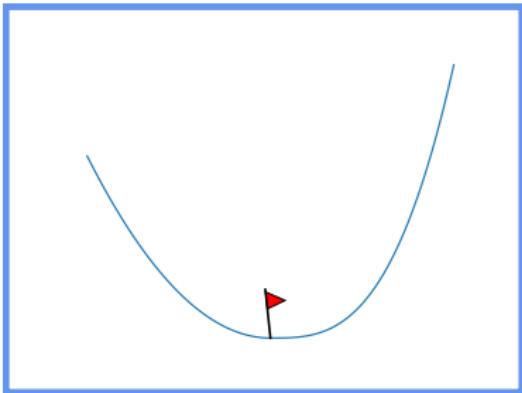
Inria

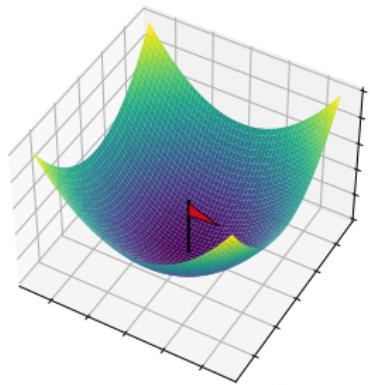


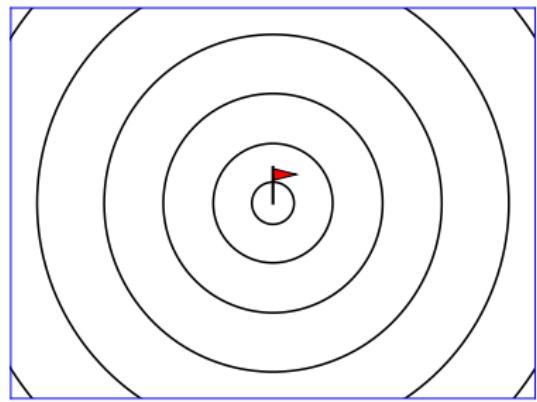
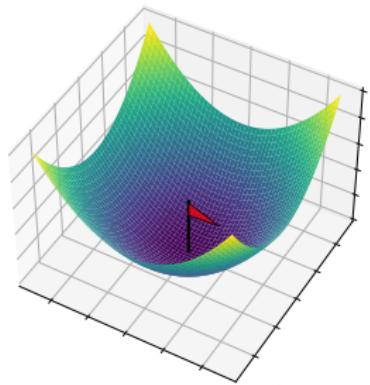












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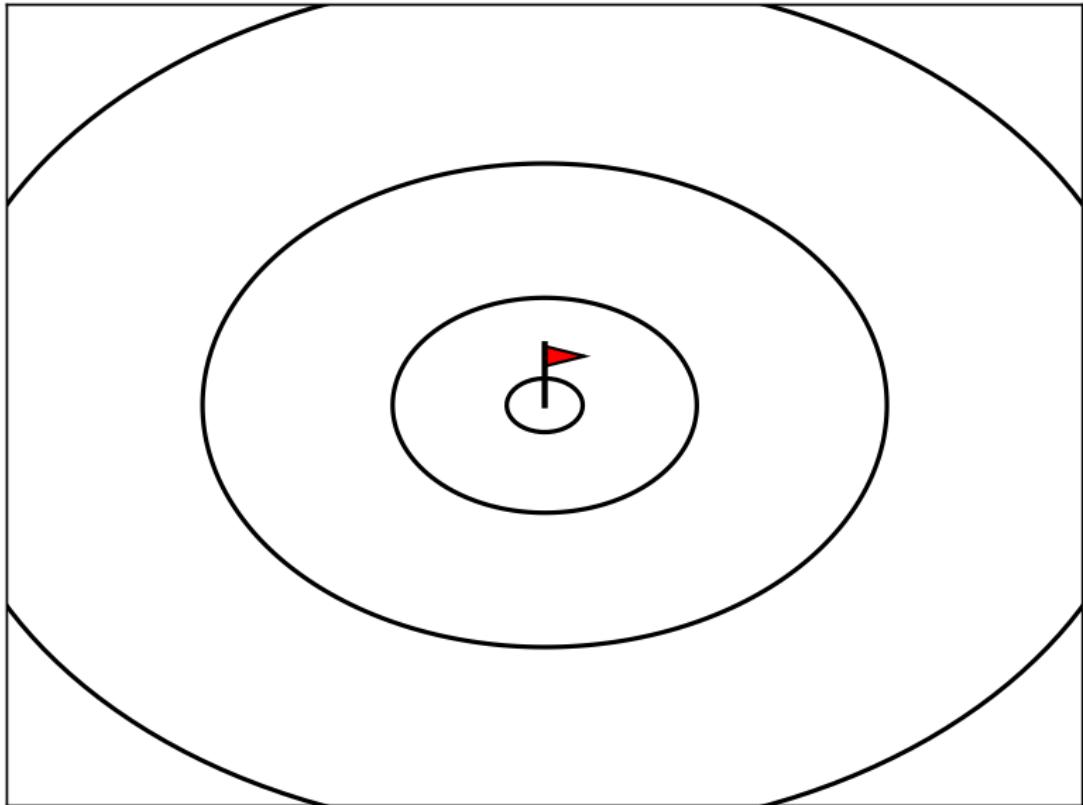
$$\cancel{\nabla f(x)} \qquad \cancel{\partial f(x)}$$

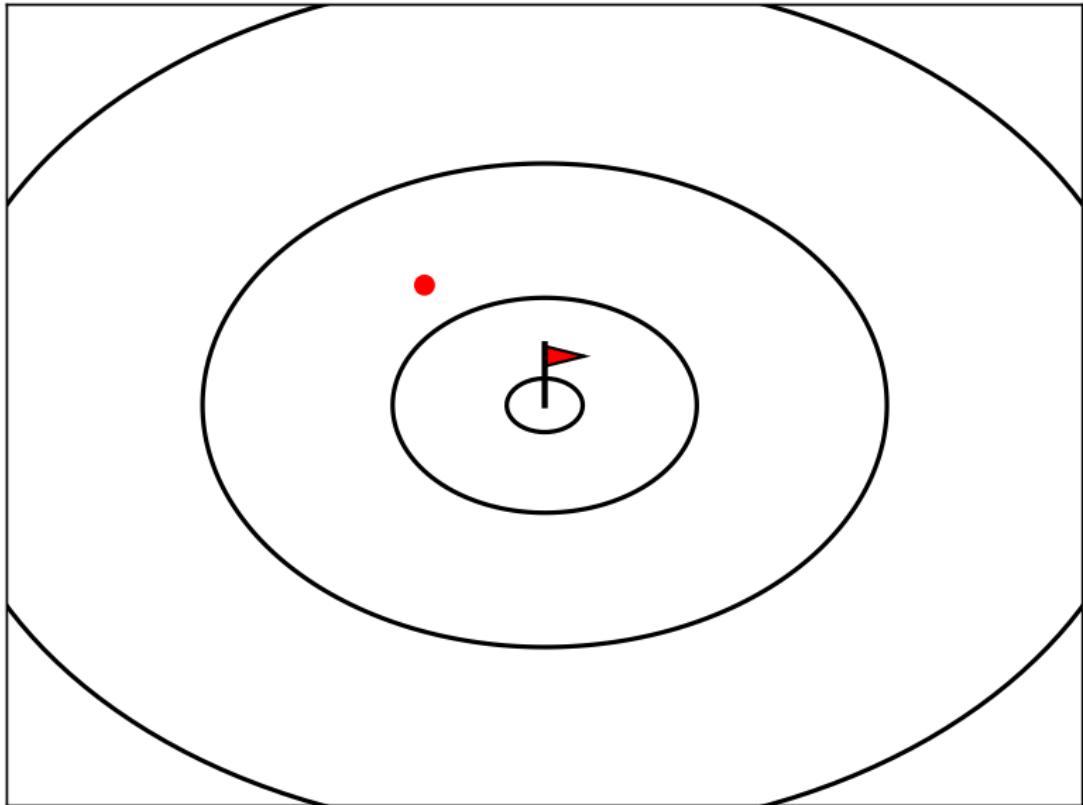
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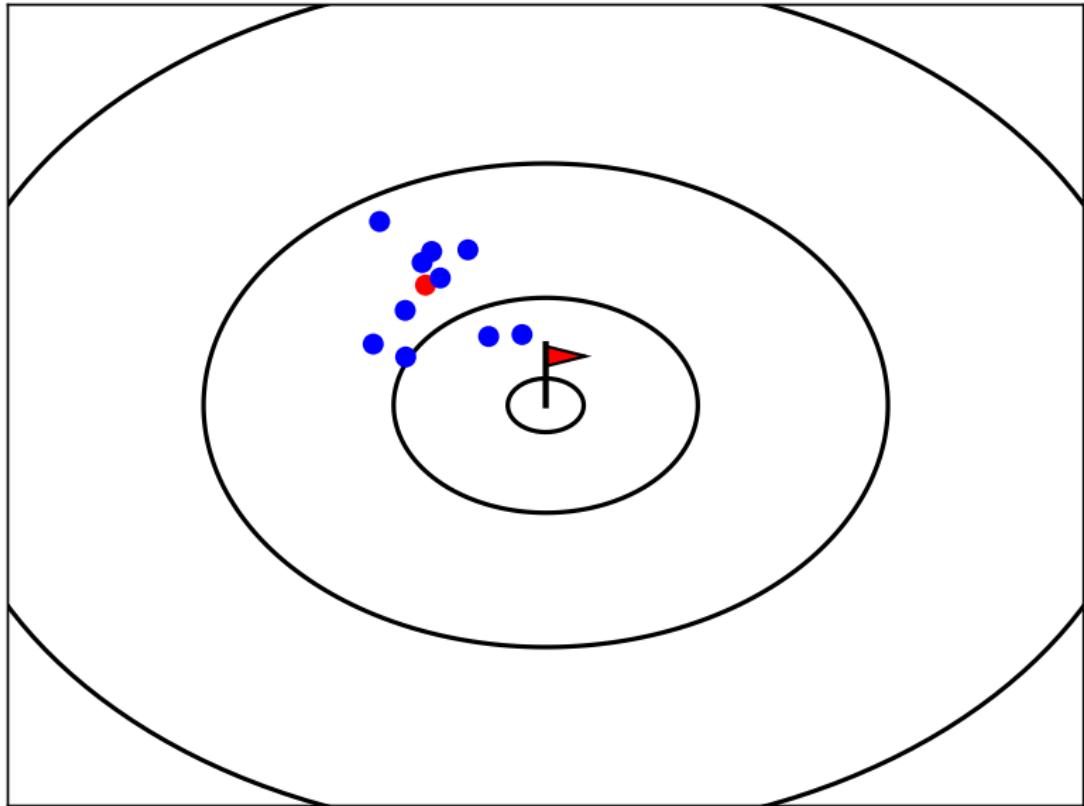
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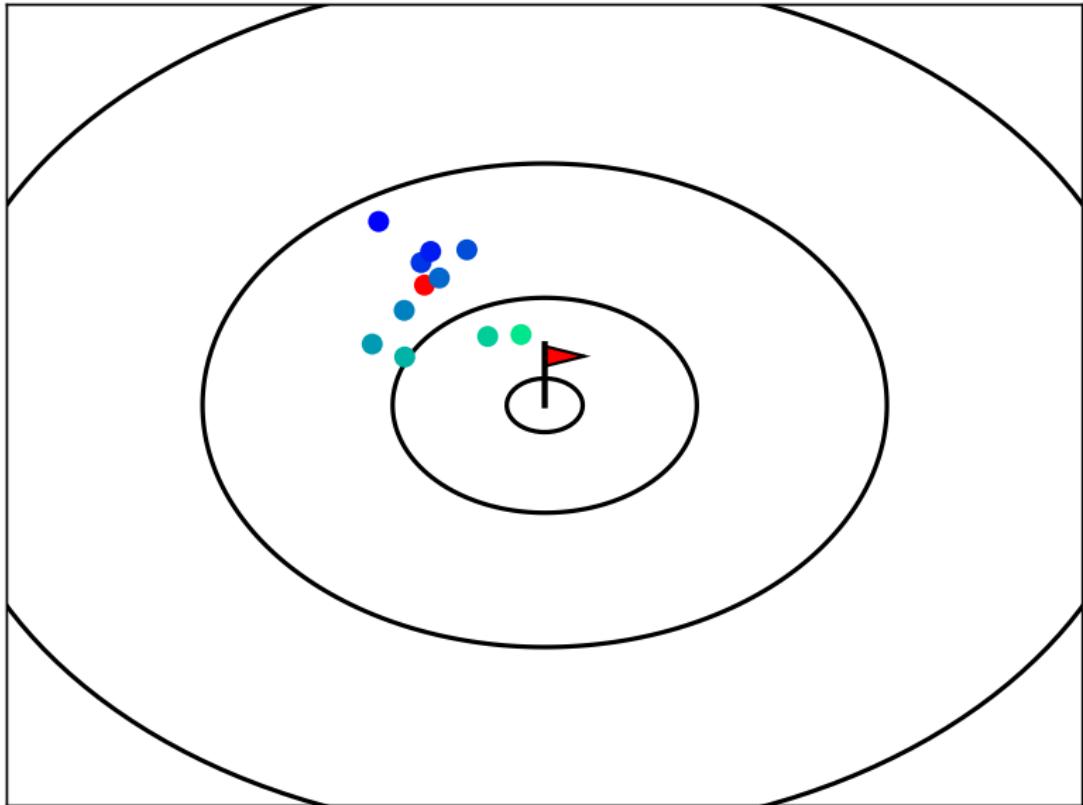
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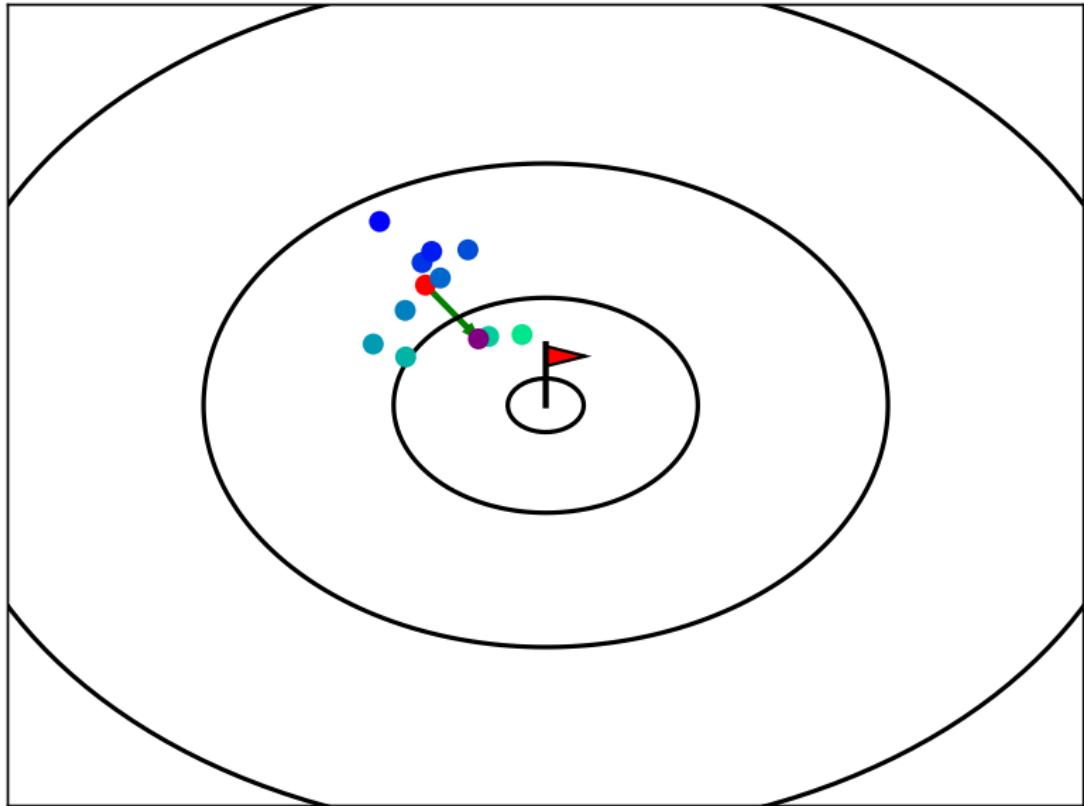
$$\text{Find } x^* \in \operatorname{Arg \min}_{x \in \mathbb{R}^d} f(x) \quad (\mathcal{P})$$





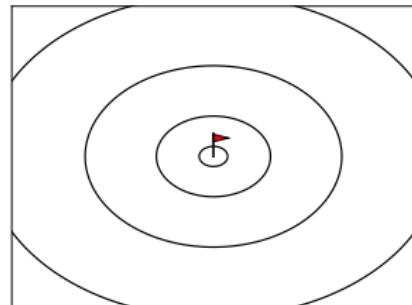






Algorithm 1 Our first ES

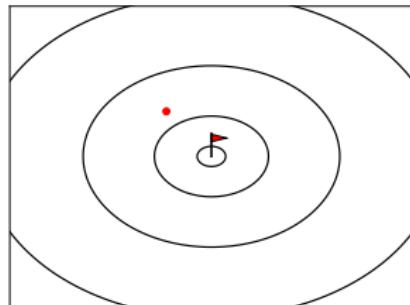
Goal: $\min_{x \in \mathbb{R}^d} f(x)$



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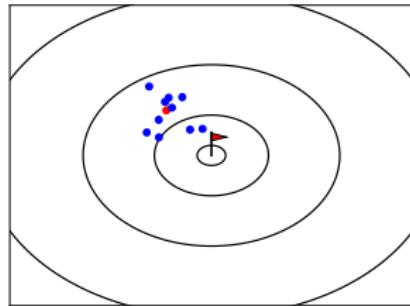


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$\lambda = \text{population size}$

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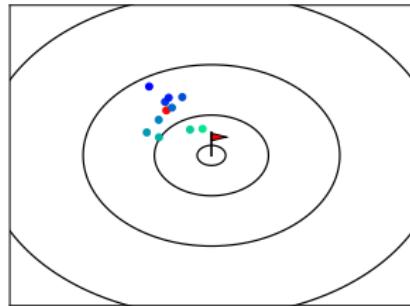
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2. Rank population:

$$f(x_{t+1}^{1:\lambda}) \leq \dots \leq f(x_{t+1}^{\lambda:\lambda})$$



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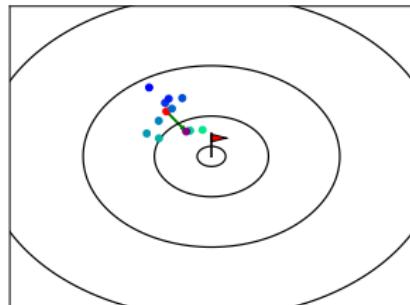
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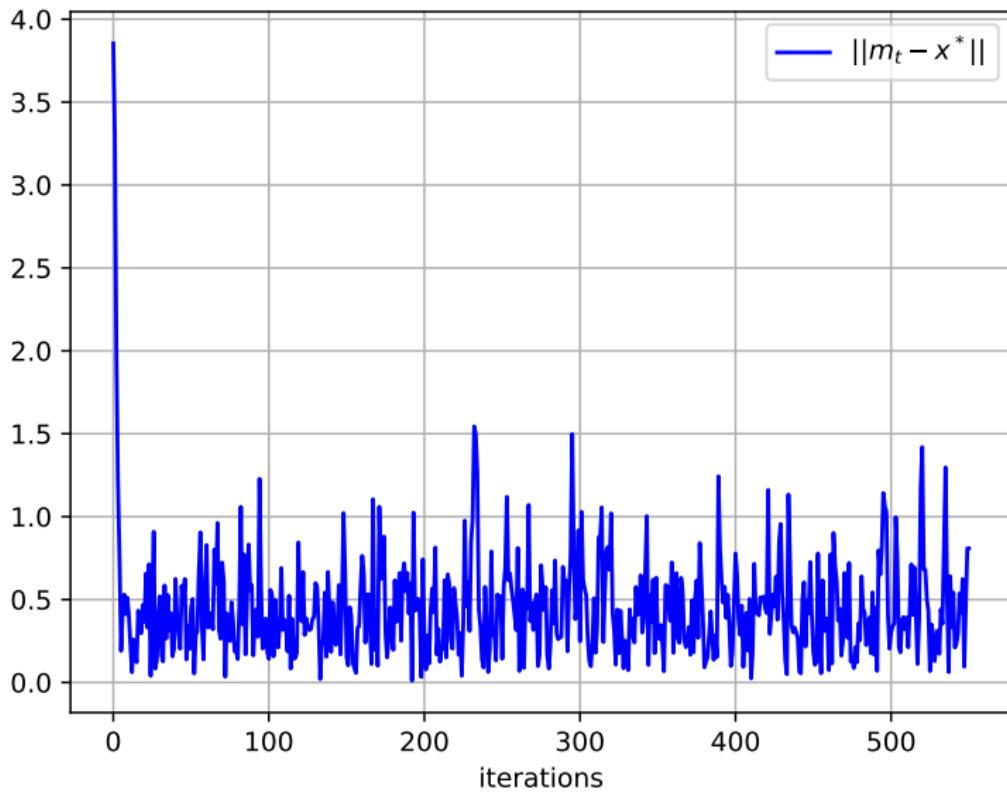
3. Update mean: $m_{t+1} = \text{Average}(x_{t+1}^{1:\lambda}, \dots, x_{t+1}^{\mu:\lambda})$

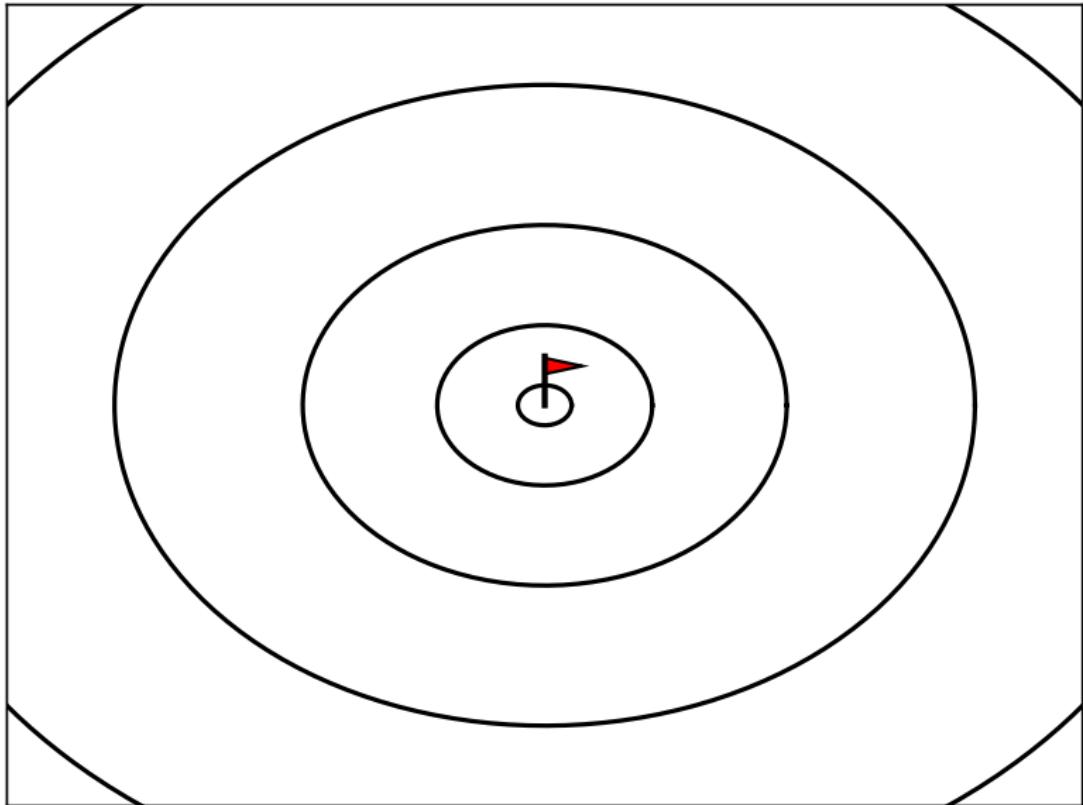


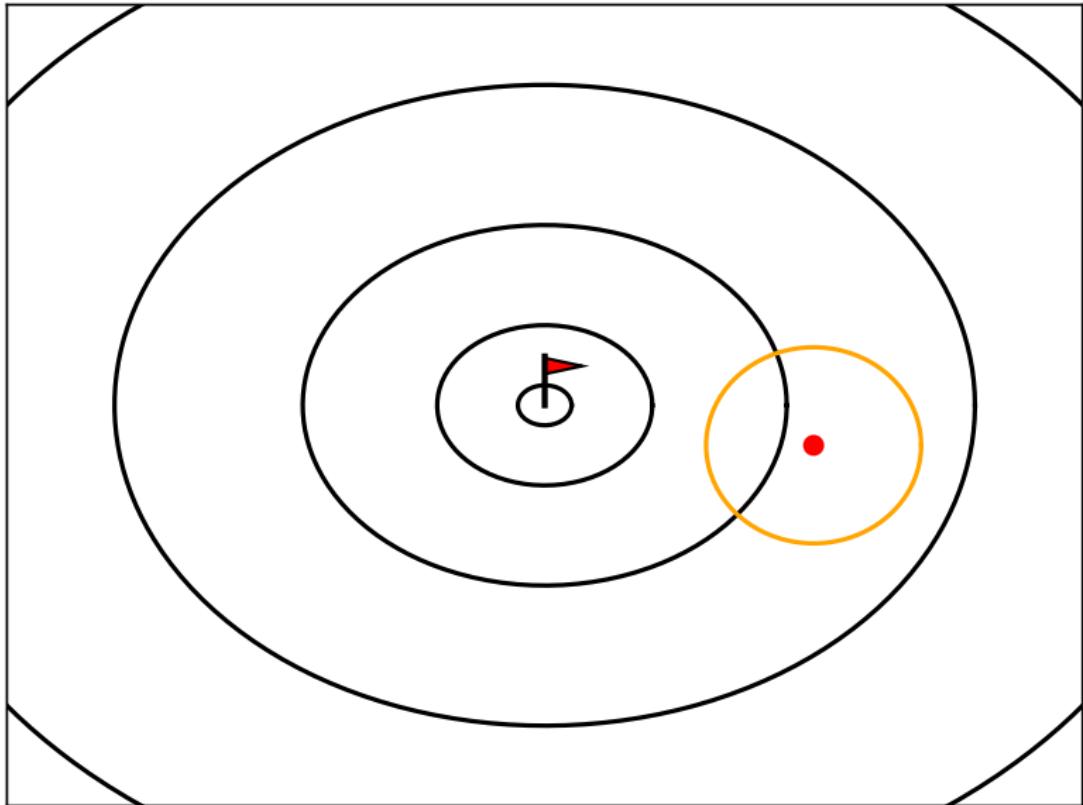
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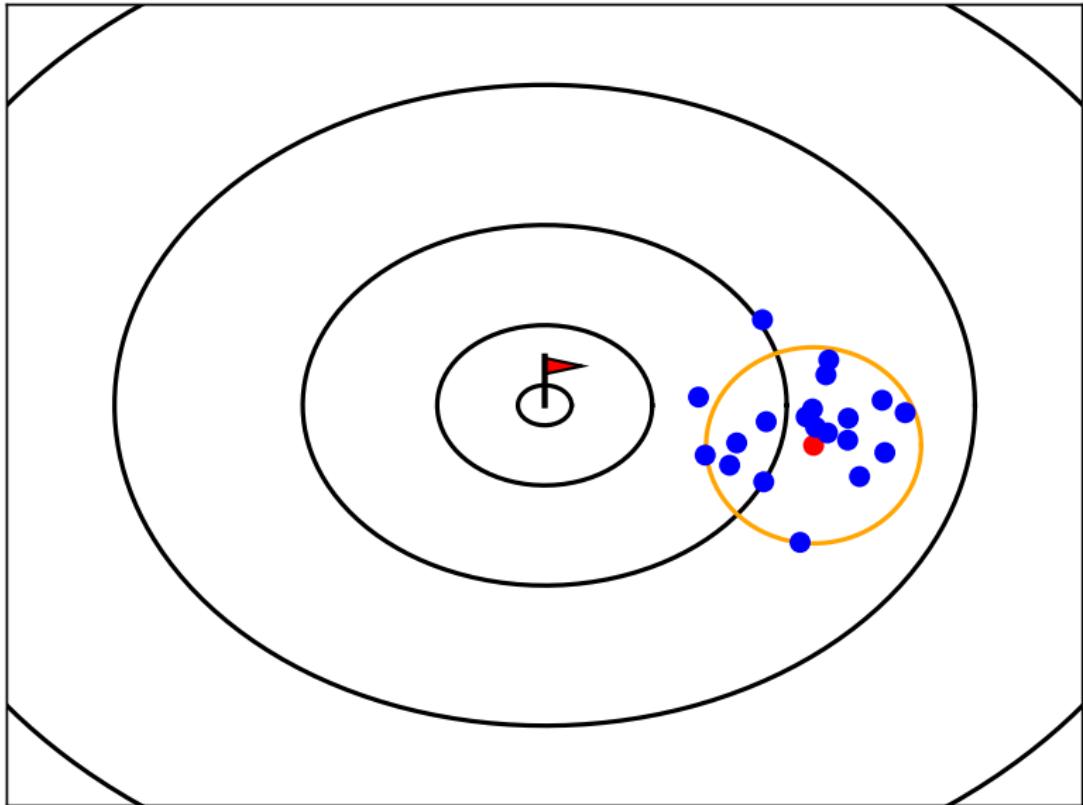
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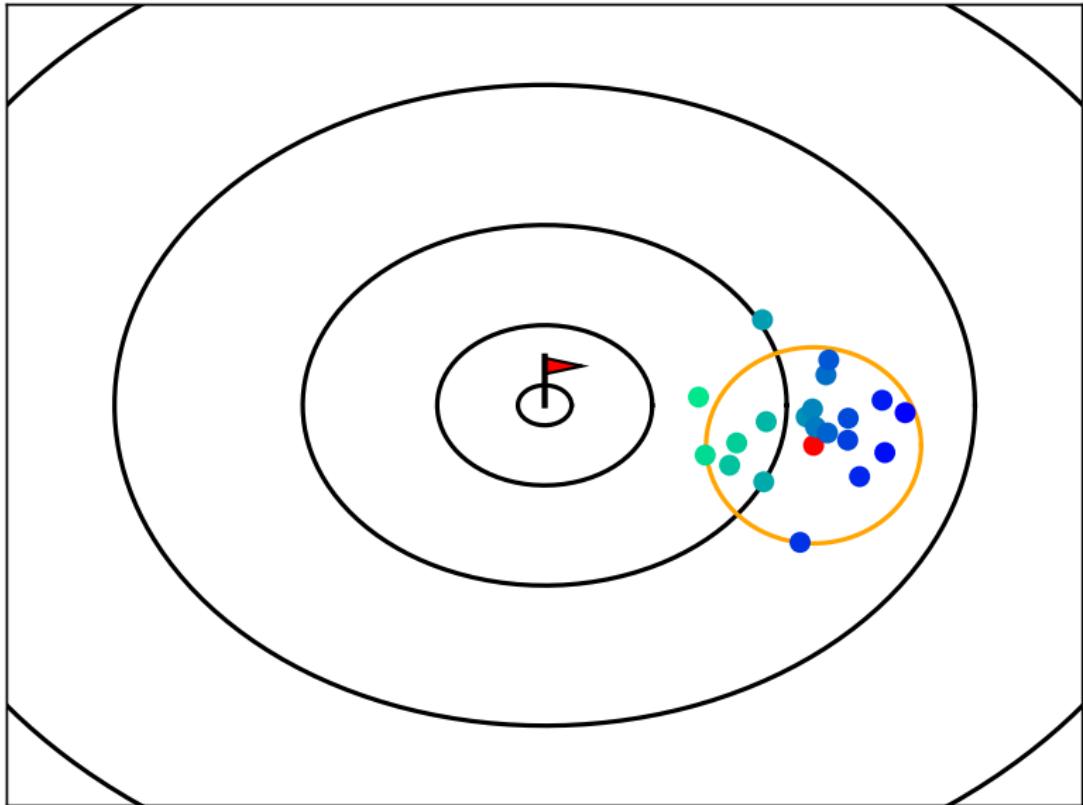
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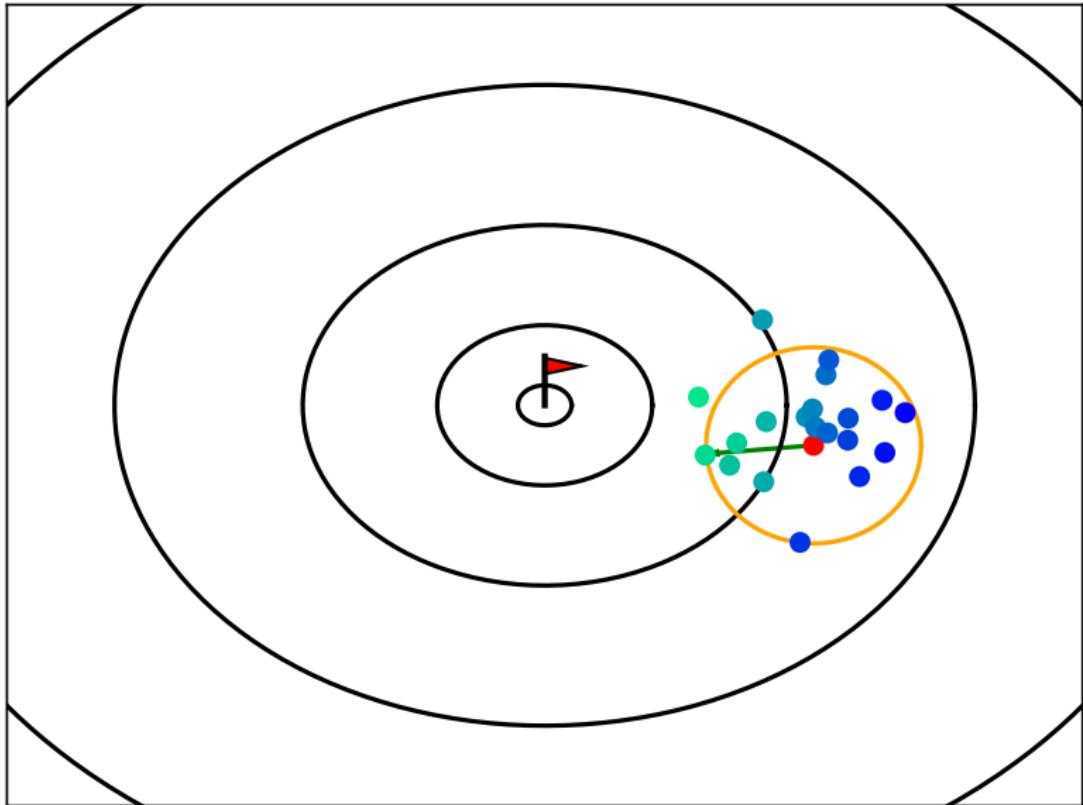


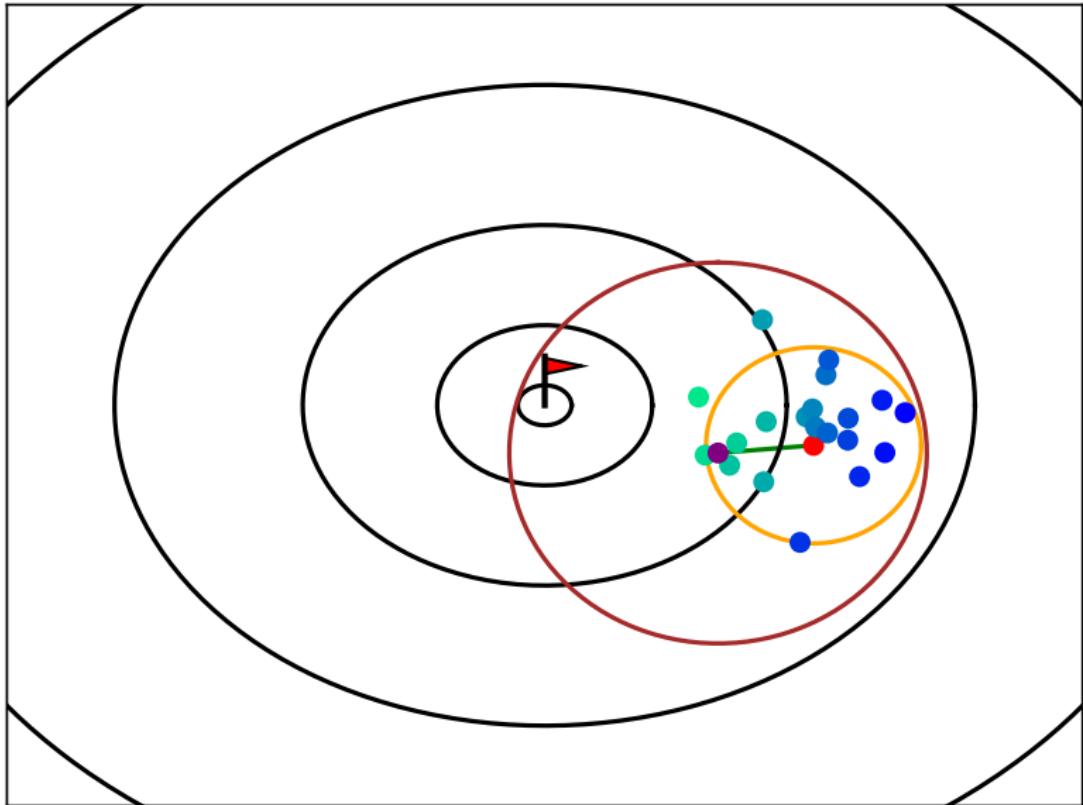


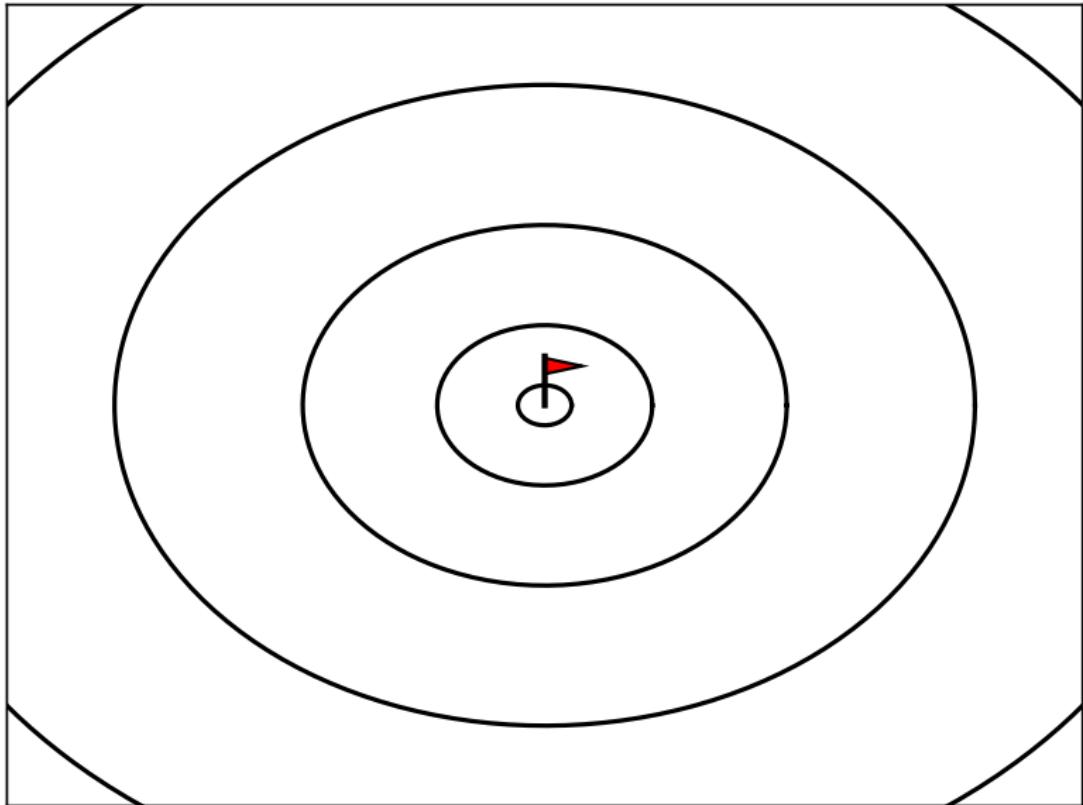


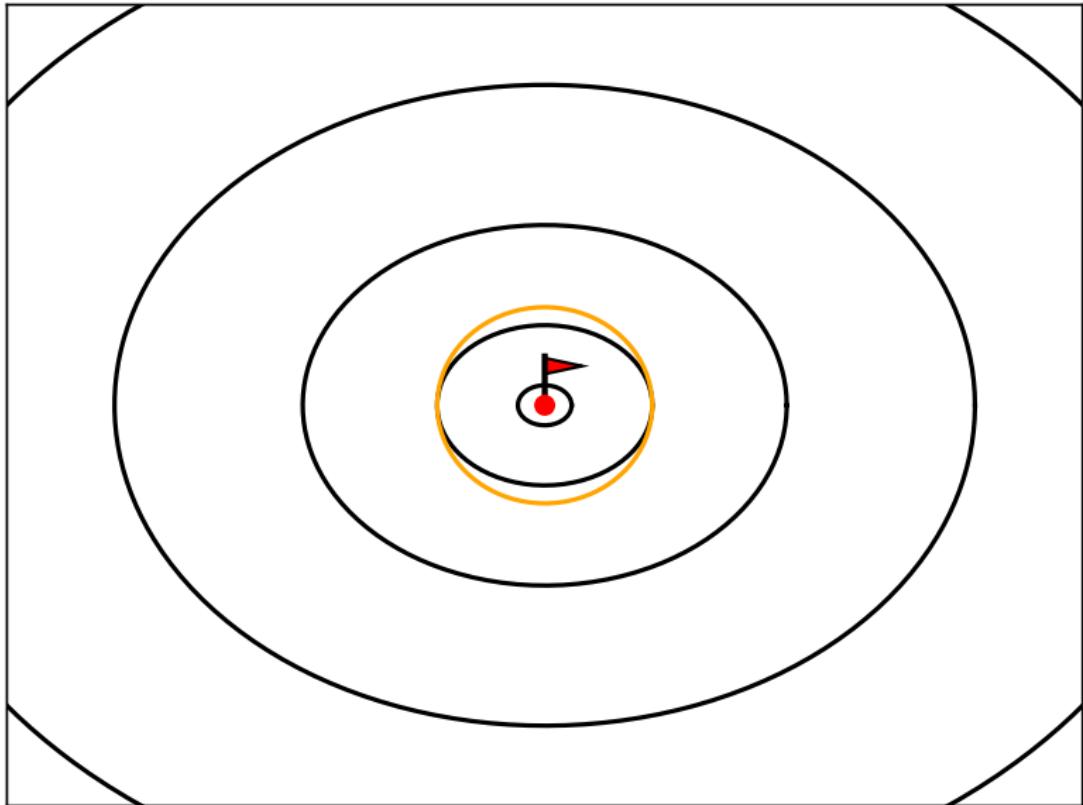


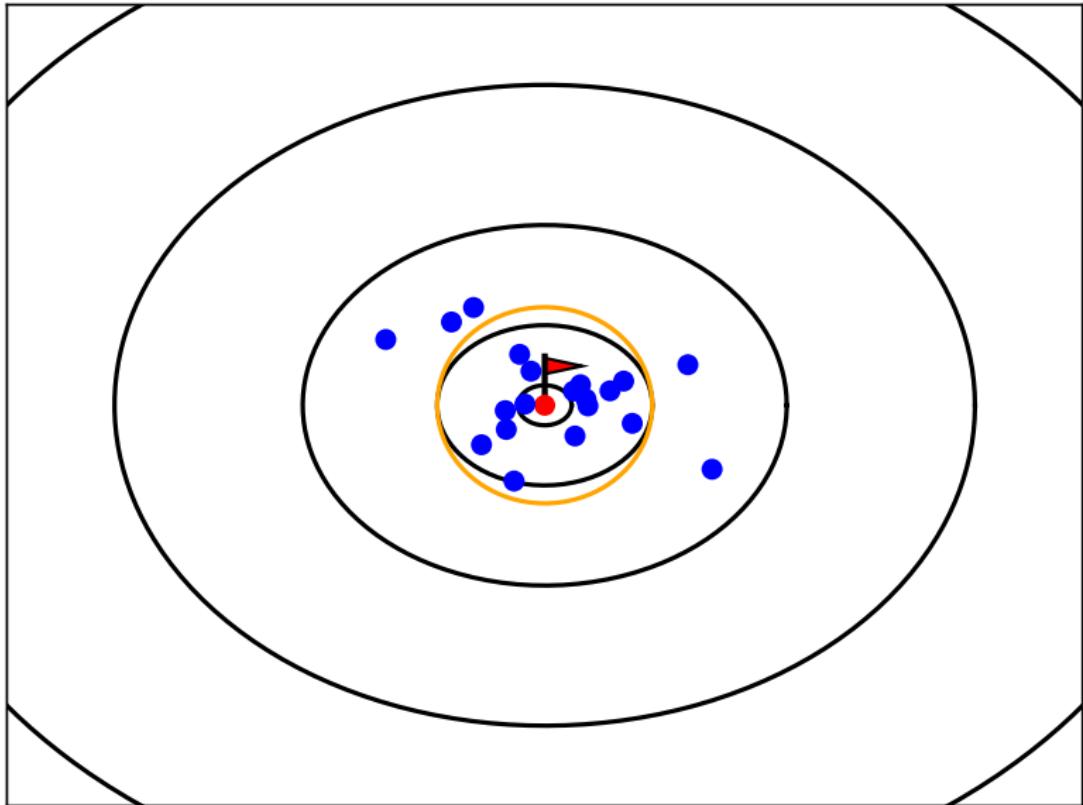


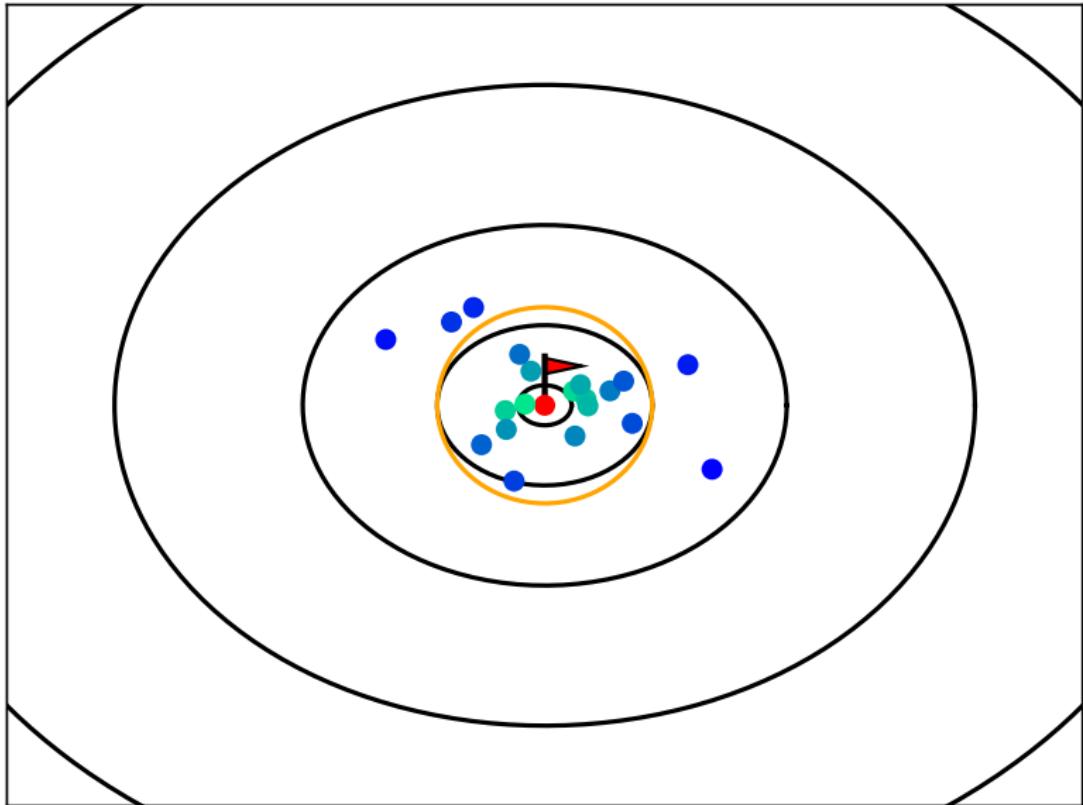


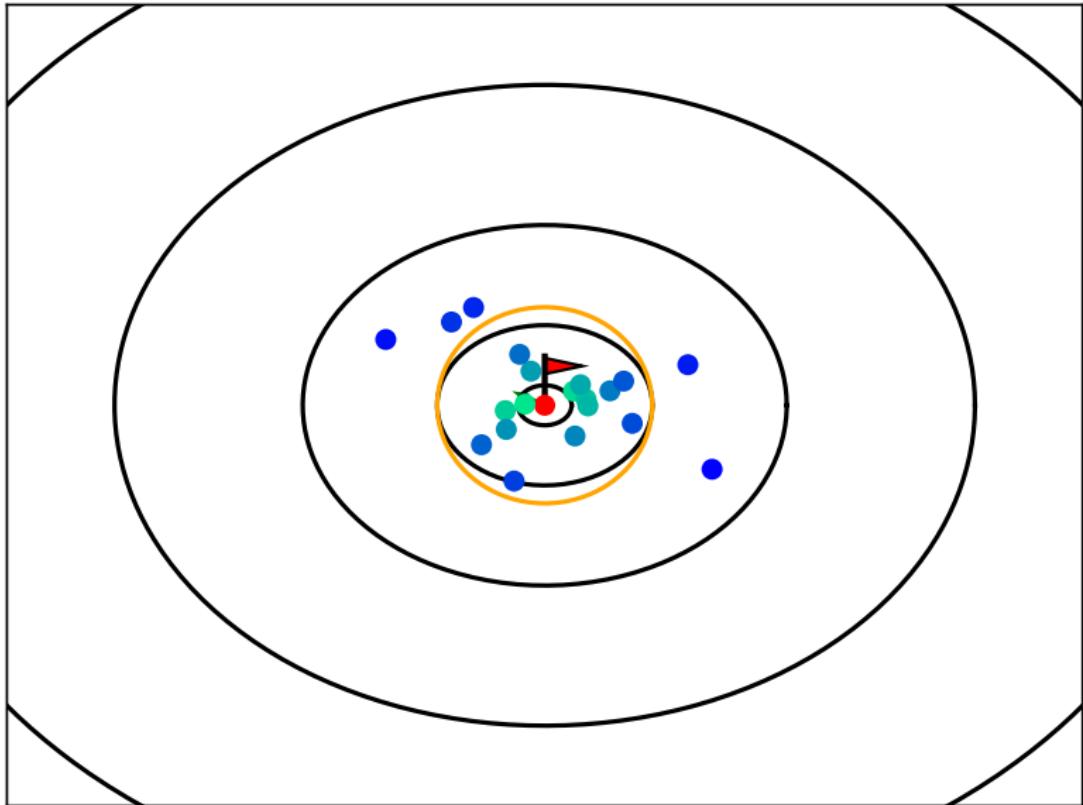


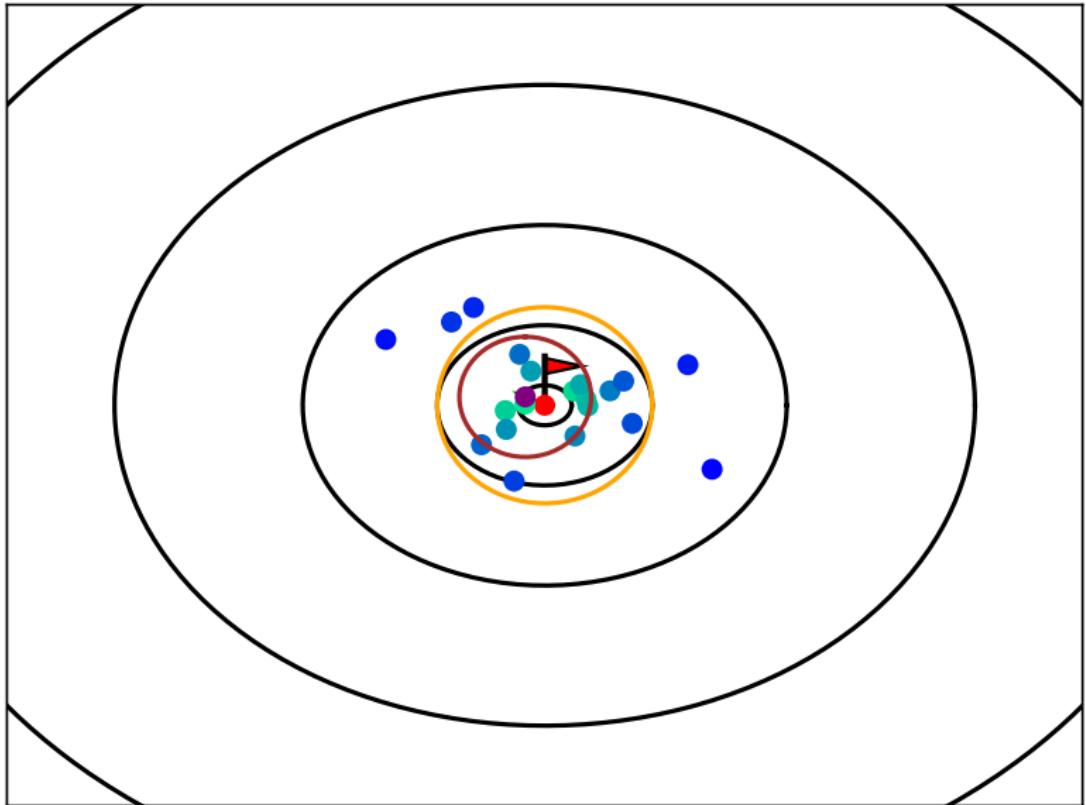






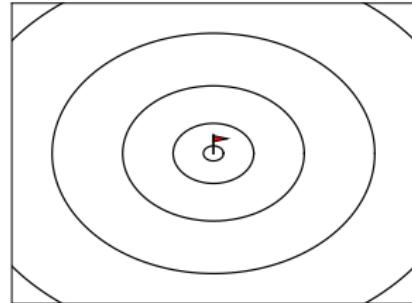






Algorithm 2 ES with step-size adaptation

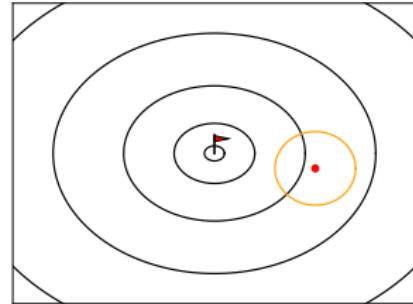
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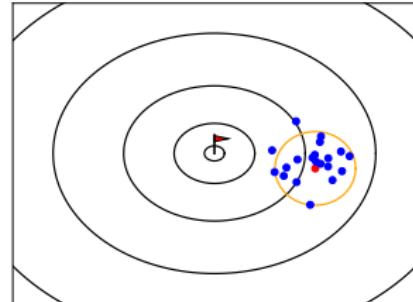


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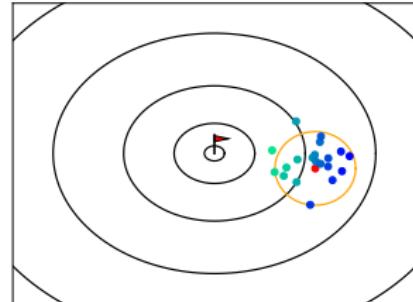
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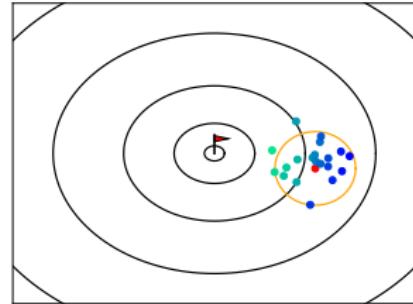
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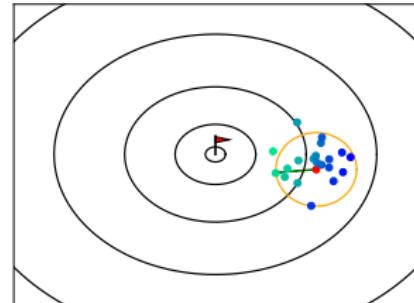
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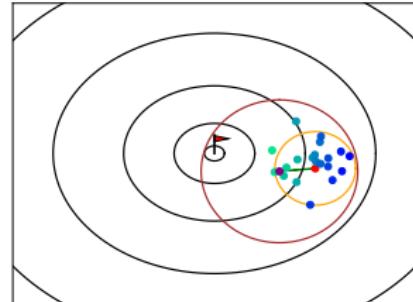
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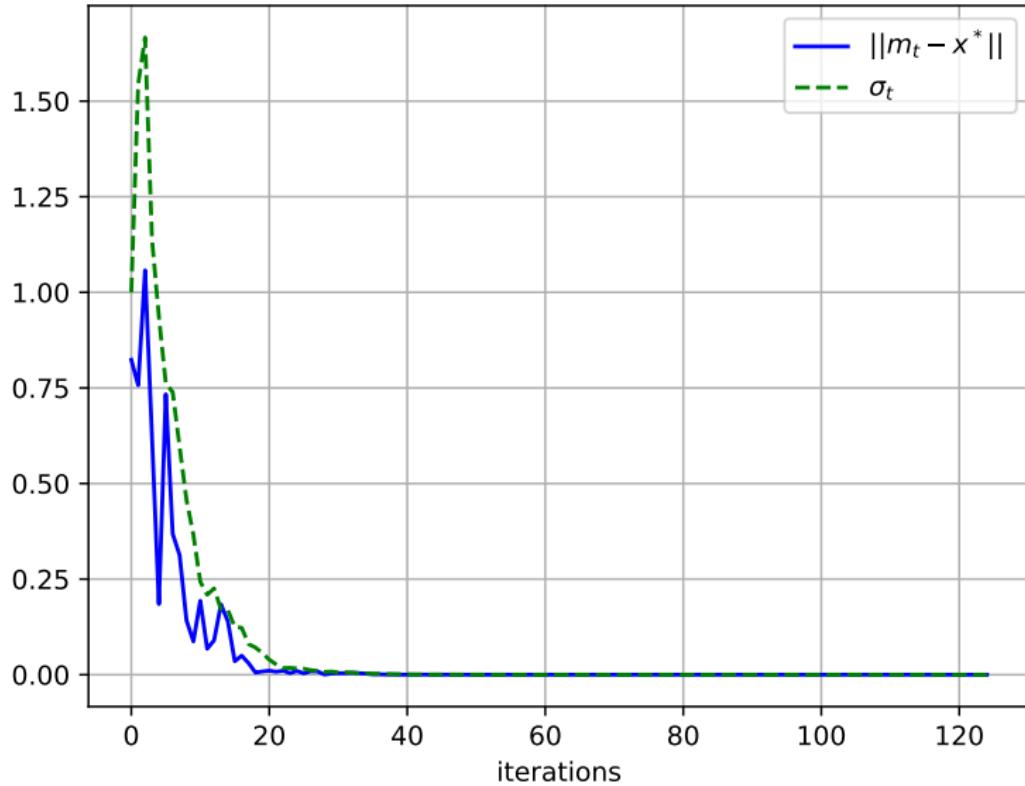
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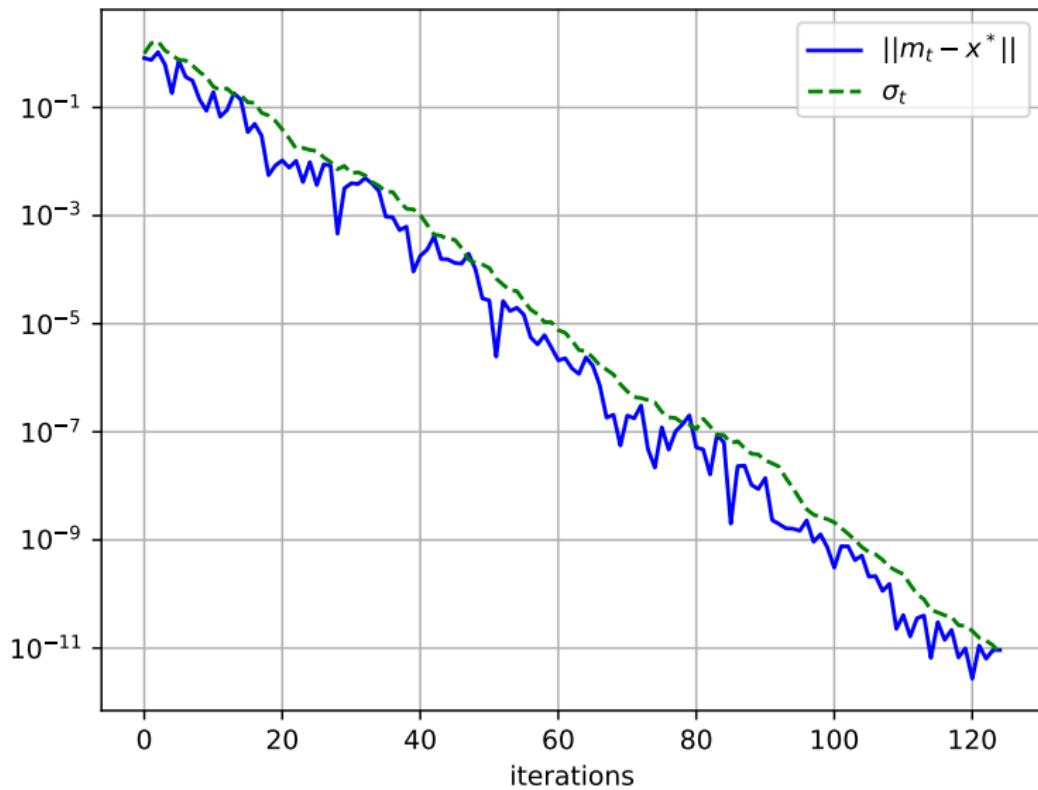
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$$f: x \mapsto x^T A x$$



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Prove:

$$\frac{\|m_{t+1} - x^*\|}{\|m_t - x^*\|} \approx \frac{\sigma_{t+1}}{\sigma_t} \approx \rho \in (0, 1).$$

Prove:

$$\log \frac{\|m_{t+1} - x^*\|}{\|m_t - x^*\|} \approx \log \frac{\sigma_{t+1}}{\sigma_t} \approx -\text{CR}.$$

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A **Markov chain** with transition kernel P is a random sequence $\{\theta_t\}_{t \in \mathbb{N}}$ such that:

$$\mathbb{P}[\theta_{t+1} \in A \mid \theta_t = x] = P(x, A).$$

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- We can define a **k -steps transition kernel** P^k which satisfies

$$\mathbb{P}[\theta_{t+k} \in A \mid \theta_t = x] = P^k(x, A)$$

If X is finite:

If $X = \{1, \dots, n\}$:

$$\nu_0 = (p_1, \dots, p_n) \quad \text{with} \quad \sum_k p_k = 1$$

represents an initial state of the Markov chain $\{\theta_k\}_{k \in \mathbb{N}}$

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$$\exists \pi, \forall \nu_0, \quad \lim_{k \rightarrow \infty} \nu_k = \pi$$

then $\{\theta_k\}_{k \in \mathbb{N}}$ is *ergodic*.

If X is **infinite**:

ν_0 **probability measure on X**

represents an initial state of the Markov chain $\{\theta_k\}_{k \in \mathbb{N}}$

After k steps:

$$\nu_k = \int \nu_0(dx) P^k(x, \cdot)$$

If

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For an ergodic Markov chain $\Theta = \{\theta_k\}_{k \in \mathbb{N}}$:

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where π is the invariant probability measure of Θ :

$$\theta_k \sim \pi \Rightarrow \theta_{k+1} \sim \pi$$

When $\Theta = \{\theta_k\}_{k \in \mathbb{N}}$ is ergodic:

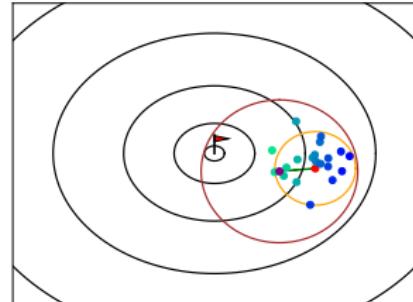
$$\lim_{T \rightarrow +\infty} \frac{1}{T} \sum_{k=0}^{T-1} g(\theta_k) = \int g(x) d\pi(x)$$

Algorithm 2 ES with step-size adaptation

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

Repeat (Given $m_t \in \mathbb{R}^d$ and $\sigma_t > 0$)

1. $x_{t+1}^1, \dots, x_{t+1}^\lambda \sim \mathcal{N}(m_t, \sigma_t^2 I_d)$
 2. sort $f(x_{t+1}^i)$:
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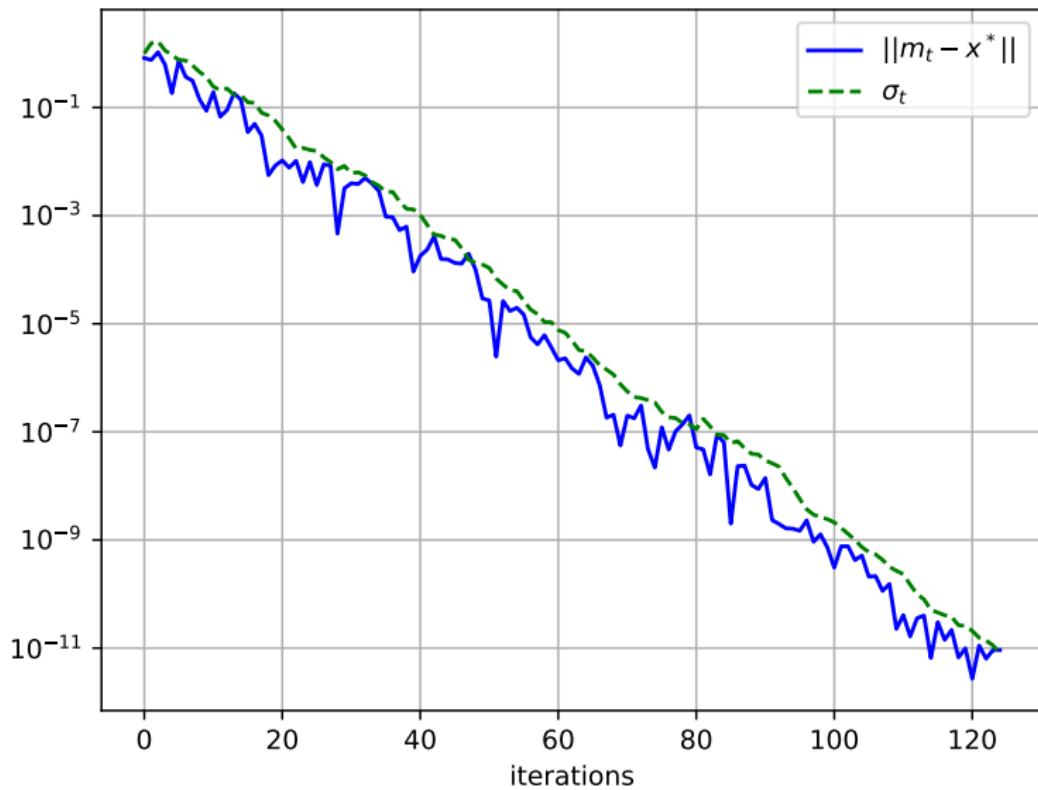
$\{(m_k, \sigma_k)\}_{k \in \mathbb{N}}$ is a Markov chain valued in $X = \mathbb{R}^d \times (0, +\infty)$

$$\lim_{k \rightarrow \infty} m_k = x^* \quad \text{and} \quad \lim_{k \rightarrow \infty} \sigma_k = 0$$

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$\delta_{(x^*, 0)}$ is **not** a probability distribution on $X = \mathbb{R}^d \times (0, +\infty)$!

$$f: x \mapsto x^T A x$$



$$z_t = \frac{m_t - x^*}{\sigma_t}$$

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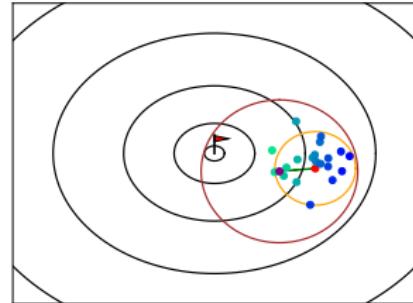
Question: $\{z_t\}_{t \in \mathbb{N}}$ is an ergodic Markov chain?

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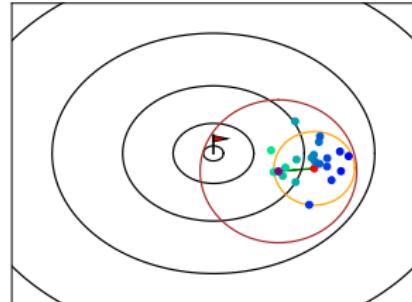
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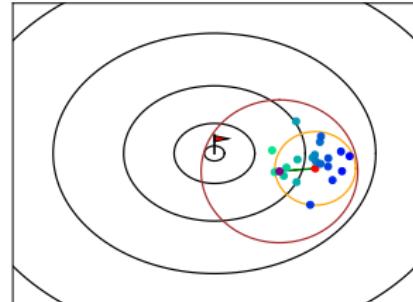
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Algorithm 3 ES with step-size adaptation

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

Repeat (Given $z_t \in \mathbb{R}^d$) :

1. $z_{t+1}^1, \dots, z_{t+1}^\lambda \sim \mathcal{N}(z_t, I_d)$
 2. sort $f(x_{t+1}^i)$:
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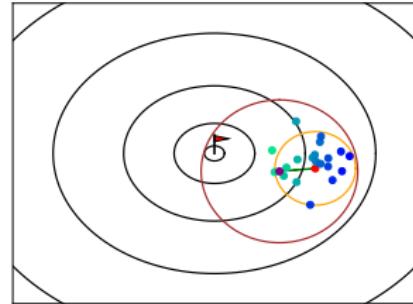
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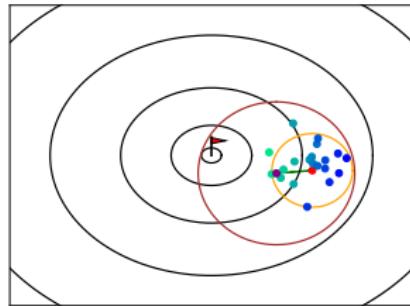
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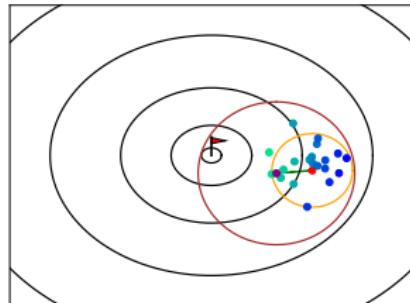
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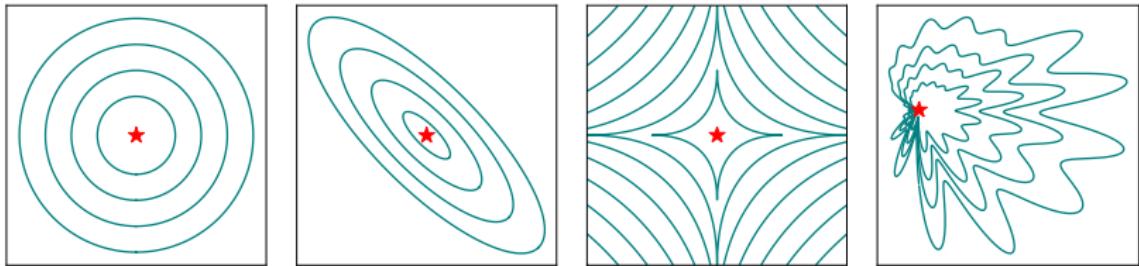
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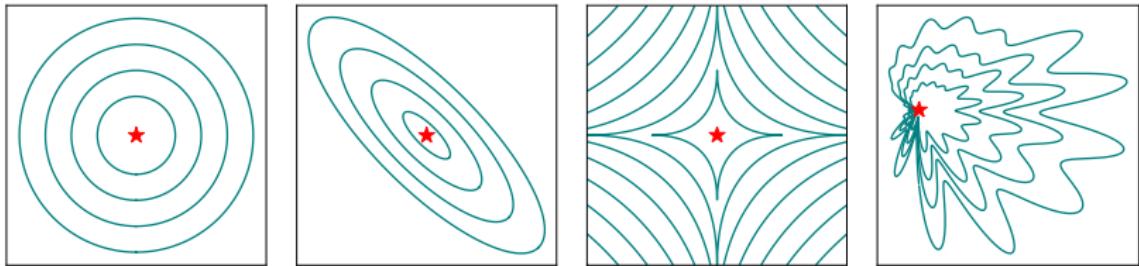


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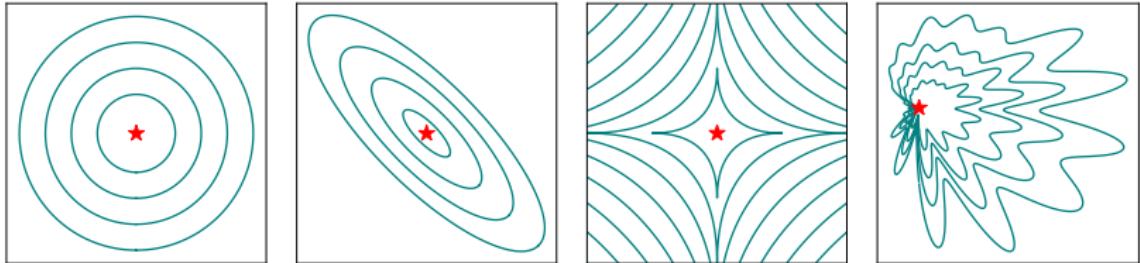
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$$f(\textcolor{red}{x}_{t+1}^{1:\lambda}) \leq \dots \leq f(\textcolor{blue}{x}_{t+1}^{\lambda:\lambda}) \stackrel{?}{\Leftrightarrow} g(\textcolor{red}{z}_{t+1}^{1:\lambda}) \leq \dots \leq g(\textcolor{blue}{z}_{t+1}^{\lambda:\lambda})$$





$$f(m_t) \leq f(x_{t+1}) \Leftrightarrow f\left(\star + \frac{m_t - \star}{\sigma_t}\right) \leq f\left(\star + \frac{x_{t+1} - \star}{\sigma_t}\right)$$



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Proposition

If $f \in \left\{ \text{[Panel 1]}, \text{[Panel 2]}, \text{[Panel 3]}, \text{[Panel 4]} \right\}$, then $\{z_t\}_{t \in \mathbb{N}}$ is a Markov chain.

$$z_t = \frac{m_t - x^*}{\sigma_t}$$

Question: $\{z_t\}_{t \in \mathbb{N}}$ is an ergodic **Markov chain**?

When X is finite:

Theorem

If $\{\theta_t\}_{t \in \mathbb{N}}$ is an irreducible, aperiodic Markov chain, then it is ergodic.

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for some volume on X .

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If

$$\left\{ \begin{array}{l} \theta_1 \in A_1 \Rightarrow \mathbb{P}[\theta_2 \in A_2] = 1 \\ \theta_2 \in A_2 \Rightarrow \mathbb{P}[\theta_3 \in A_3] = 1 \\ \vdots \\ \theta_T \in A_T \Rightarrow \mathbb{P}[\theta_{T+1} \in A_1] = 1 \end{array} \right.$$

Then period = T .

When period = 1,

$\{\theta_t\}$ is **aperiodic**.

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If $\{\theta_t\}_{t \in \mathbb{N}}$ is an irreducible, aperiodic Markov chain, then it is ergodic if

$$\mathbb{E}[V(\theta_{t+1}) \mid \theta_t] \leq (1 - \varepsilon)V(\theta_t) \quad \text{if } \theta_t \notin \text{small set}$$

for some $V : X \rightarrow [1, +\infty]$.

Proposition: for $\{z_t\}_{t \in \mathbb{N}}$, compact sets are small

When X is infinite:

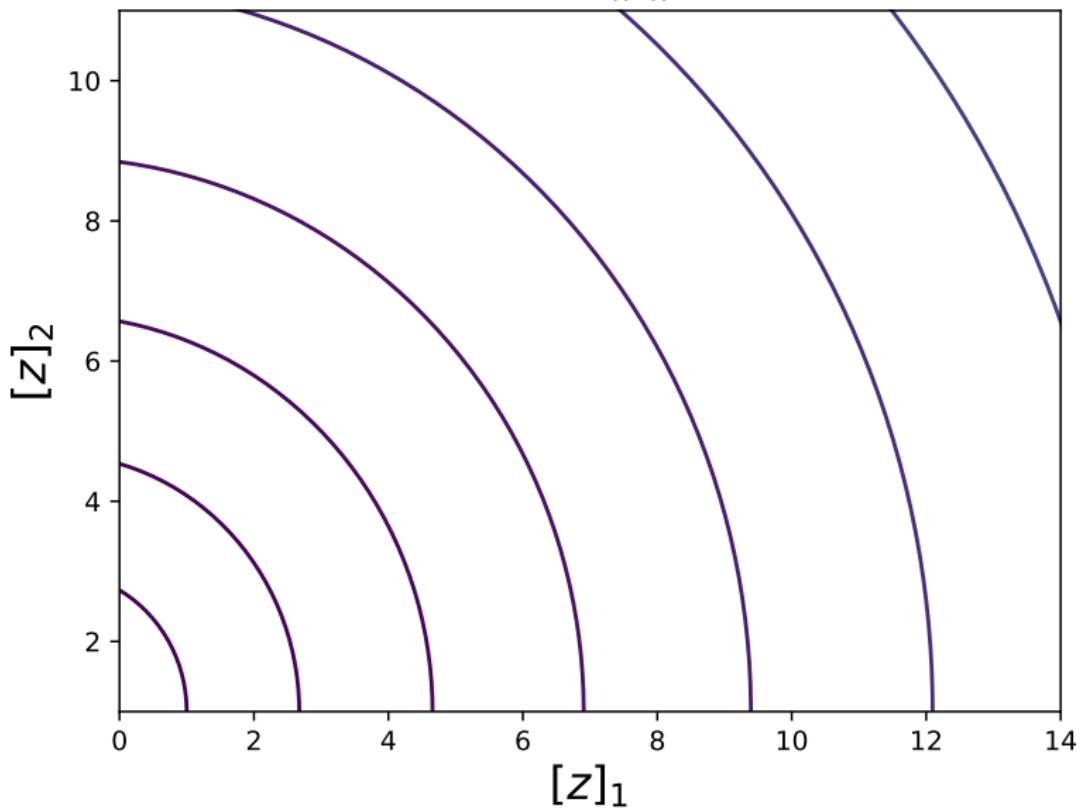
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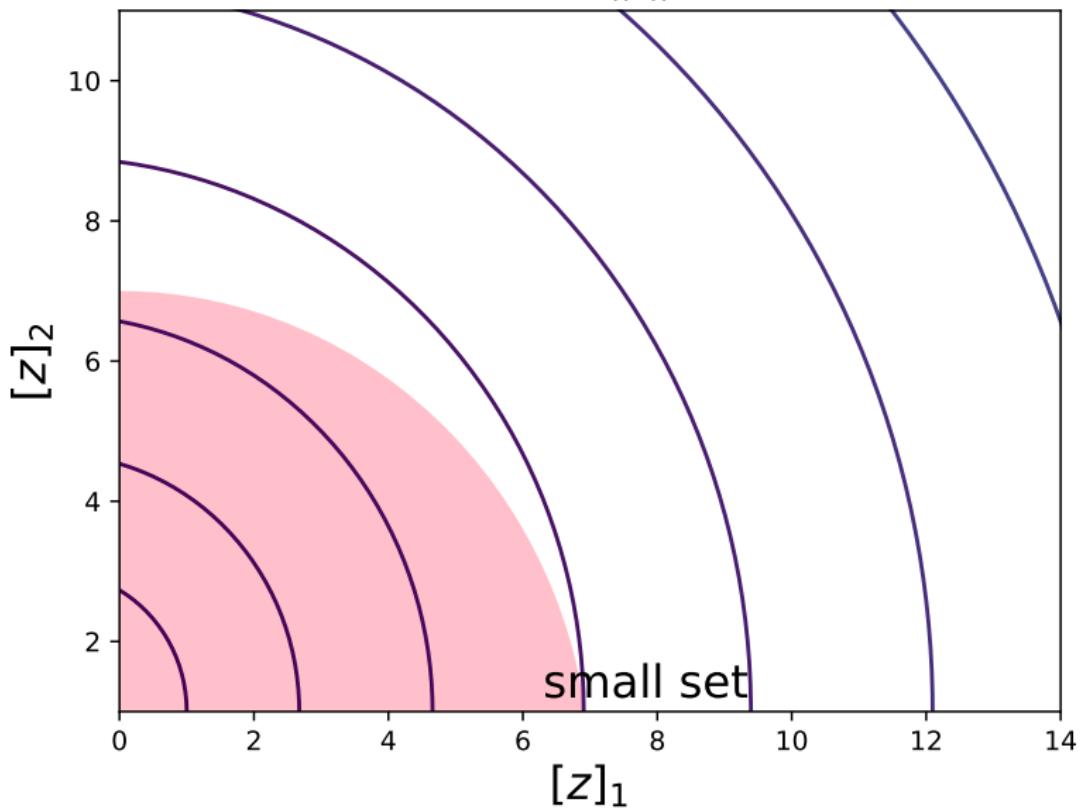
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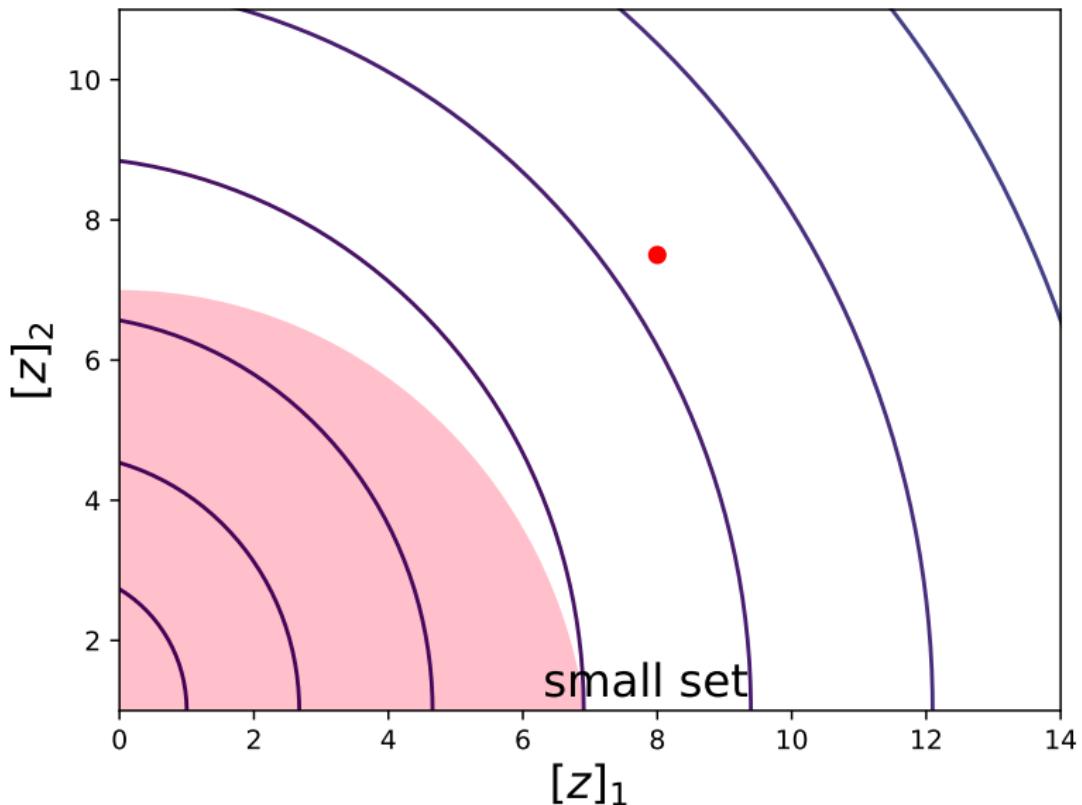
$$V(z) = ||z||$$



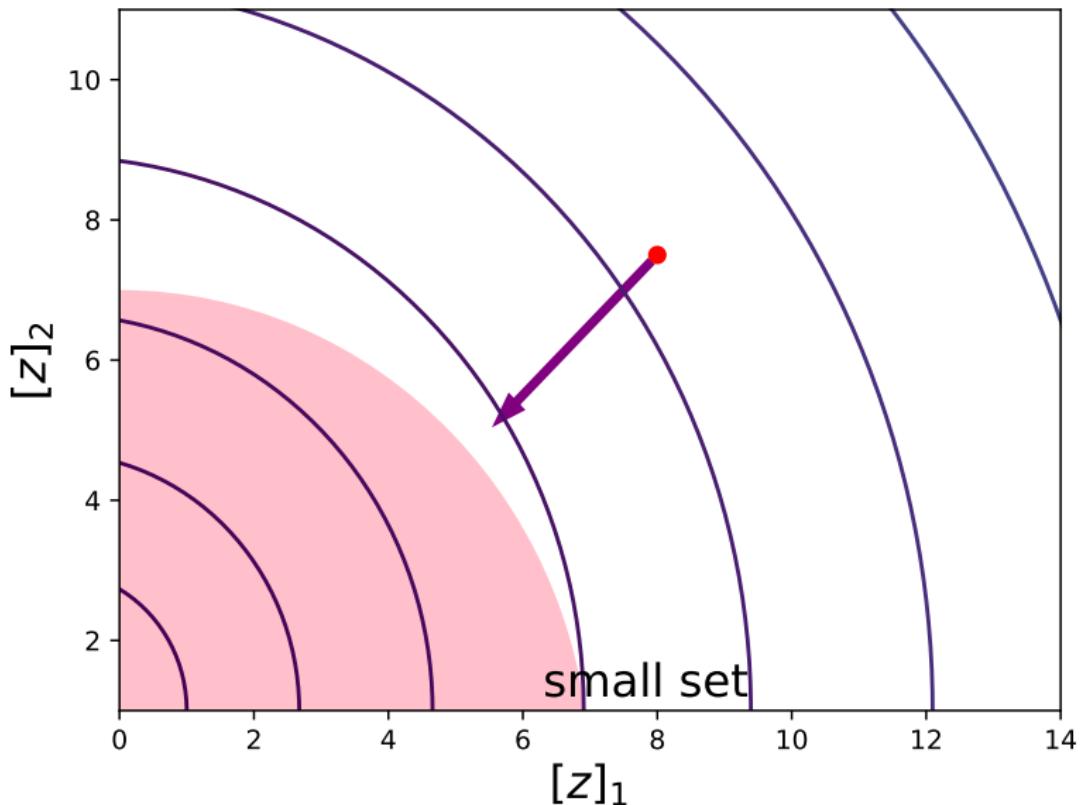
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$$\theta_{k+1} = F(\theta_k, x_{k+1}) \quad (\mathbf{CM}(F))$$

where $x_{k+1} \sim p_{\theta_k}$

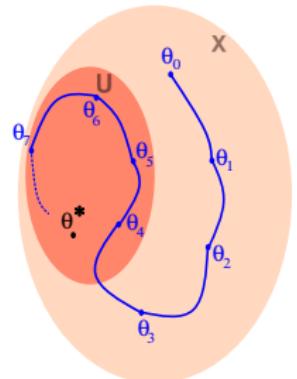
$$\begin{aligned}\theta_{k+1} &= F(\theta_k, x_{k+1}) && (\mathbf{CM}(F)) \\ &= F_{k+1}(\theta_0, x_1, \dots, x_{k+1})\end{aligned}$$

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θ^* is **attracting** when

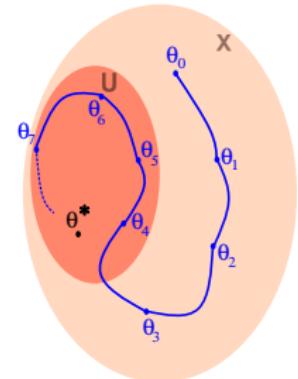
θ^* is **attracting** when

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Theorem

If

- $\exists \theta^*$ *attracting*
- $\exists x_1^*, \dots, x_k^*$

such that $F_k(\theta^*, \cdot)$ is a **submersion** at $x_{1..k}^*$,

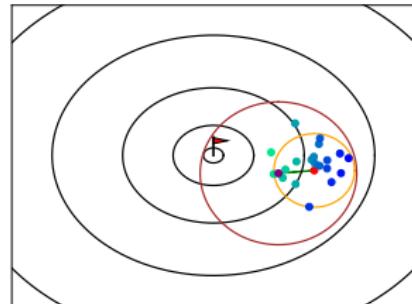
then, $\{\theta_t\}_{t \in \mathbb{N}}$ is **irreducible** and **aperiodic**.

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

Repeat (Given $z_t \in \mathbb{R}^d$) :

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$$z_{k+1} = F(z_k,z_{k+1}^{1:\lambda},\dots,z_{k+1}^{\lambda:\lambda})$$

$$z_{k+1} = F(z_k, z_{k+1}^{1:\lambda}, \dots, z_{k+1}^{\lambda:\lambda})$$

Proposition

0 is attracting

Proof.

Take $z_k^{i:\lambda} = 0$. Then

$$z_{k+1} = \frac{\text{Average}(0, \dots, 0)}{\text{normalization}} = 0$$

□

$$z_{k+1} = F(z_k, z_{k+1}^{1:\lambda}, \dots, z_{k+1}^{\lambda:\lambda})$$

Proposition

0 is attracting, and $F(0, \cdot)$ is submersive at 0 .

Proof.

$$F(0, h^1, \dots, h^\lambda) = 0 + \text{Average}(h^1, \dots, h^\lambda) + o(h^1, \dots, h^\lambda)$$

□

Corollary

If $f \in \left\{ \text{[Diagram 1]}, \text{[Diagram 2]}, \text{[Diagram 3]}, \text{[Diagram 4]} \right\}$, $\{z_t\}_{t \in \mathbb{N}}$ is irreducible and aperiodic.

Scheme of proof:

1. irreducibility and aperiodicity of $\{z_t\}_{t \in \mathbb{N}}$
2. **drift condition:** $\exists K \subset \mathbb{R}^d$ **compact and** $V: \mathbb{R}^d \rightarrow [1, +\infty]$

$$\mathbb{E}[V(z_1)] \leq (1 - \varepsilon)V(z_0) \quad \forall z_0 \notin K$$

3. deduce convergence from the ergodicity

Proposition

If $f \in \left\{ \begin{array}{c} \text{[Diagram of a spiral]} \\ \text{[Diagram of a circle with a dot]} \\ \text{[Diagram of a chaotic attractor]} \end{array} \right\}$:

$$\mathbb{E}[\|z_{t+1}\| \mid z_t] \leq (1 - \varepsilon) \times \|z_t\| \quad \text{if } \|z_t\| \gg 1$$

Proposition

If $f \in \left\{ \begin{array}{c} \text{[Diagram of a point fixed by a rotation]} \\ \text{[Diagram of a point repelled by a rotation]} \\ \text{[Diagram of a chaotic attractor]} \end{array} \right\}$:

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3. **deduce convergence from the ergodicity**

Theorem

If $f \in \left\{ \text{[Diagram 1]}, \text{[Diagram 2]}, \text{[Diagram 3]} \right\}$, ES converges linearly (or geometrically):

$$\lim_{t \rightarrow \infty} \frac{1}{t} \log \frac{\|m_t - x^*\|}{\|m_0 - x^*\|} = \lim_{t \rightarrow \infty} \mathbb{E} \left[\log \frac{\|m_{t+1} - x^*\|}{\|m_t - x^*\|} \right] = -\text{CR}.$$

Proof.

$$\frac{1}{T} \log \frac{\|m_T - x^*\|}{\|m_0 - x^*\|}$$

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$$\frac{1}{T} \log \frac{\|m_T - x^*\|}{\|m_0 - x^*\|} = \frac{1}{T} \sum_{t=0}^{T-1} \log \|m_{t+1} - x^*\| - \log \|m_t - x^*\|$$

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Proof.

$$\lim_{T \rightarrow \infty} \frac{1}{T} \log \frac{\|m_T - x^*\|}{\|m_0 - x^*\|} = \mathbb{E}_{z_t \sim \pi} [\log \|z_{t+1}\| - \log \|z_t\| + \uparrow (\|z_{t+1} - z_t\|)]$$

□

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Proof.

$$\lim_{T \rightarrow \infty} \frac{1}{T} \log \frac{\|m_T - x^*\|}{\|m_0 - x^*\|} = \mathbb{E}_{z_t \sim \pi} [\uparrow (\|z_{t+1} - z_t\|)]$$

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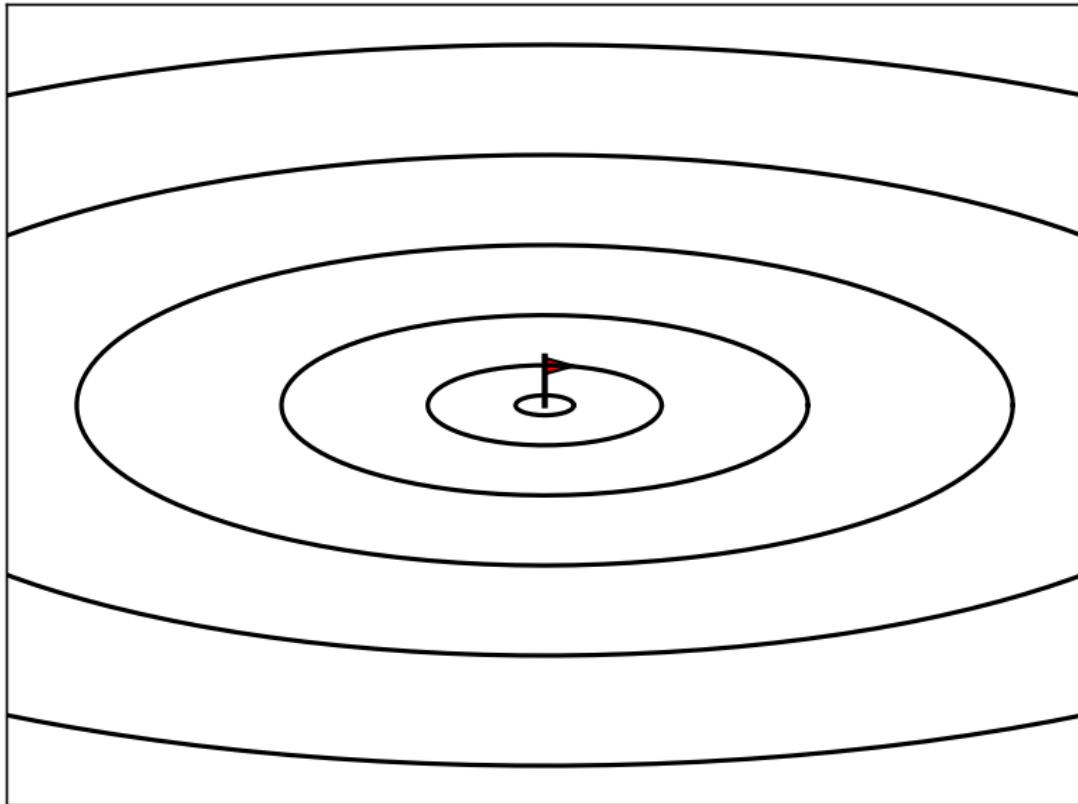
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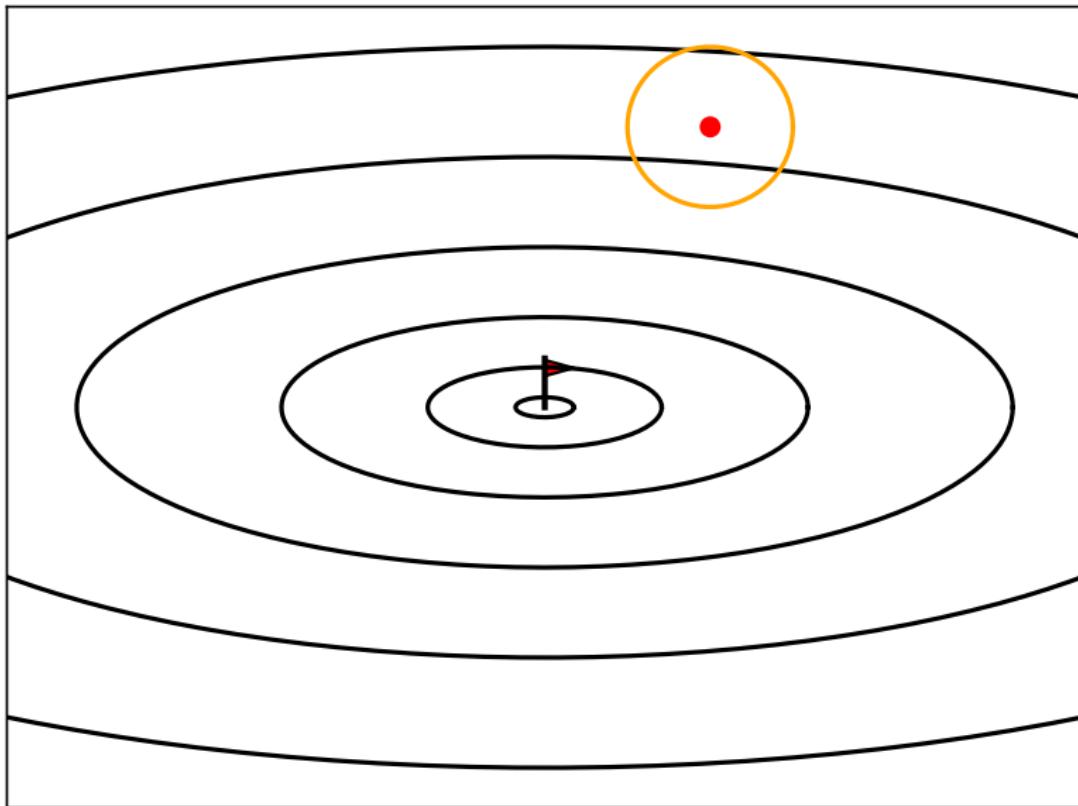
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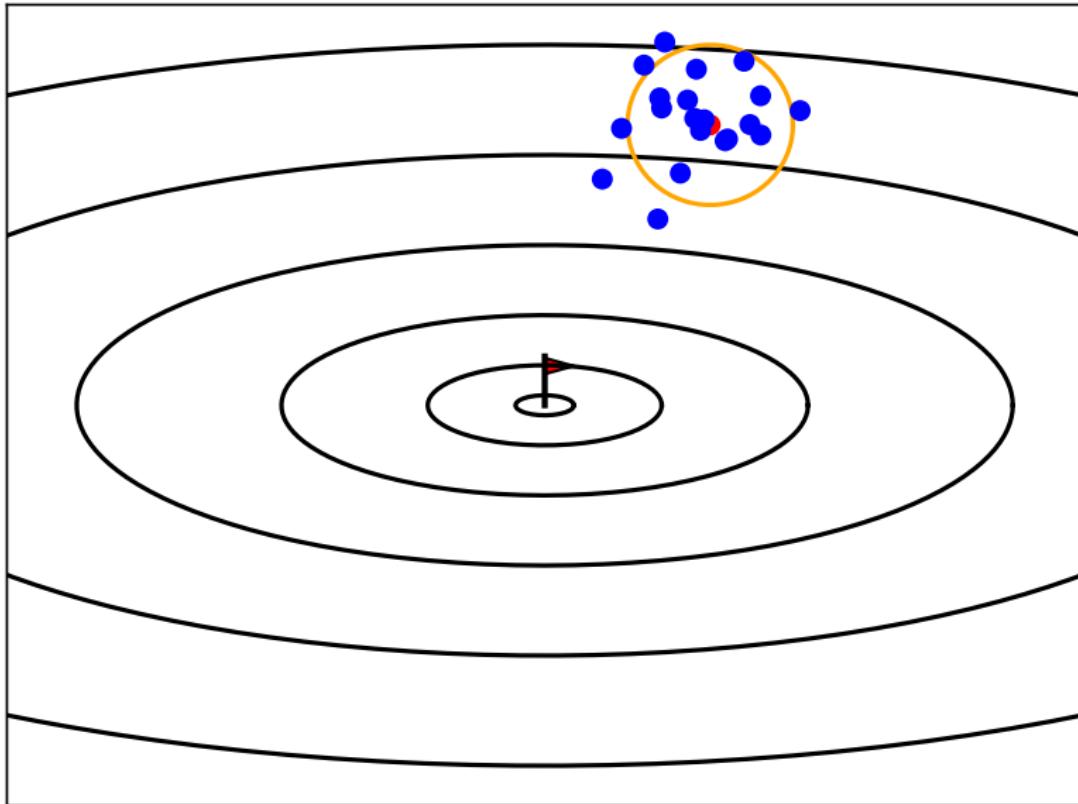
$$\lim_{T \rightarrow \infty} \frac{1}{T} \log \frac{\|m_T - x^*\|}{\|m_0 - x^*\|} = \mathbb{E}_{z_t \sim \pi} [\uparrow (\|z_{t+1} - z_t\|)]$$

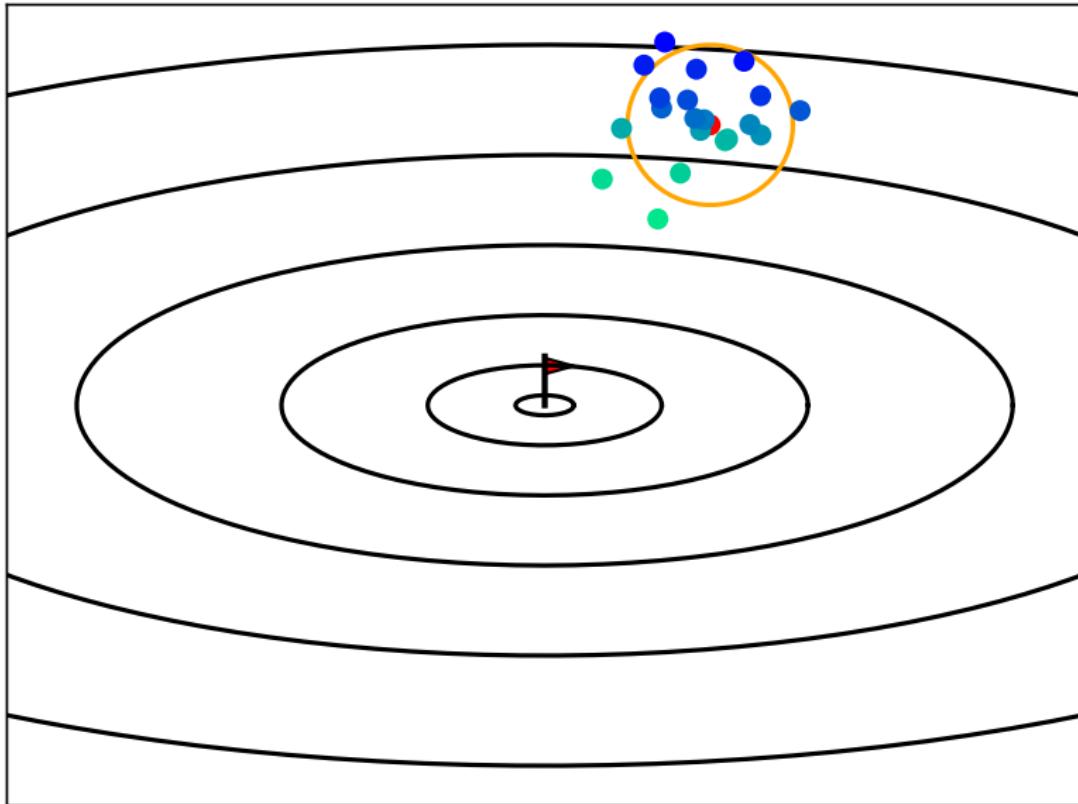
$$\text{CR} = -\mathbb{E}_{z_t \sim \pi} \uparrow (\|z_{t+1} - z_t\|)$$

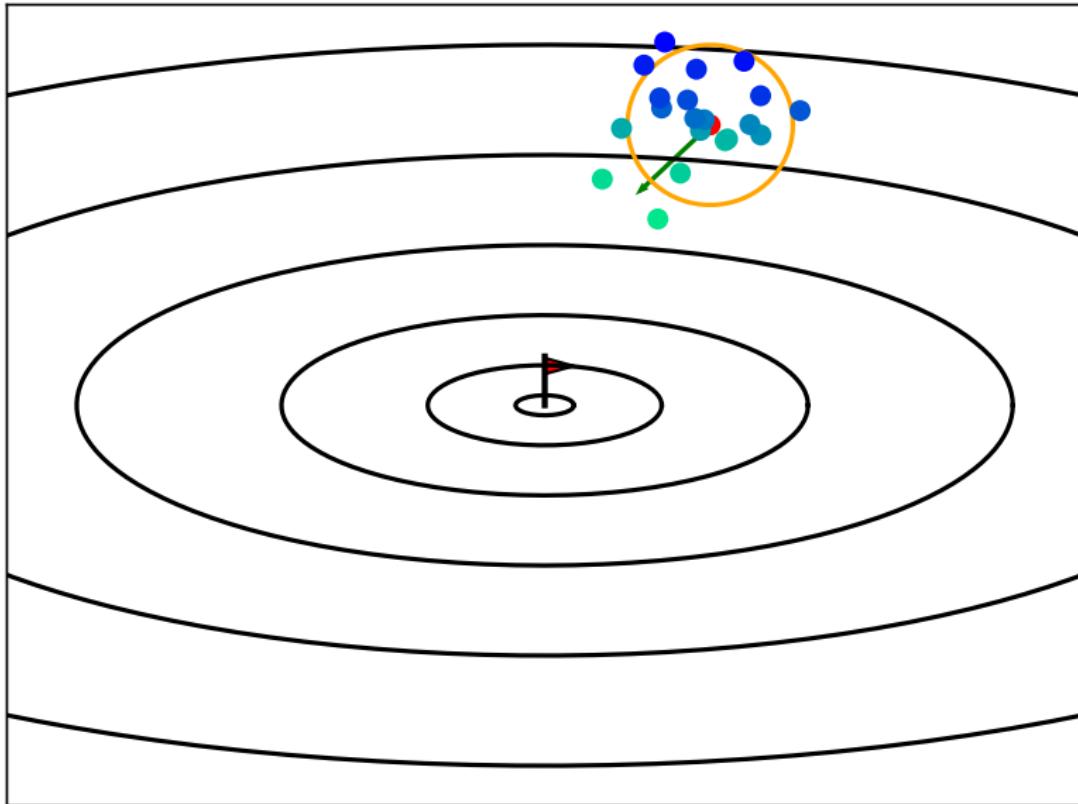
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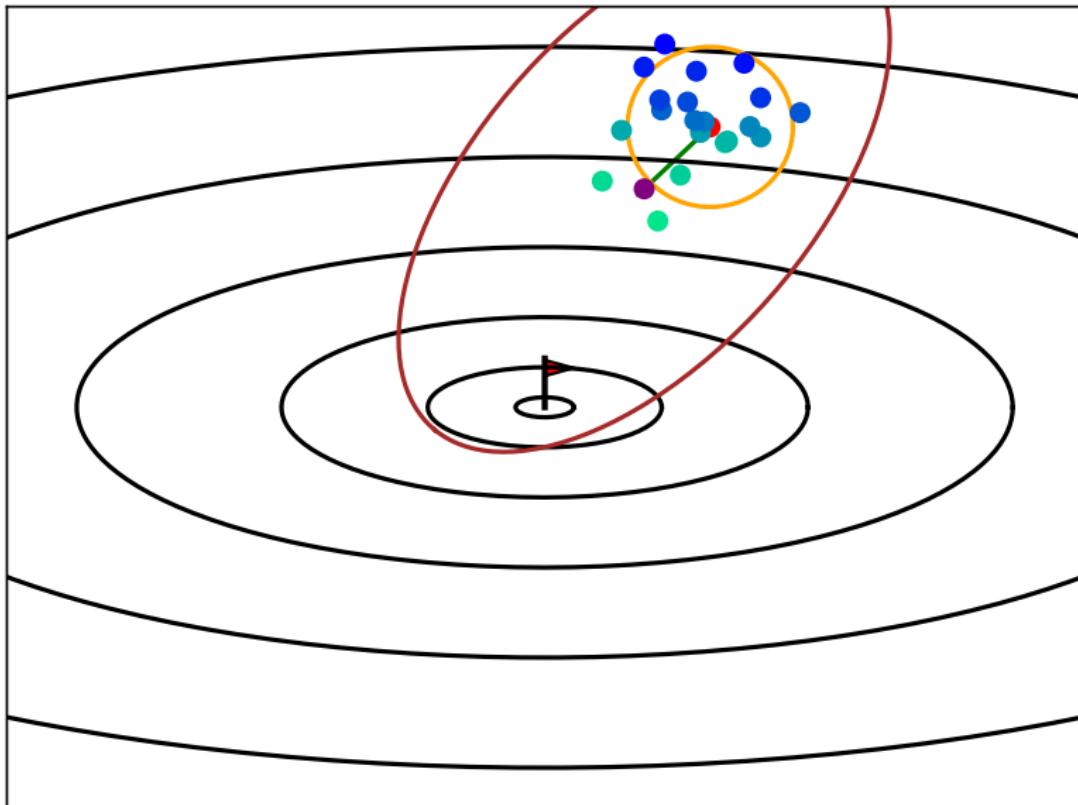












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where C_t is the covariance matrix at iteration t

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$x_{t+1}^{1:\lambda}$ is the best point among $\{x_{t+1}^1, \dots, x_{t+1}^\lambda\}$

Idea: sample more in the direction $x_{t+1}^{1:\lambda} - m_t$ at iteration $t + 1$

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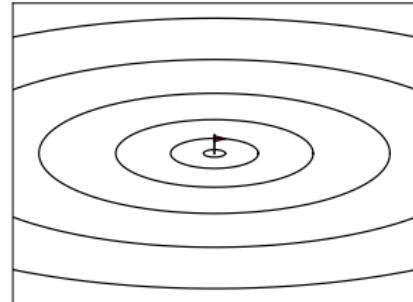
$$\overleftrightarrow{v} = v \otimes v = v \times v^\top$$

$$C_{t+1} = \text{Positive combination} \left(C_t, \overleftrightarrow{x_{t+1}^{1:\lambda} - m_t} \right)$$

favors more the sampling in the direction $x_{t+1}^{1:\lambda} - m_t$ than C_t

Algorithm 4 ES with covariance matrix adaptation

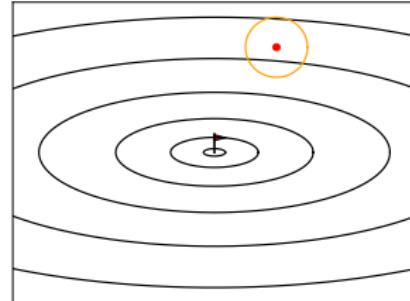
Goal: $\min_{x \in \mathbb{R}^d} f(x)$



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Repeat ($m_t \in \mathbb{R}^d$, $\sigma_t > 0$, $C_t \succ 0$)

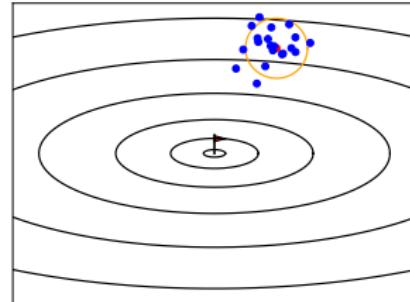


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Repeat ($m_t \in \mathbb{R}^d$, $\sigma_t > 0$, $C_t \succ 0$)

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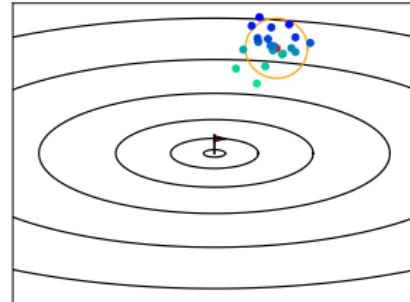
λ = population size

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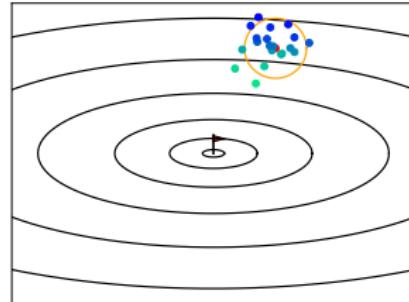
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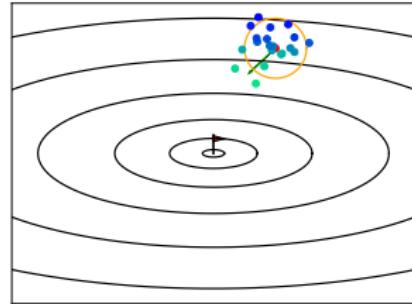
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λ = population size

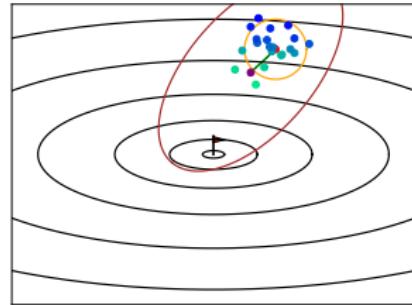
μ = parent number

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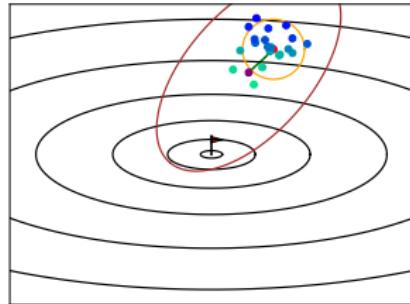
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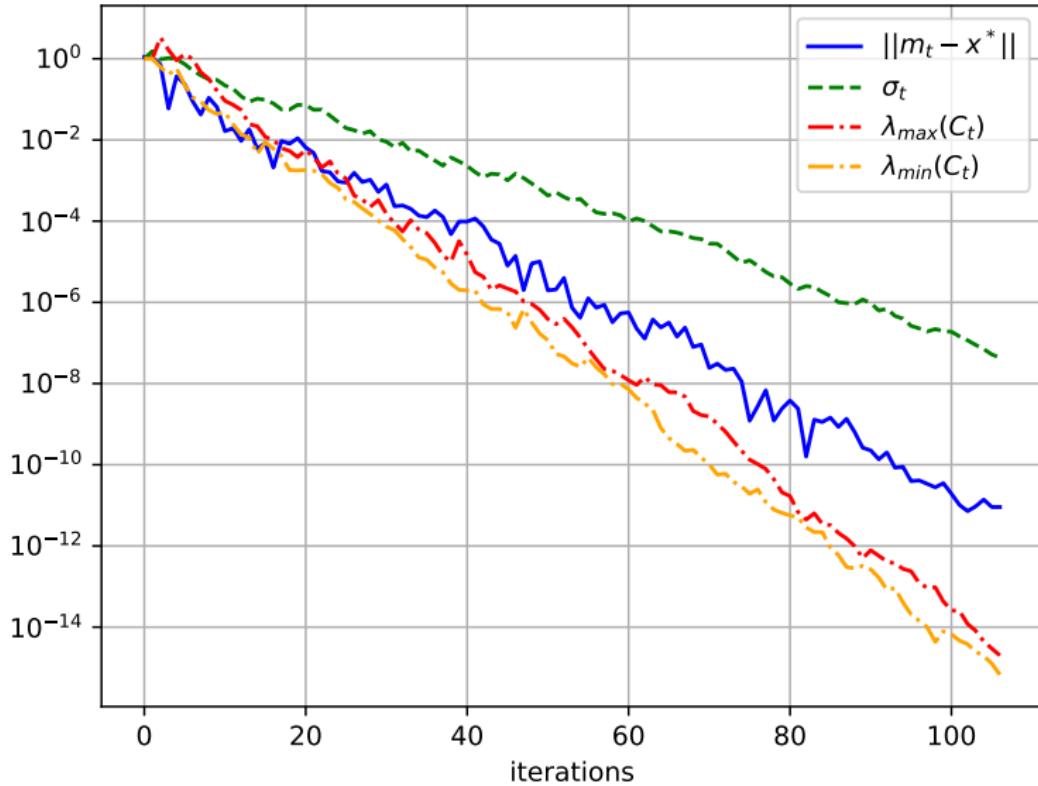
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2. sort $f(x_{t+1}^i)$:
 $f(x_{t+1}^{1:\lambda}) \leq \dots \leq f(x_{t+1}^{\lambda:\lambda})$
3. $m_{t+1} = \text{Average}(x_{t+1}^{1:\lambda}, \dots, x_{t+1}^{\mu:\lambda})$
4. $\sigma_{t+1} = \sigma_t \times \text{increasing function}(\|m_{t+1} - m_t\|)$
5. $C_{t+1} = \text{Positive combination}\left(C_t, \text{Average}\left[\overleftrightarrow{(x_{t+1}^{i:\lambda} - m_t)}\right]\right)$

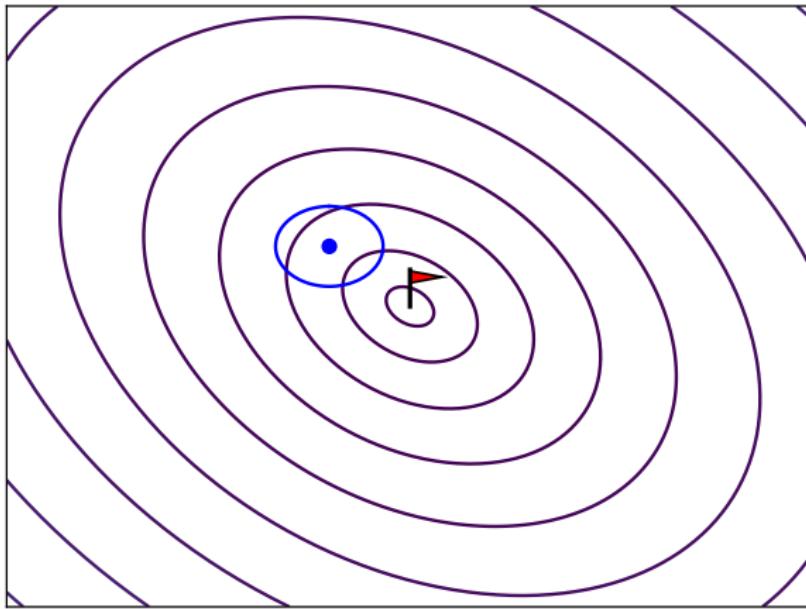


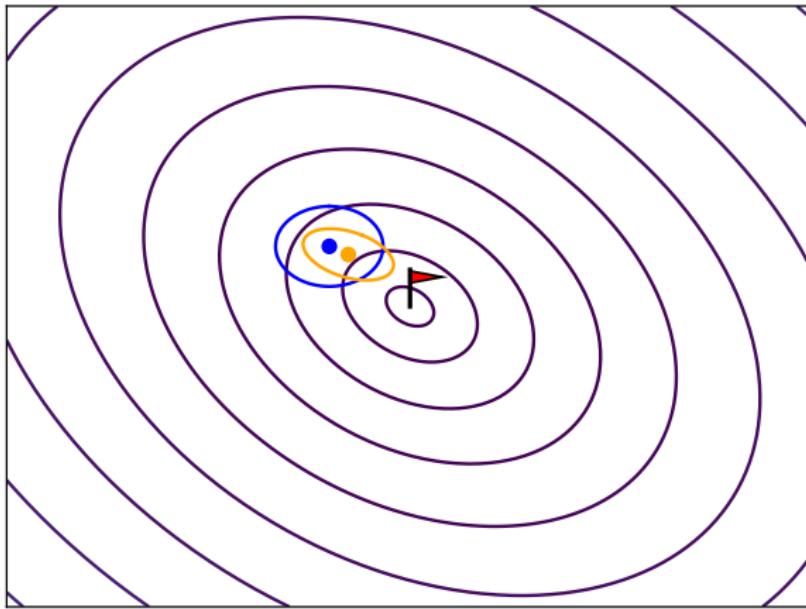
λ = population size

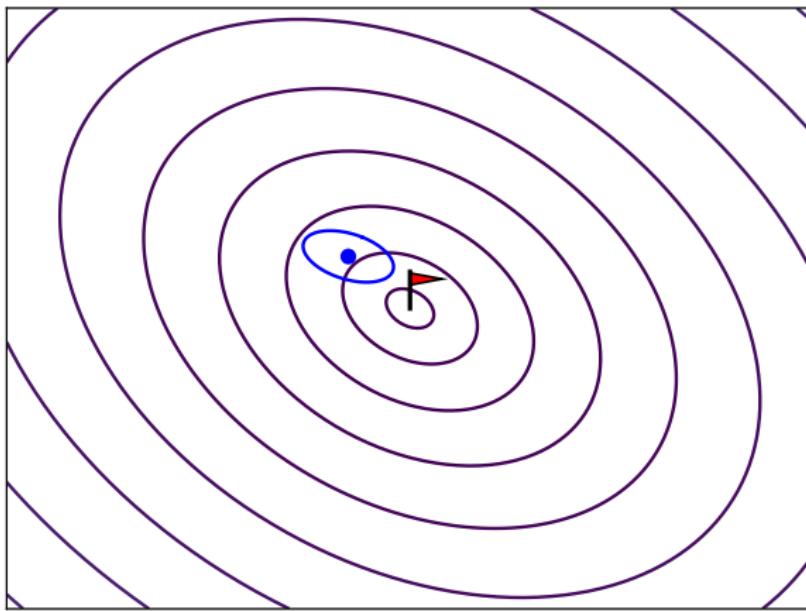
μ = parent number

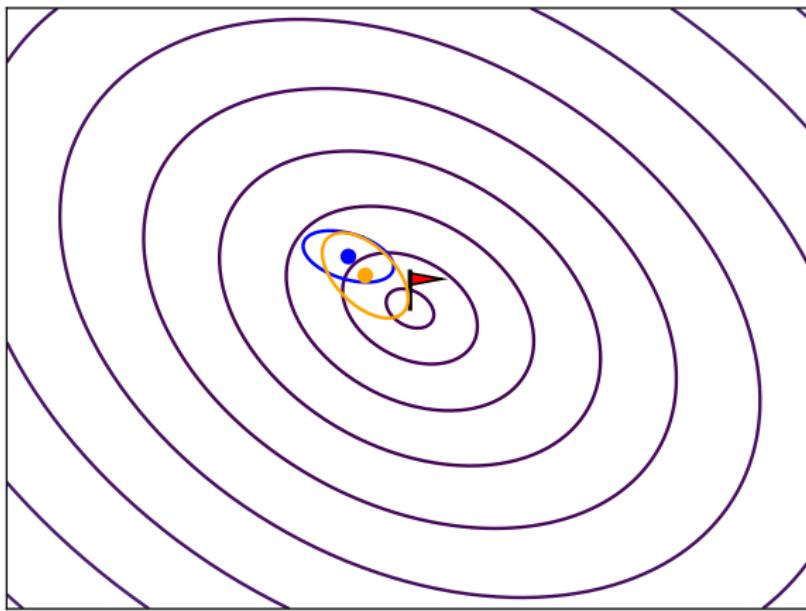
$$f: x \mapsto x^T A x$$

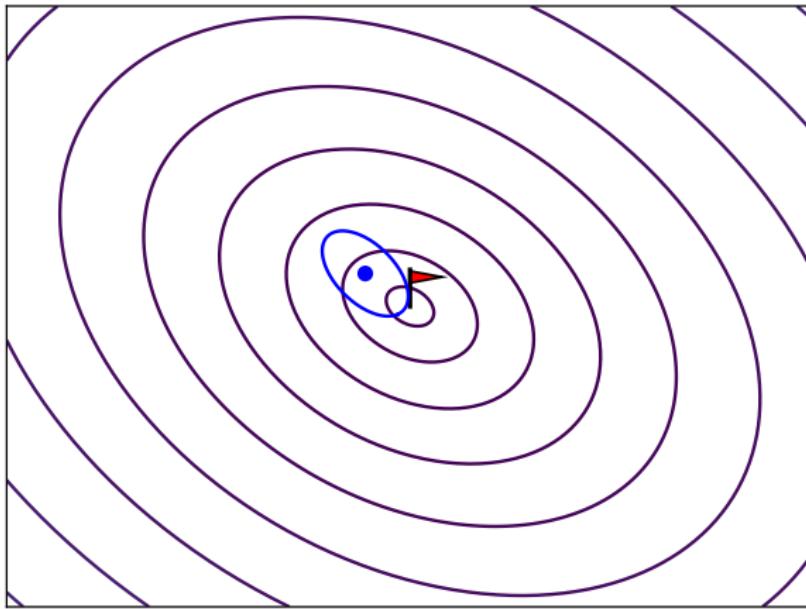


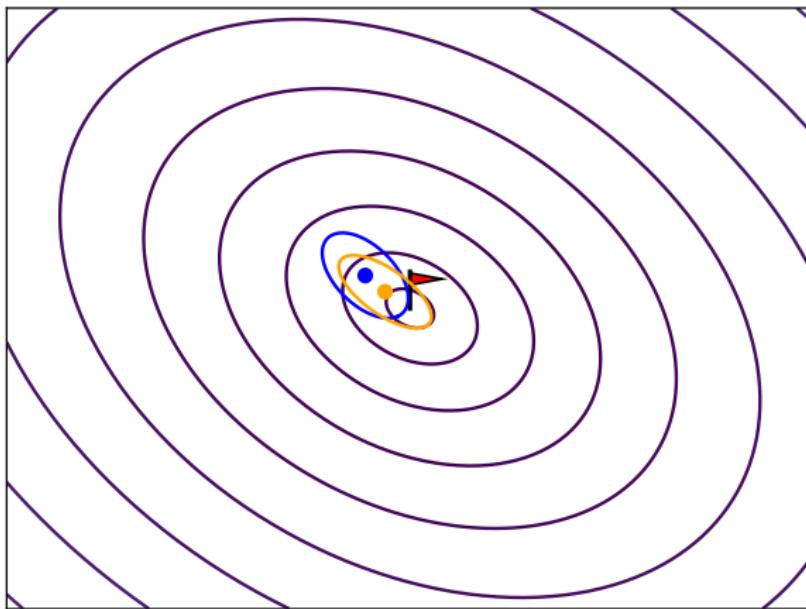


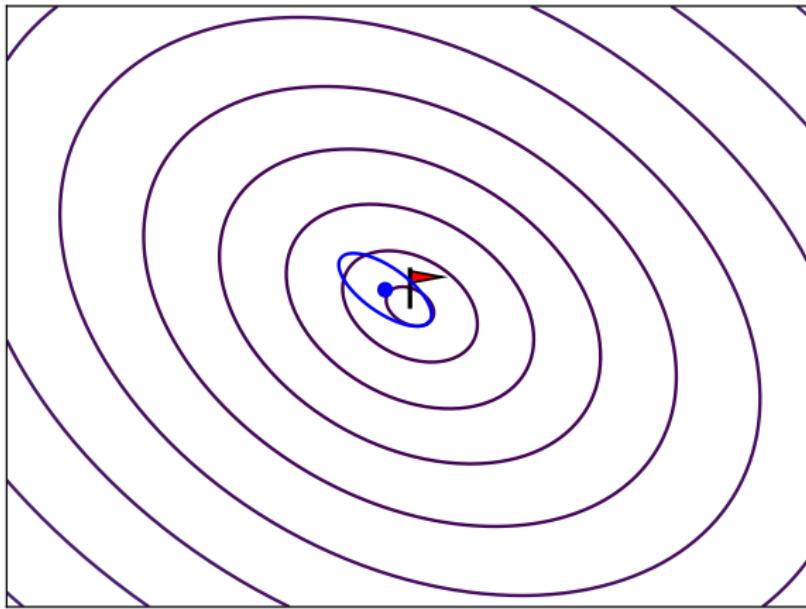


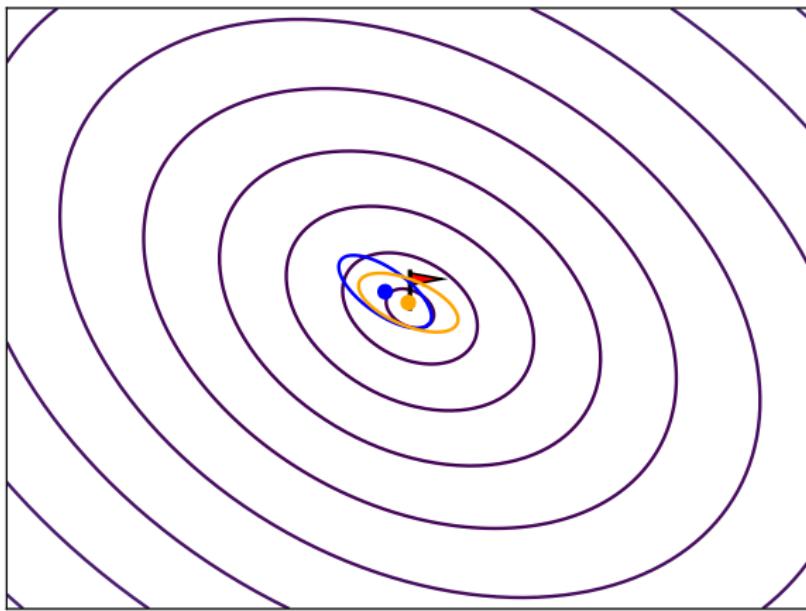


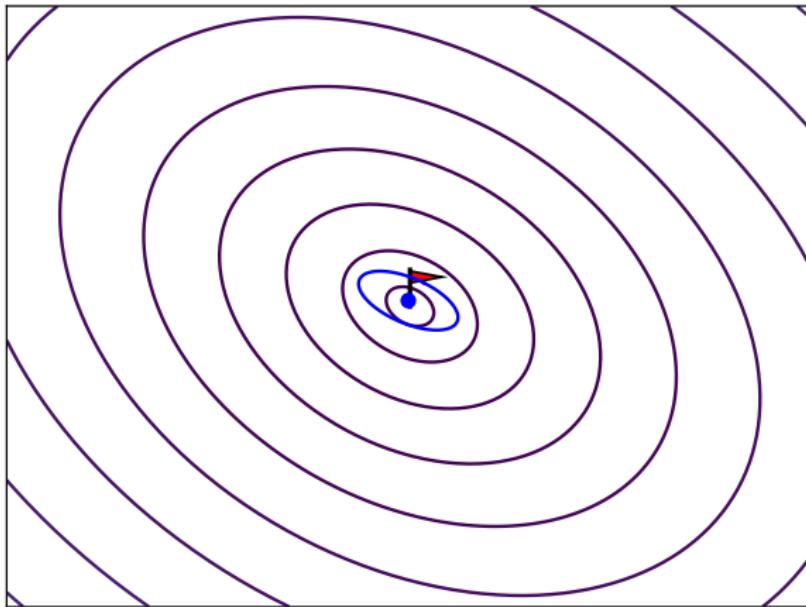


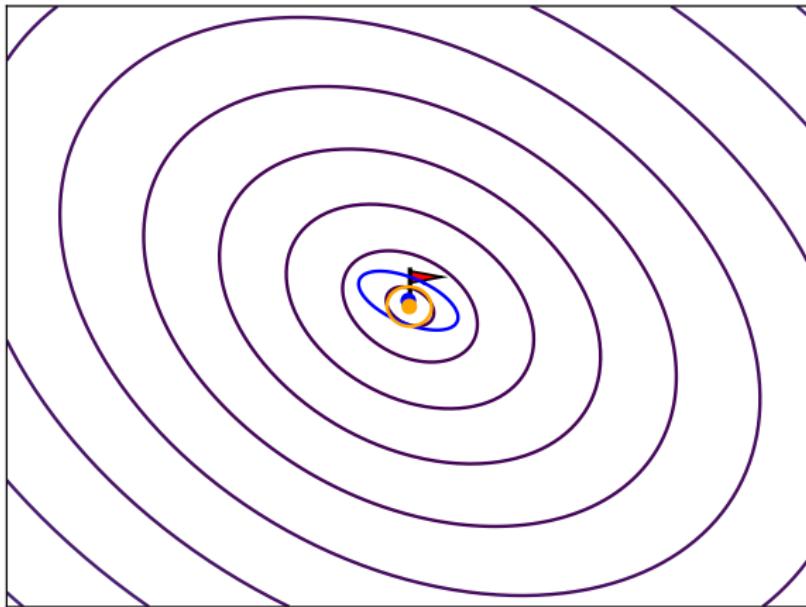


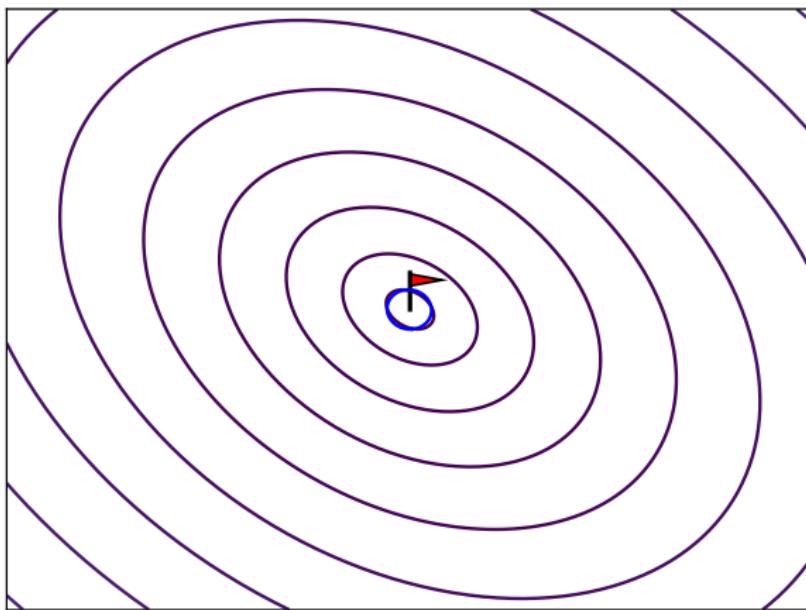


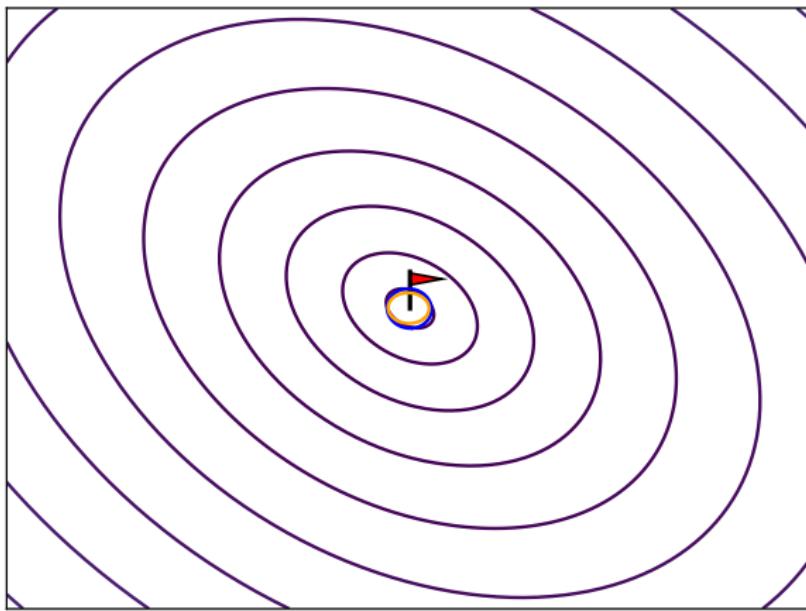


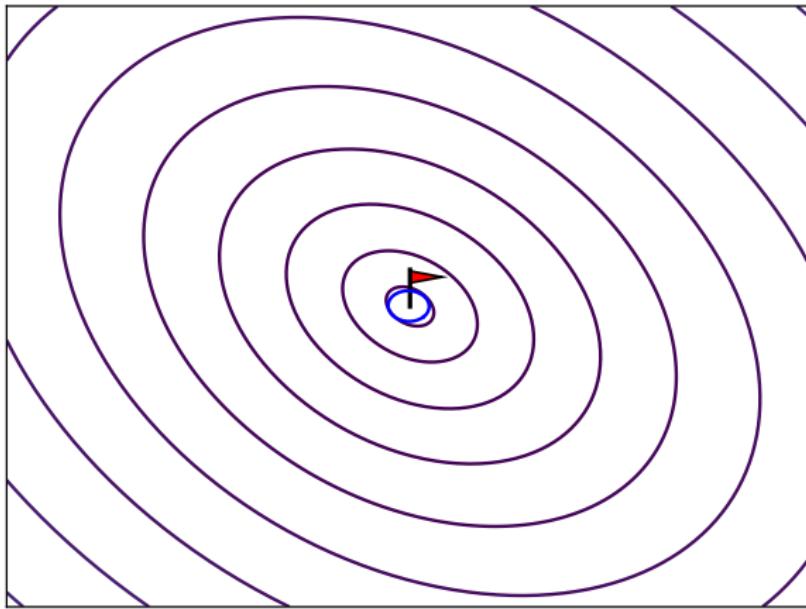


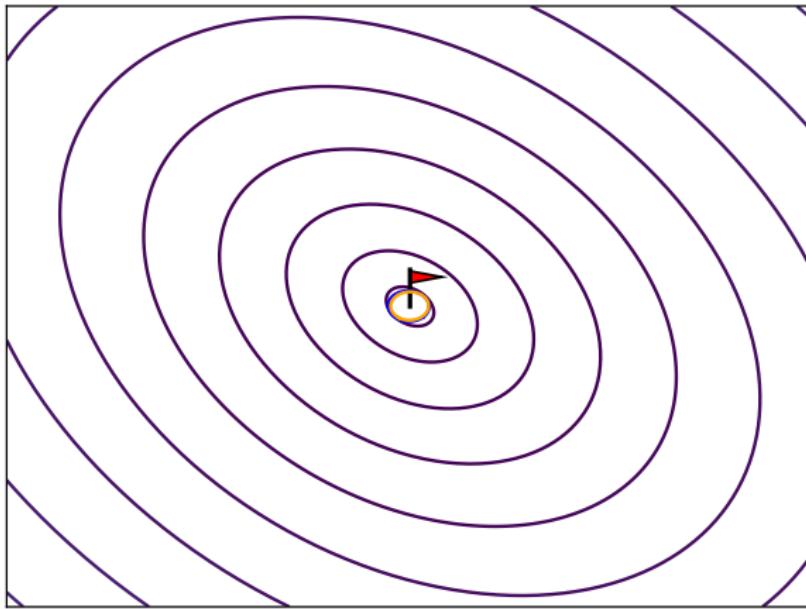


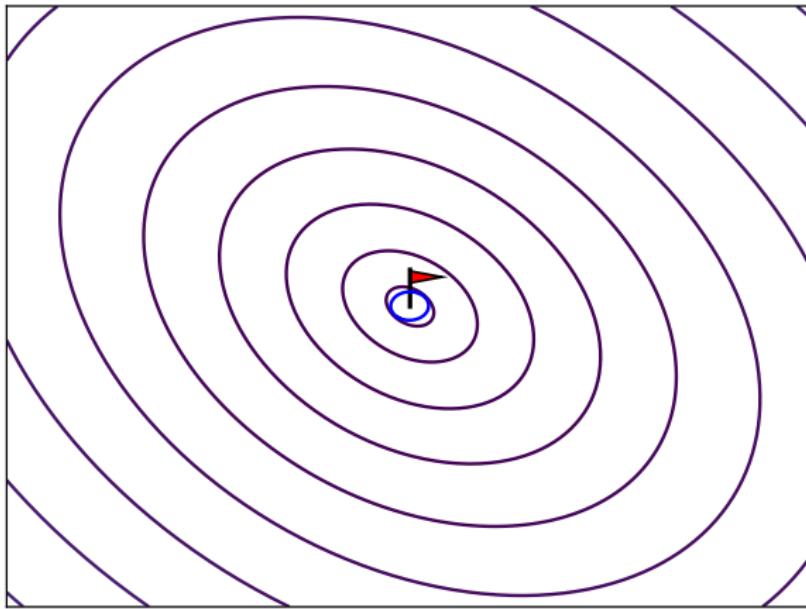


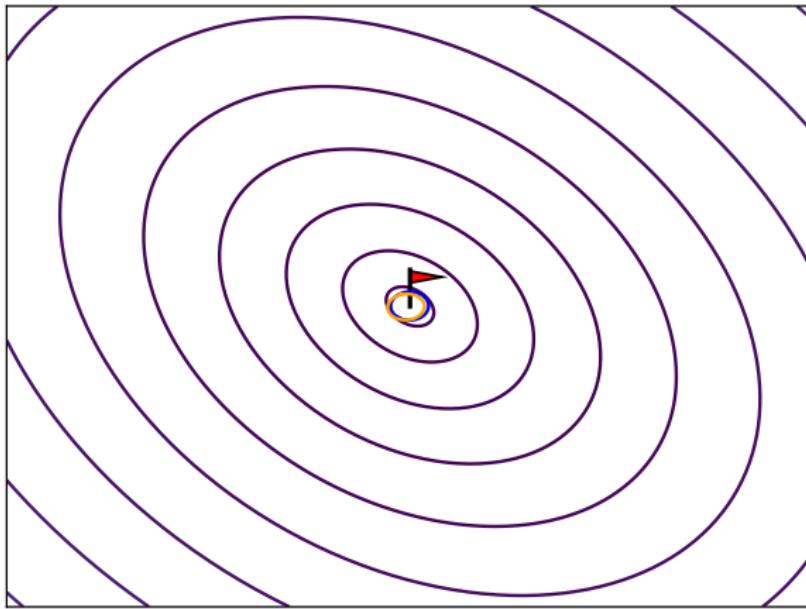


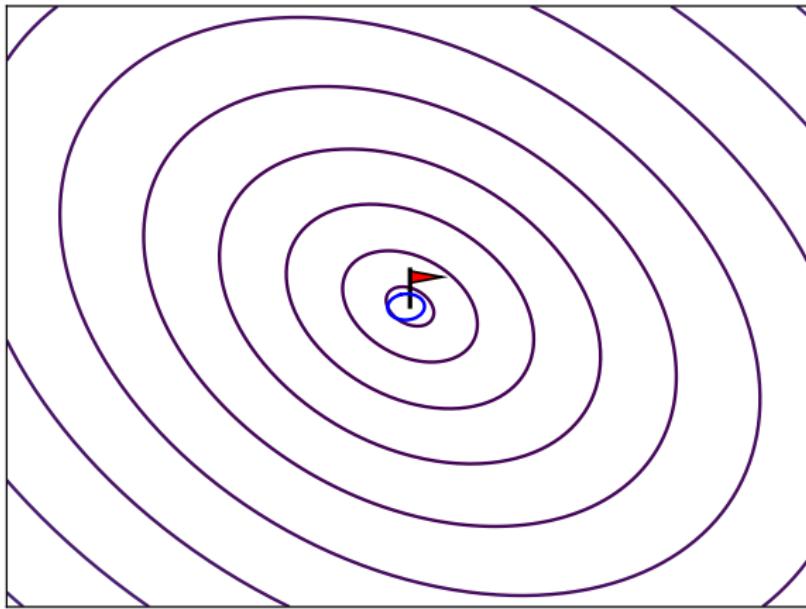


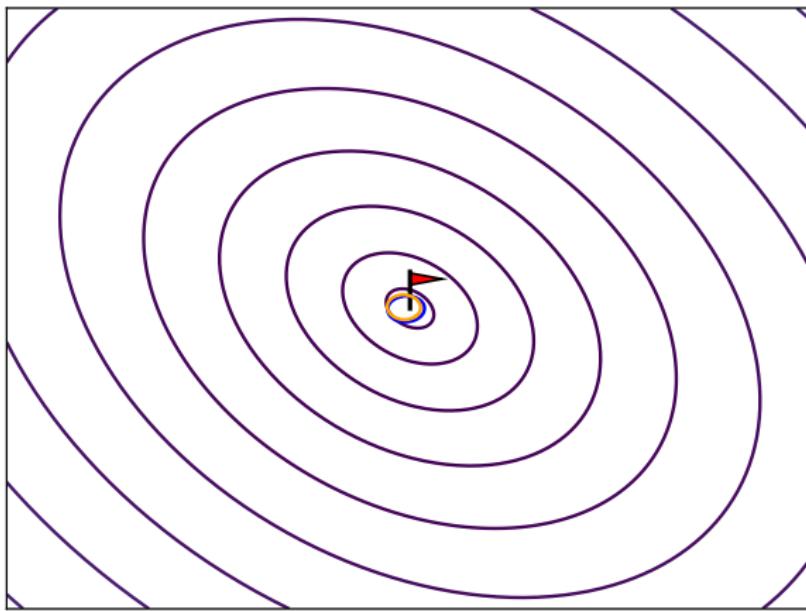


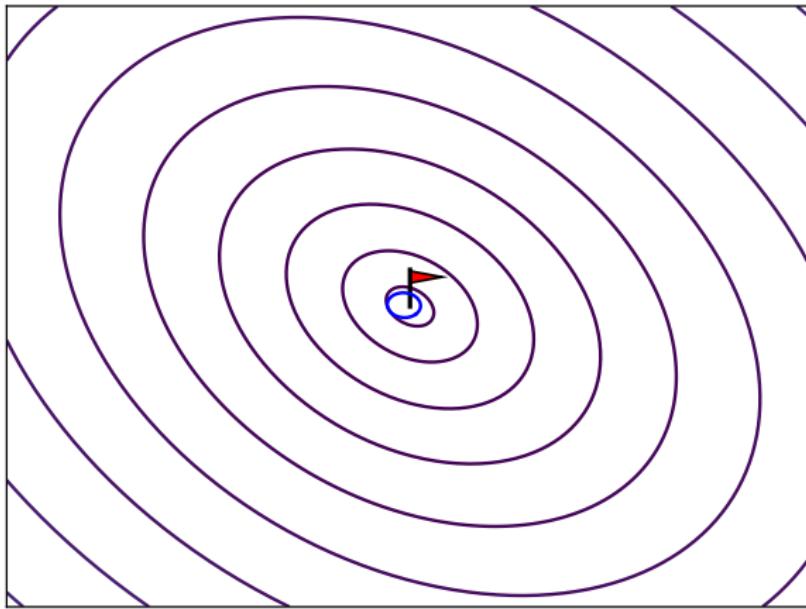


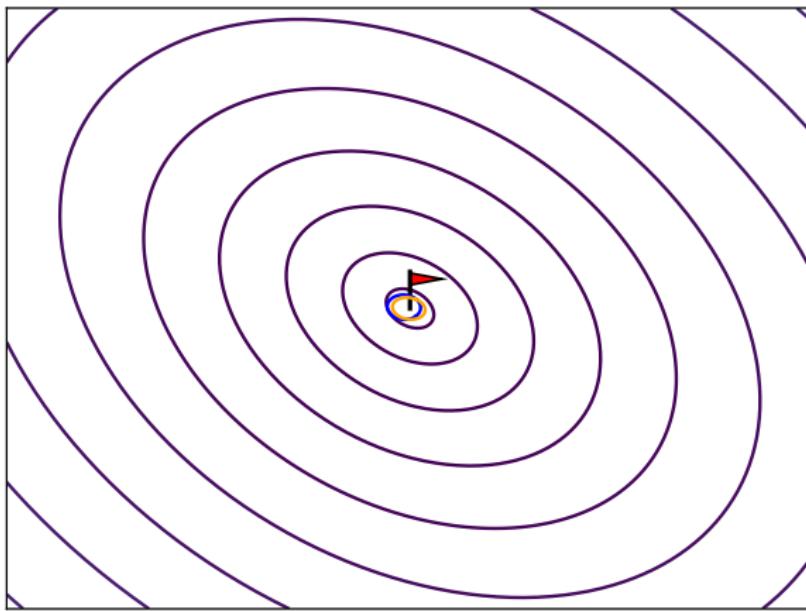


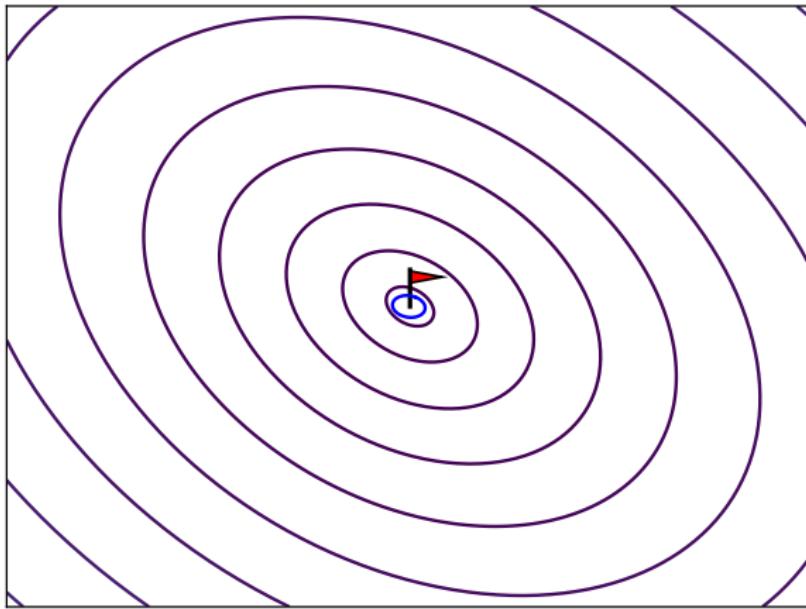


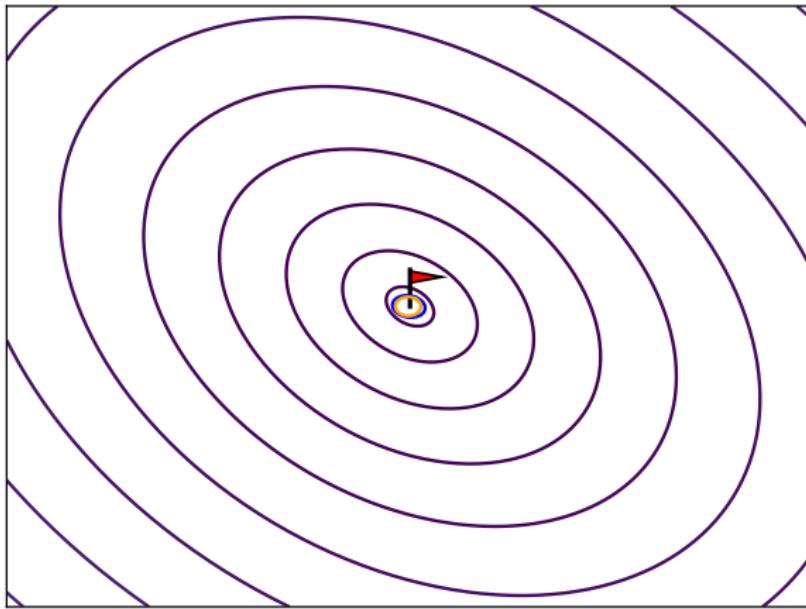


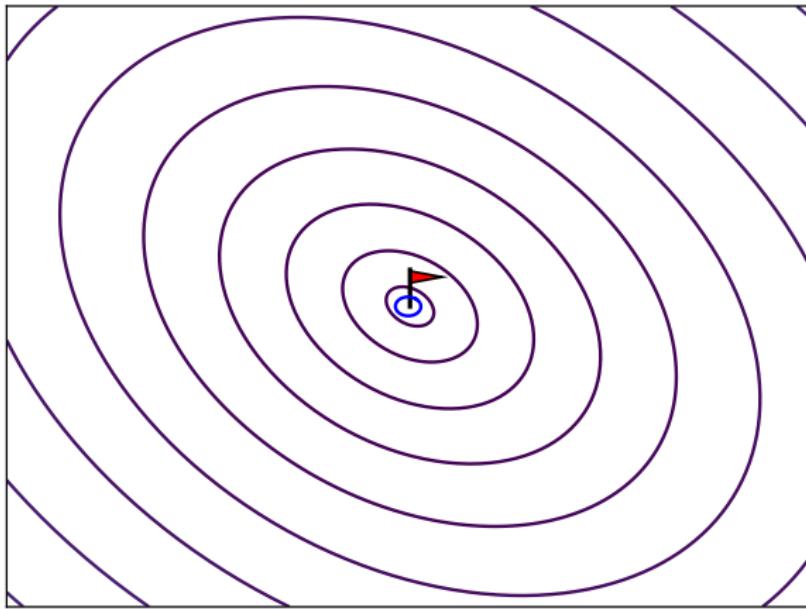


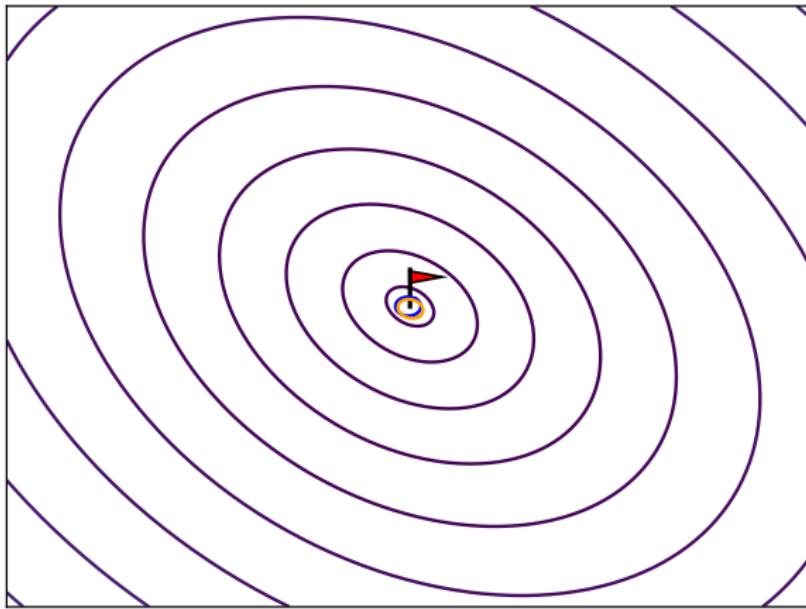


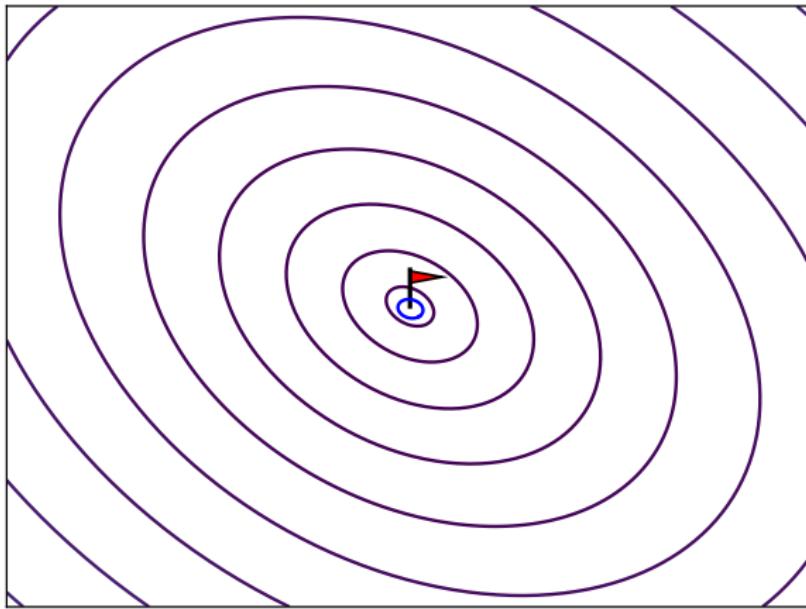


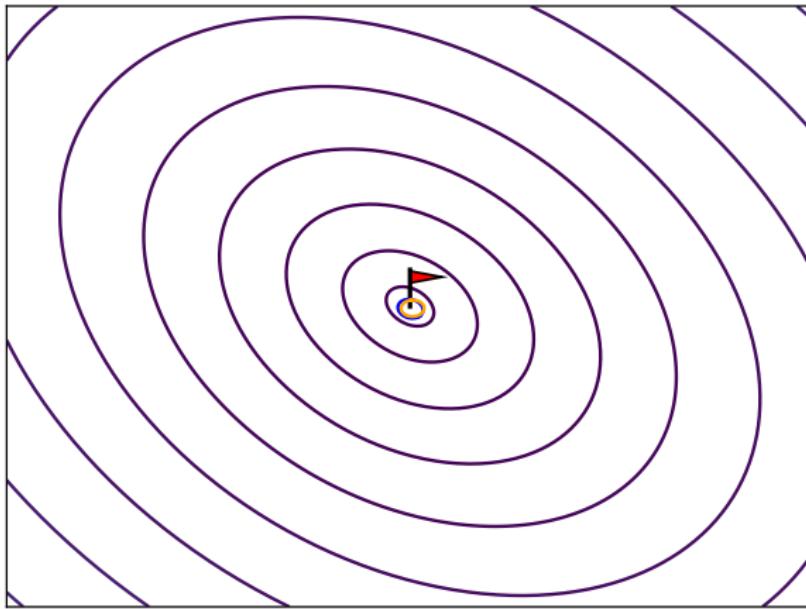












Observations:

$$\lim_{t \rightarrow \infty} m_t = x^*$$

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For the proof: we rely (again) on Markov chains

$$z_t = \frac{m_t - x^*}{\sigma_t \sqrt{\lambda_{\min}(C_t)}}$$

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$$\Sigma_t = \frac{C_t}{\lambda_{\min}(C_t)}$$

Proposition

If $f \in \left\{ \text{, } \text{, } \text{, } \text{} \right\}$, then $\{(z_t, \Sigma_t)\}_{t \in \mathbb{N}}$ is a Markov chain.

Scheme of proof:

1. irreducibility and aperiodicity of $\{(z_t, \Sigma_t)\}_{t \in \mathbb{N}}$
2. drift condition: $\exists K \subset \mathbb{R}^d \times \lambda_{\min}^{-1}(\{1\})$ compact and
 $V: \mathbb{R}^d \times \lambda_{\min}^{-1}(\{1\}) \rightarrow [1, +\infty]$

$$\mathbb{E}[V(z_1, \Sigma_1)] \leq (1 - \varepsilon)V(z_0, \Sigma_0) \quad \forall (z_0, \Sigma_0) \notin K$$

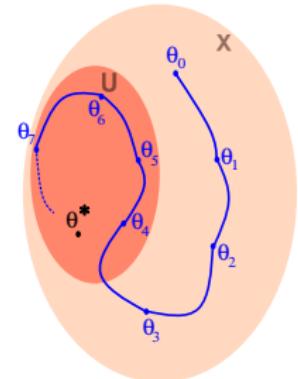
3. deduce convergence from the ergodicity

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3. deduce convergence from the ergodicity

θ^* is **attracting** when

$$\exists x_1, x_2, \dots, \lim_{k \rightarrow \infty} F_k(\theta_0, x_{1..k}) = \theta^*$$



Theorem

If

- $\exists \theta^*$ *attracting*
- $\exists x_1^*, \dots, x_k^*$

such that $F_k(\theta^*, \cdot)$ is a **submersion** at $x_{1..k}^*$,

then, $\{\theta_t\}_{t \in \mathbb{N}}$ is **irreducible** and **aperiodic**.

$$(z_{k+1}, \Sigma_{k+1}) = F(z_k, \Sigma_k, z_{k+1}^{1:\lambda}, \dots, z_{k+1}^{\lambda:\lambda})$$

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$(0, I_d)$ is attracting

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$(0, I_d)$ is attracting, and $F_k(0, I_d, \cdot)$ is submersive somewhere.

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Proposition

$(0, I_d)$ is attracting, and $F_k(0, I_d, \cdot)$ is submersive somewhere.

Corollary

If $f \in \left\{ \begin{array}{c} \text{[Diagram of a spiral attractor]} \\ \text{[Diagram of a limit cycle attractor]} \\ \text{[Diagram of a quasiperiodic pattern]} \\ \text{[Diagram of a chaotic attractor]} \end{array} \right\}$, $\{z_t, \Sigma_t\}_{t \in \mathbb{N}}$ is irreducible and aperiodic.

Scheme of proof:

1. irreducibility and aperiodicity of $\{(z_t, \Sigma_t)\}_{t \in \mathbb{N}}$
2. **drift condition:** $\exists K \subset \mathbb{R}^d \times \lambda_{\min}^{-1}(\{1\})$ **compact and**
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$$V(z, \Sigma) = \text{linear combination}(\|z\|^2, \|\Sigma\|)$$

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Proposition

If $f = \boxed{\circlearrowleft}$, then:

$$\mathbb{E}[V(z_{t+1}, \Sigma_{t+1}) \mid z_t, \Sigma_t] \leq (1 - \varepsilon) \times V(z_t, \Sigma_t)$$

when $\|z_t\| \gg 1$ or $\|\Sigma_t\| \gg 1$

When $\|\Sigma_t\| \gg \|z_t\|^2$:

When $\lambda_{\max}(\Sigma_t) \gg \|z_t\|^2$:

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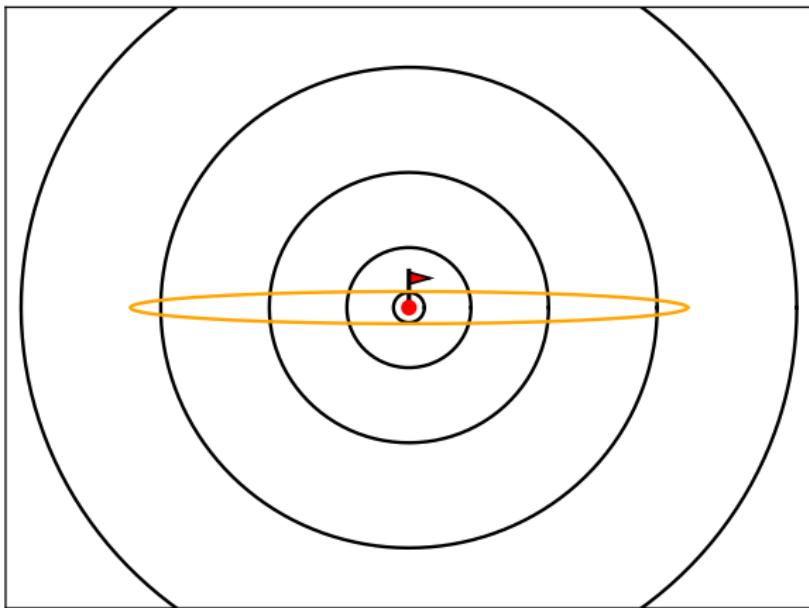
$$\begin{aligned}\mathbb{E}_t [\text{linear combination}(\|z_{t+1}\|^2, \|\Sigma_{t+1}\|)] \\ \leq (1 - \varepsilon) \times \text{linear combination}(\|z_t\|^2, \|\Sigma_t\|)\end{aligned}$$

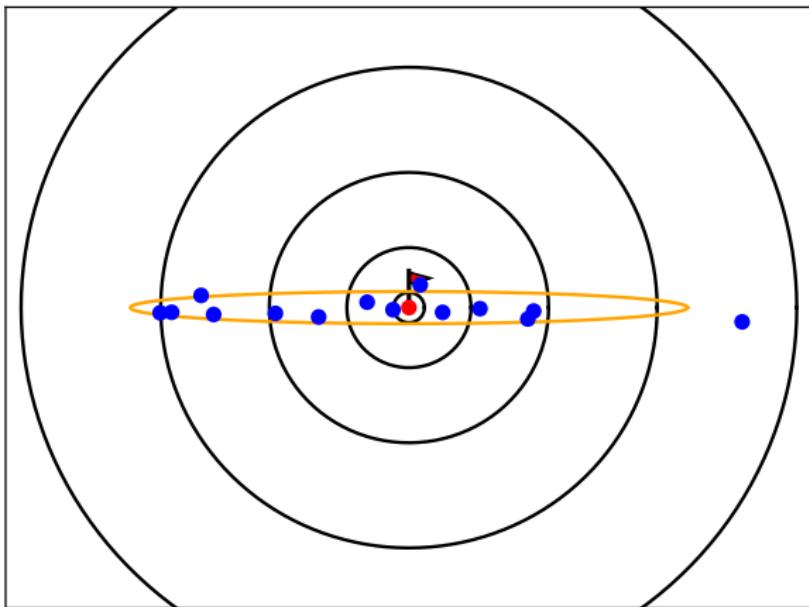
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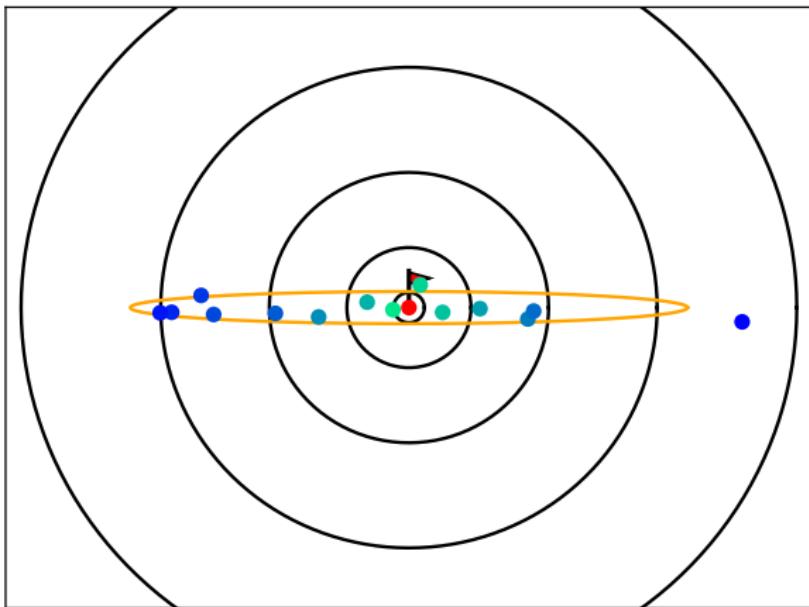
$$\mathbb{E}_t [\|\Sigma_{t+1}\|] \leq (1 - \varepsilon) \times \|\Sigma_t\|$$

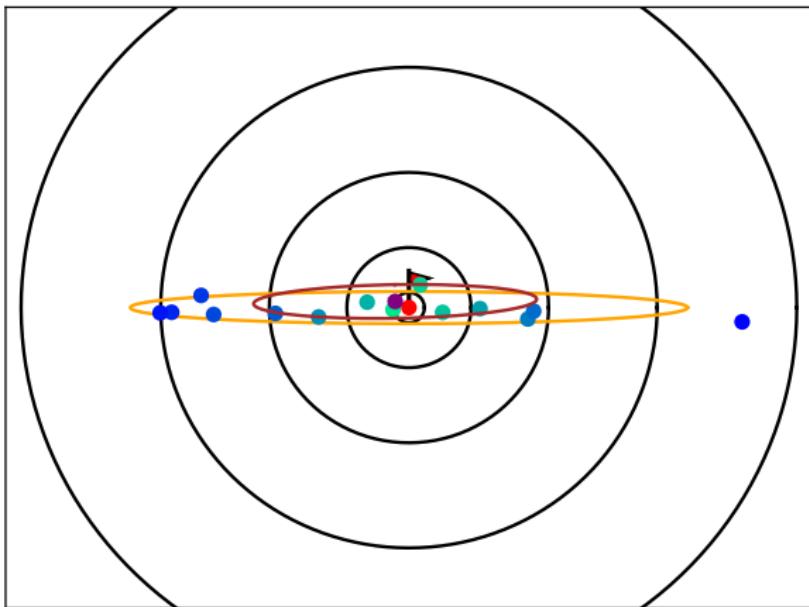
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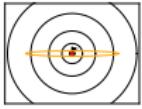








Proposition

When :

$$\mathbb{E} [\lambda_{\max}(\Sigma_{t+1})] \leq (1 - \varepsilon) \times \lambda_{\max}(\Sigma_t)$$

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$$\text{normalization} = \frac{\sigma_{t+1}}{\sigma_t} \sqrt{\frac{\lambda_{\min}(C_{t+1})}{\lambda_{\min}(C_t)}}$$

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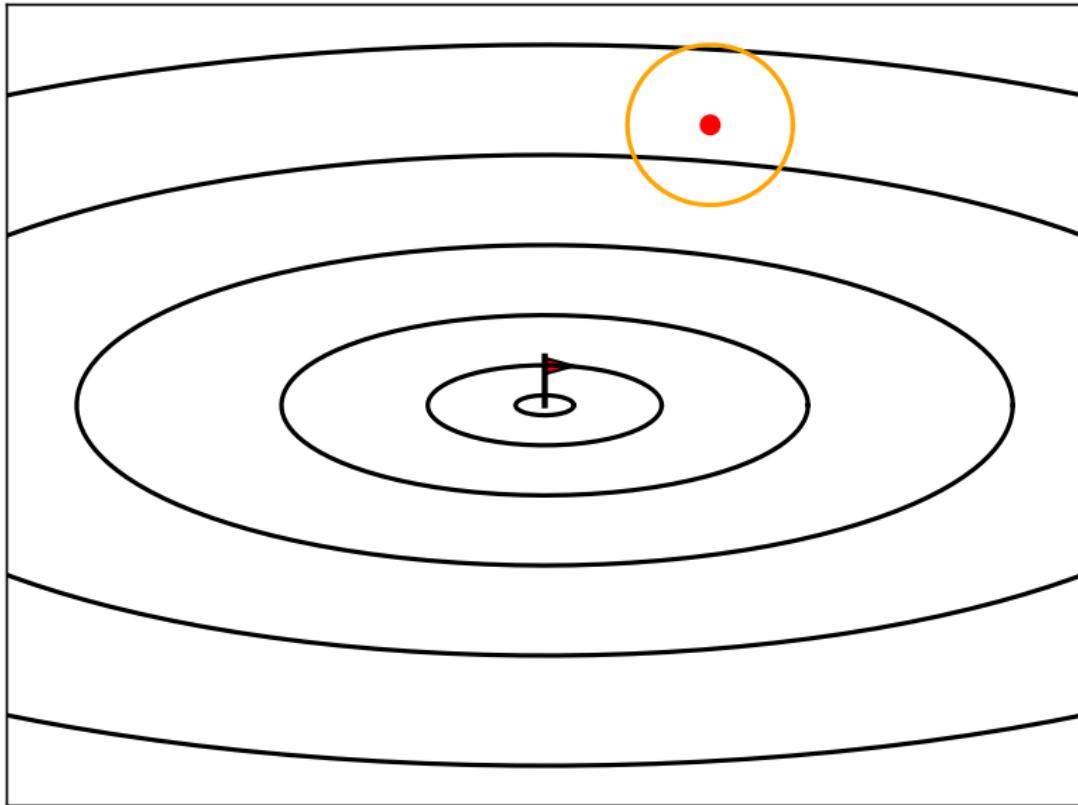
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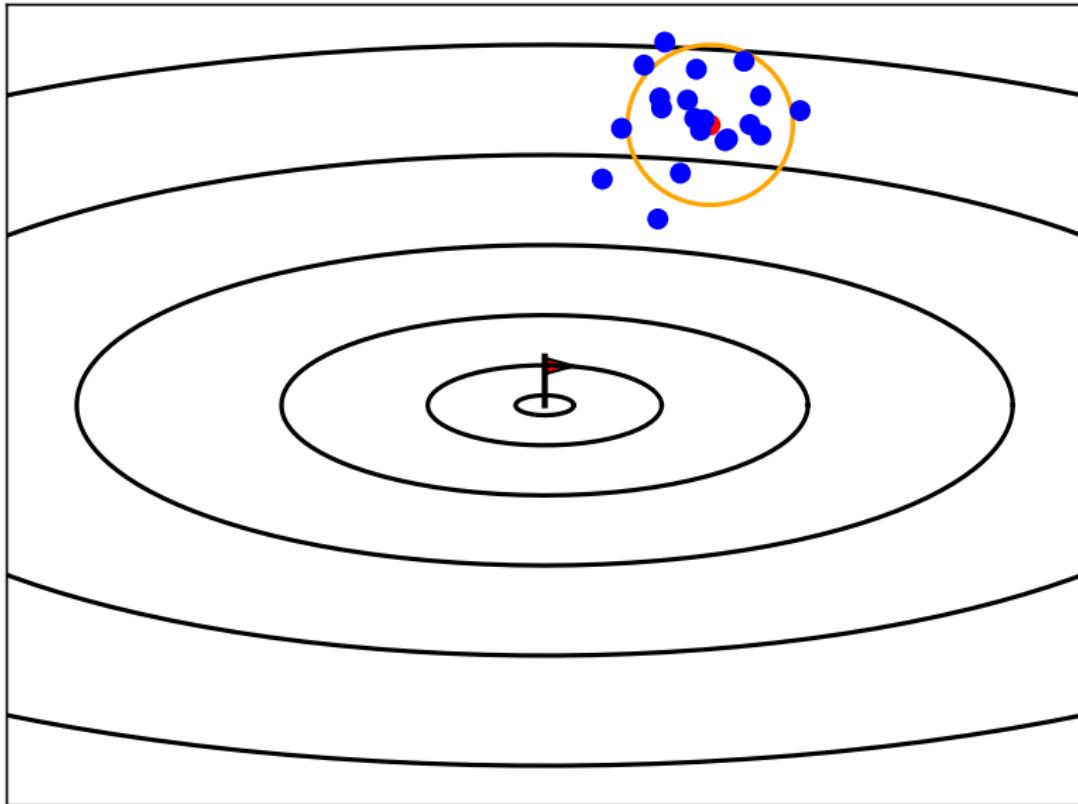
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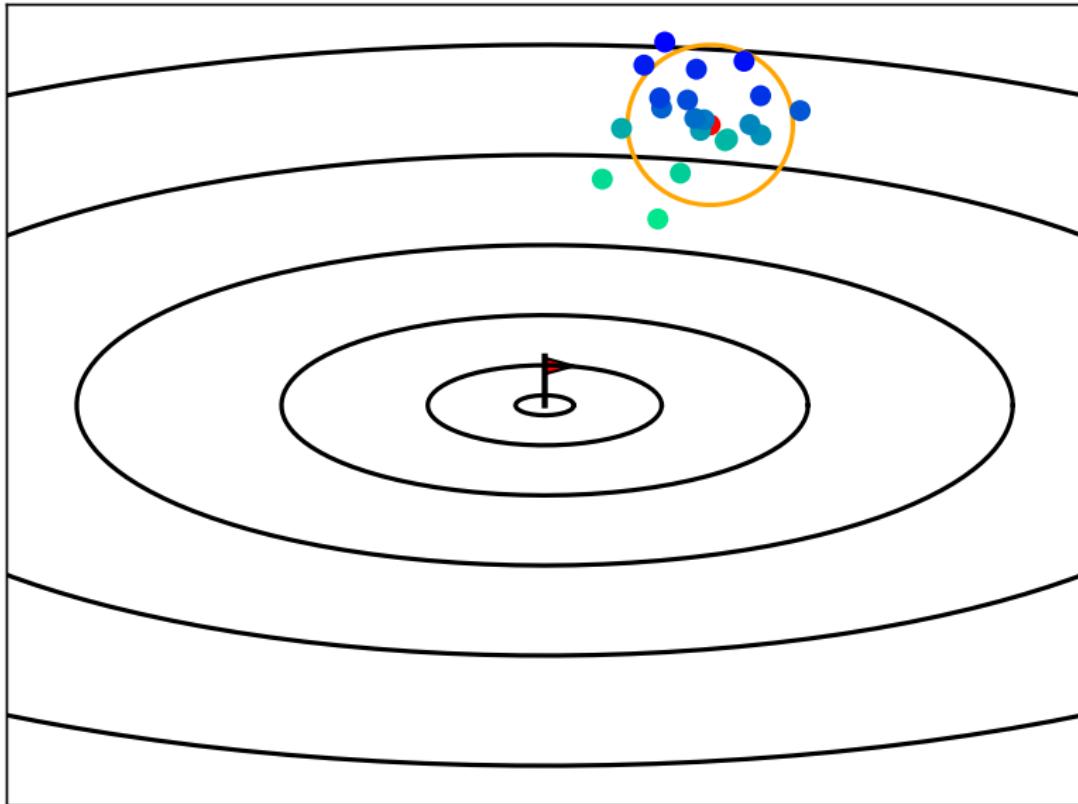
$$\text{normalization} = \underbrace{\frac{\sigma_{t+1}}{\sigma_t}} \sqrt{\frac{\lambda_{\min}(C_{t+1})}{\lambda_{\min}(C_t)}}$$

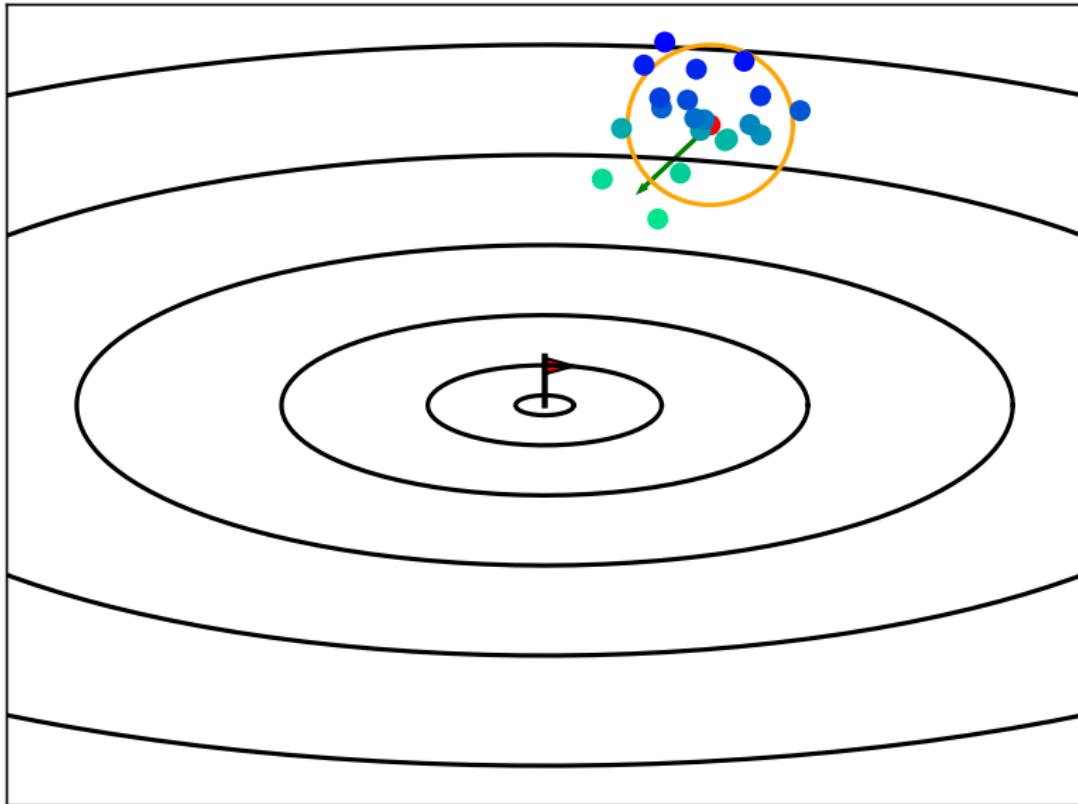
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$$\frac{\sigma_{t+1}}{\sigma_t} = \text{increasing function}(\|z_{t+1} - z_t\|)$$





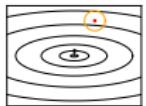




$$\frac{\sigma_{t+1}}{\sigma_t} = \text{increasing function}(\|z_{t+1} - z_t\|)$$

Proposition

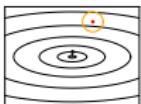
When



$$\mathbb{E}[\|z_{t+1} - z_t\|] \geq constant.$$

$$\frac{\sigma_{t+1}}{\sigma_t} = \text{increasing function}(\|z_{t+1} - z_t\|)$$

Proposition



When

$$\mathbb{E}[\|z_{t+1} - z_t\|] \geq \text{constant}.$$

Corollary

\exists increasing function s.t.:

$$\mathbb{E} [\|z_{t+1}\|^2] \leq (1 - \varepsilon) \times \|z_t\|^2$$

$$V(z, \Sigma) = \text{linear combination}(\|z\|^2, \|\Sigma\|)$$

Proposition

If $f = \boxed{\circlearrowleft}$, then:

$$\mathbb{E}[V(z_{t+1}, \Sigma_{t+1}) \mid z_t, \Sigma_t] \leq (1 - \varepsilon) \times V(z_t, \Sigma_t)$$

when $\|z_t\| \gg 1$ or $\|\Sigma_t\| \gg 1$

Corollary

If $f = \boxed{\text{red dot in green circle}}$, $\{(z_t, \Sigma_t)\}_{t \in \mathbb{N}}$ is ergodic.

Scheme of proof:

1. irreducibility and aperiodicity of $\{(z_t, \Sigma_t)\}_{t \in \mathbb{N}}$
2. drift condition: $\exists K \subset \mathbb{R}^d \times \lambda_{\min}^{-1}(\{1\})$ compact and
 $V: \mathbb{R}^d \times \lambda_{\min}^{-1}(\{1\}) \rightarrow [1, +\infty]$

$$\mathbb{E}[V(z_1, \Sigma_1)] \leq (1 - \varepsilon)V(z_0, \Sigma_0) \quad \forall (z_0, \Sigma_0) \notin K$$

3. **deduce convergence from the ergodicity**

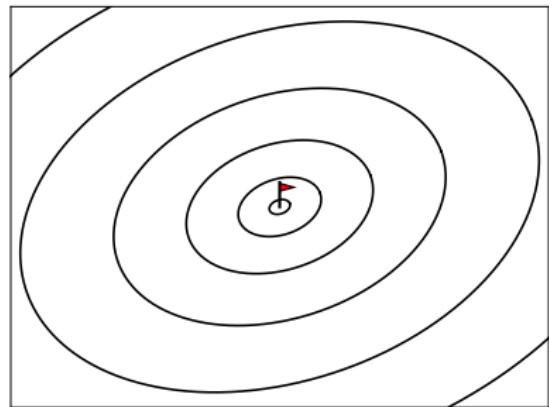
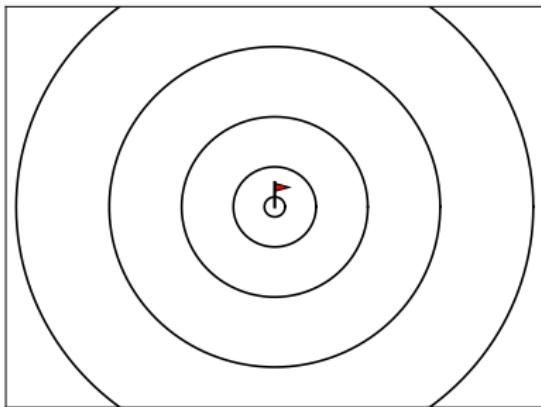
Theorem

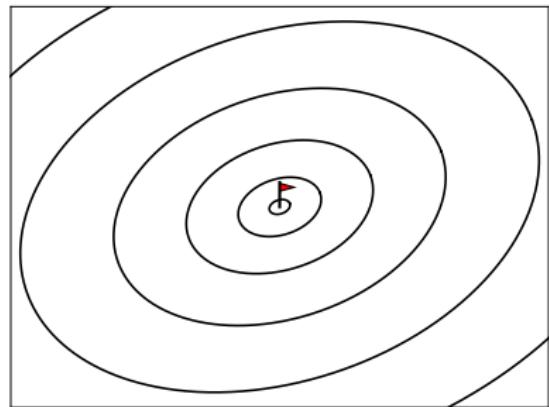
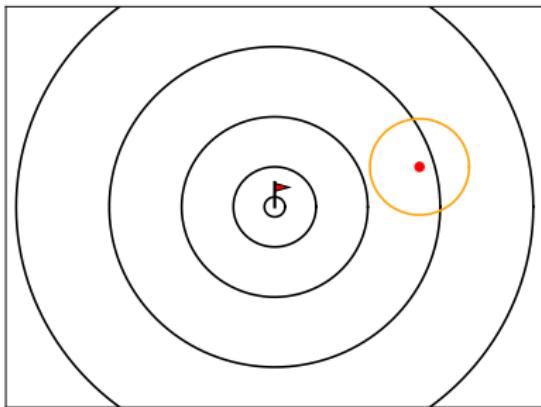
If $f = \text{circle icon}$, CMA-ES converges linearly (or geometrically).

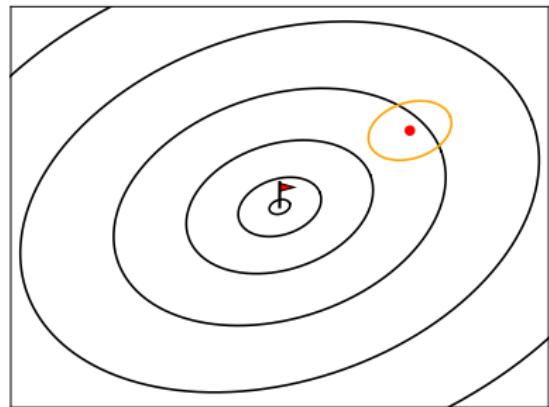
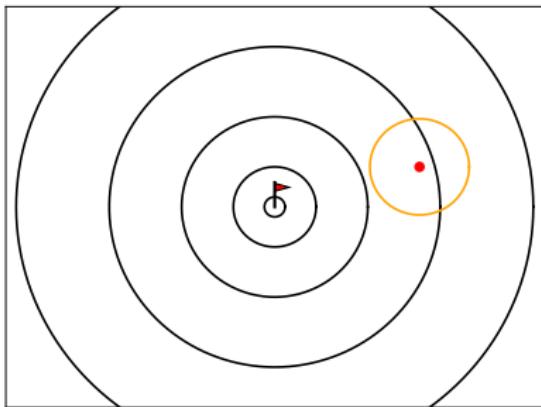
Theorem

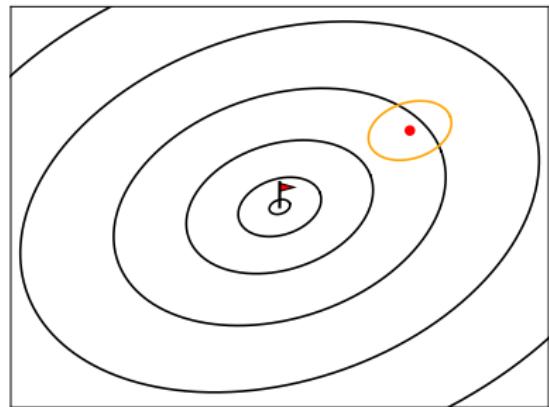
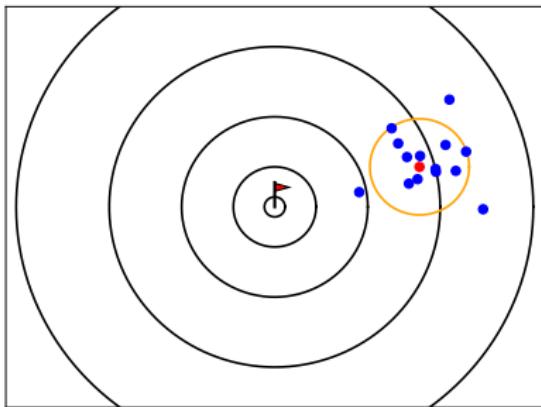
If $f = \text{circle}$, CMA-ES converges linearly (or geometrically).

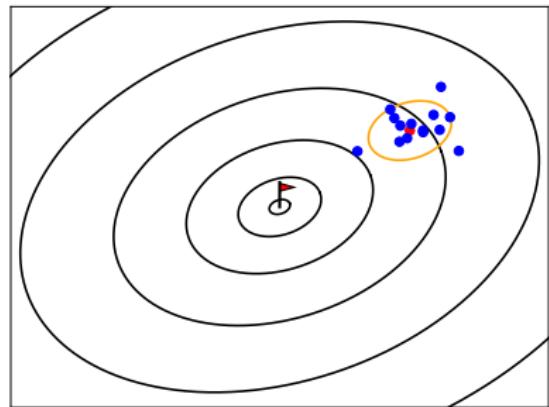
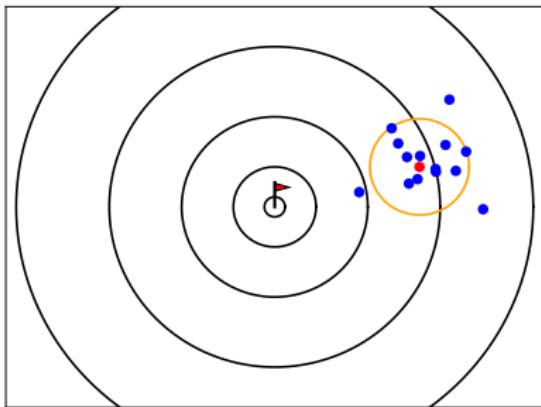
Question: how to extend to $f = \boxed{\text{ }}$?

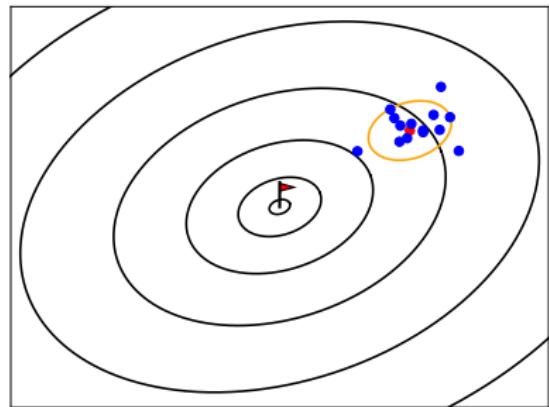
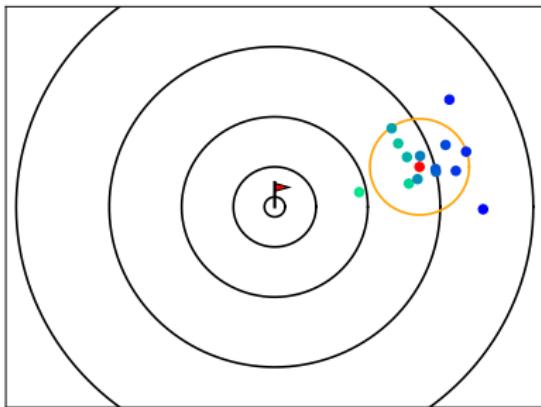


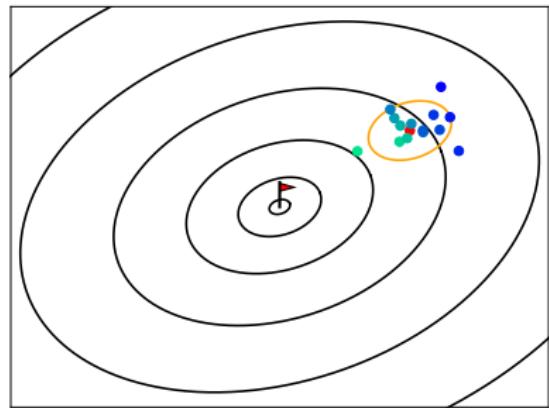
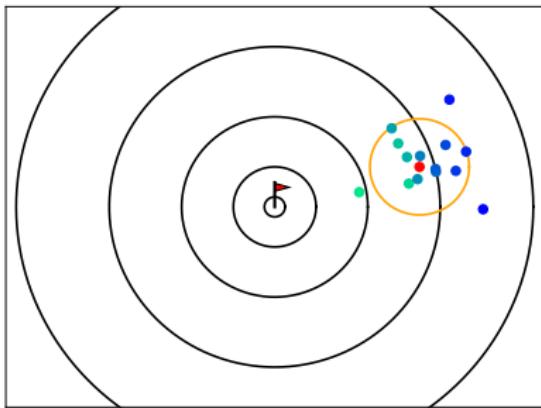


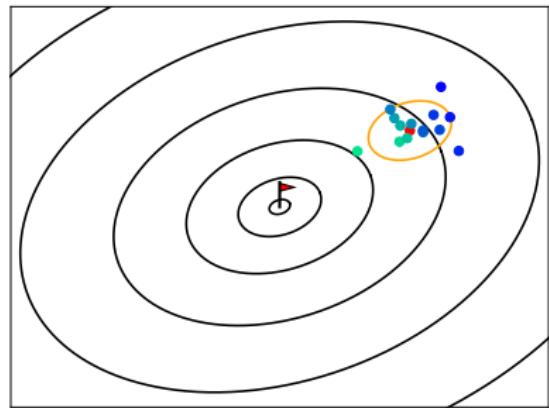
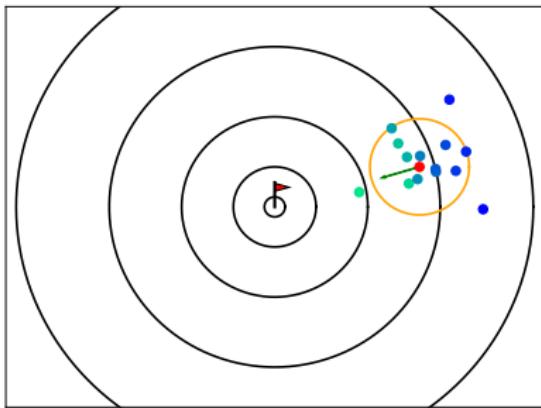


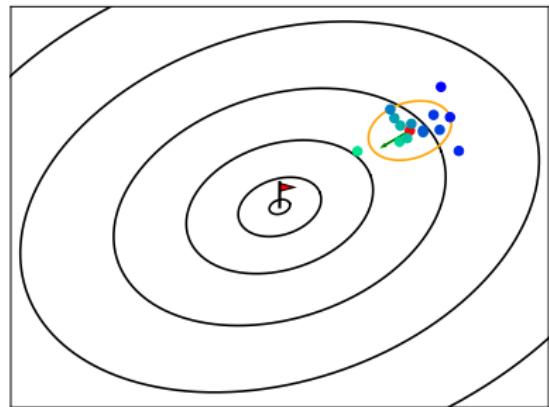
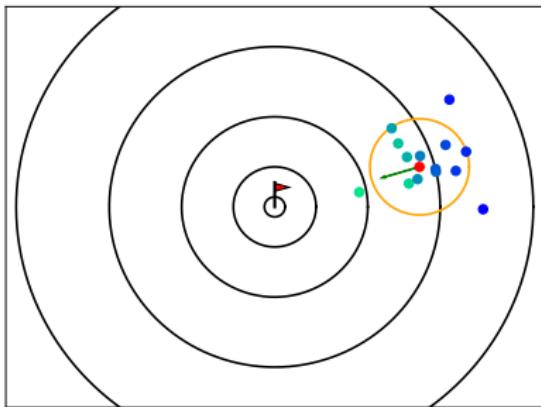


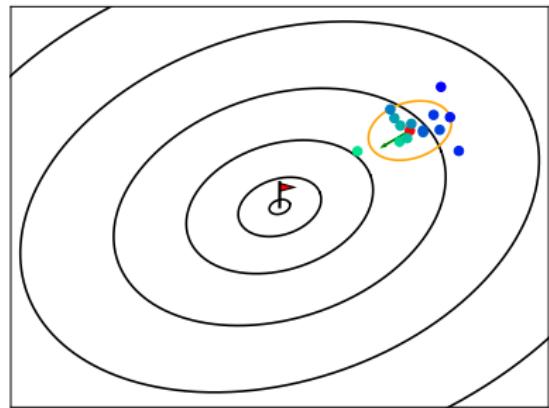
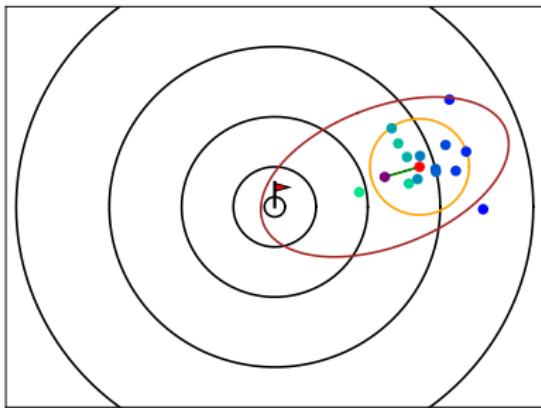


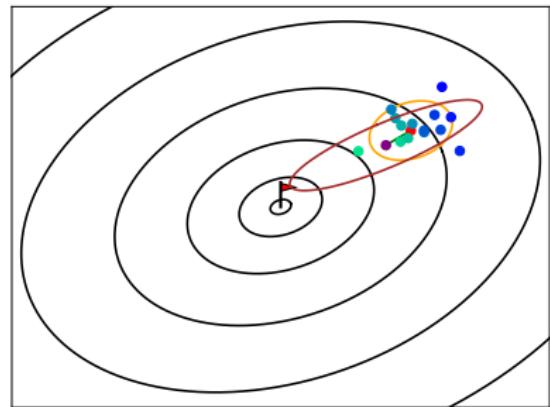
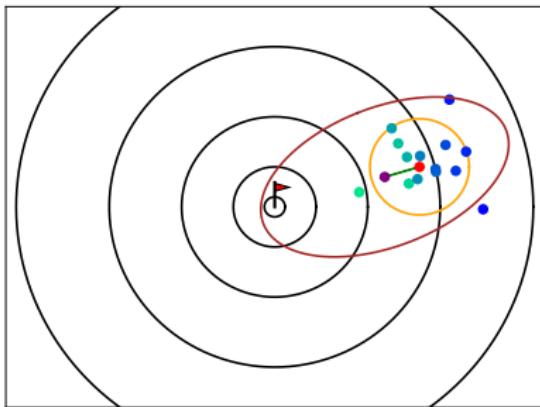












$$\begin{array}{ccc}
 (m_0, C_0) & \xrightarrow{\min f(x)} & (m_1, C_1) \\
 \downarrow \Psi & & \uparrow \Psi^{-1} \\
 (m'_0, C'_0) & \xrightarrow{\min f(Bx + b)} & (m'_1, C'_1)
 \end{array}$$

Algorithm 1 Our first ES

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

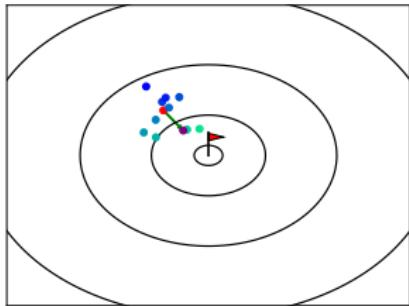
Repeat: (Given $m_t \in \mathbb{R}^d$)

1. $x_{t+1}^1, \dots, x_{t+1}^\lambda \sim \mathcal{N}(m_t, I_d)$

2. Rank population:

$$f(x_{t+1}^{1:\lambda}) \leq \dots \leq f(x_{t+1}^{\lambda:\lambda})$$

3. Update mean: $m_{t+1} = \text{Average}(x_{t+1}^{1:\lambda}, \dots, x_{t+1}^{\mu:\lambda})$



λ = population size

μ = parent number

Algorithm 1 Our first ES

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

Repeat: (Given $m_t \in \mathbb{R}^d$, $C_t \in \mathcal{S}_{++}^d$)

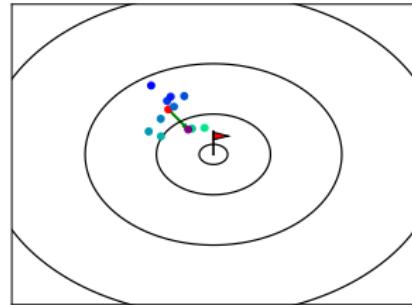
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$$f(x_{t+1}^{1:\lambda}) \leq \dots \leq f(x_{t+1}^{\lambda:\lambda})$$

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4. $C_{t+1} = C_t$



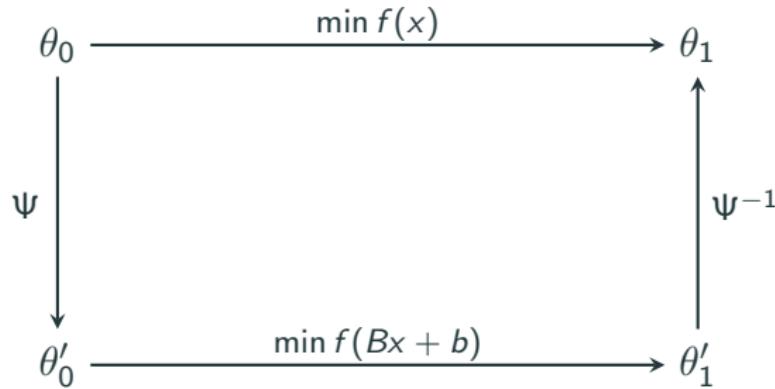
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Definition

An algorithm $\Theta = \{\theta_t\}_{t \in \mathbb{N}}$ is affine-invariant if

(i)



(ii) From θ_0 , Θ can reach a trajectory which starts at $\theta'_0 = \Psi(\theta_0)$.

Theorem

CMA-ES is affine-invariant.

Theorem

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Theorem

If $f \in \left\{ \begin{array}{c} \text{[Diagram of concentric ellipses]} \\ \text{[Diagram of rotated ellipses]} \end{array} \right\}$:

$$\lim_{t \rightarrow \infty} m_t = x^* \quad \text{geometrically}$$

Theorem

$f \in \left\{ \begin{array}{c} \text{[Diagram of a function with a single minimum]} \\ \text{[Diagram of a function with two minima]} \end{array} \right\} :$

$$\lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{C_t}{normalization} \right] \propto Hessian^{-1}(f)$$

Proof.

□

Theorem

$f \in \left\{ \begin{array}{c} \text{Diagram A} \\ \text{Diagram B} \end{array} \right\}$:

$$\lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{C_t}{normalization} \right] \propto Hessian^{-1}(f)$$

Proof.

When $f = \boxed{\text{Diagram A}}$:

□

Theorem

$f \in \left\{ \begin{array}{c} \text{[Diagram: Concentric circles centered at red dot]} \\ \text{[Diagram: Ellipse centered at red dot]} \end{array} \right\} :$

$$\lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{C_t}{\text{normalization}} \right] \propto \text{Hessian}^{-1}(f)$$

Proof.

When $f = \boxed{\text{[Diagram: Concentric circles centered at red dot]}}$:

$$R \times \boxed{\text{[Diagram: Concentric circles centered at red dot]}} = \boxed{\text{[Diagram: Concentric circles centered at red dot]}}$$

for R a rotation matrix.

□

Theorem

$f \in \left\{ \begin{array}{c} \text{Diagram A} \\ \text{Diagram B} \end{array} \right\} :$

$$\lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{C_t}{\text{normalization}} \right] \propto \text{Hessian}^{-1}(f)$$

Proof.

When $f = \text{Diagram A}$:

$$R \times \text{Diagram A} = \text{Diagram A}$$

for R a rotation matrix.

$$RC_t R^\top \text{ behaves like } C_t$$

□

Theorem

$f \in \left\{ \begin{array}{c} \text{[Diagram: Concentric circles centered at red dot]} \\ \text{[Diagram: Elliptical contours centered at red dot]} \end{array} \right\}$:

$$\lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{C_t}{\text{normalization}} \right] \propto \text{Hessian}^{-1}(f)$$

Proof.

When $f = \text{[Diagram: Concentric circles centered at red dot]}$:

$$R \times \text{[Diagram: Concentric circles centered at red dot]} = \text{[Diagram: Concentric circles centered at red dot]}$$

for R a rotation matrix.

$$\lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{RC_tR^\top}{\text{normalization}} \right] = \lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{C_t}{\text{normalization}} \right]$$

□

Theorem

$f \in \left\{ \begin{array}{c} \text{Diagram A} \\ \text{Diagram B} \end{array} \right\}$:

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Proof.

When $f = \text{Diagram A}$:

$$R \times \text{Diagram A} = \text{Diagram A}$$

for R a rotation matrix.

$$R \times \lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{C_t}{\text{normalization}} \right] = \lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{C_t}{\text{normalization}} \right] \times R$$

□

Theorem

$f \in \left\{ \begin{array}{c} \text{Diagram A} \\ \text{Diagram B} \end{array} \right\}$:

$$\lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{C_t}{\text{normalization}} \right] \propto \text{Hessian}^{-1}(f)$$

Proof.

When $f = \text{Diagram A}$:

$$R \times \text{Diagram A} = \text{Diagram A}$$

for R a rotation matrix.

$$\lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{C_t}{\text{normalization}} \right] \propto I_d$$

□

Theorem

$f \in \left\{ \begin{array}{c} \text{Diagram A} \\ \text{Diagram B} \end{array} \right\}$:

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Proof.

When $f = \text{Diagram A}$:

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When $f = \text{Diagram B}$:

□

Theorem

$f \in \left\{ \begin{array}{c} \text{Diagram A} \\ \text{Diagram B} \end{array} \right\}$:

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Proof.

When $f = \text{Diagram A}$:

$$\lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{C_t}{\text{normalization}} \right] \propto I_d$$

When $f = \text{Diagram B}$:

C_t behaves like $\text{Hessian}^{-1/2} C_t(\text{Diagram A}) \text{Hessian}^{-1/2}$

□

Theorem

$f \in \left\{ \begin{array}{c} \text{Diagram A} \\ \text{Diagram B} \end{array} \right\}$:

$$\lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{C_t}{\text{normalization}} \right] \propto \text{Hessian}^{-1}(f)$$

Proof.

When $f = \text{Diagram A}$:

$$\lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{C_t}{\text{normalization}} \right] \propto I_d$$

When $f = \text{Diagram B}$:

$$\lim_{t \rightarrow +\infty} \mathbb{E} \left[\frac{C_t}{\text{normalization}} \right] \propto \text{Hessian}^{-1}(f)$$

□

$$\sigma_{t+1} = \sigma_t \times \text{increasing function}(\|m_{t+1} - m_t\|)$$

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Goal: remember previous iterations to update σ .

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Goal: remember previous iterations to update σ .

$$\text{path}_{t+1}^\sigma = \text{linear function}(\text{path}_t^\sigma, m_{t+1} - m_t)$$

New update:

$$\boxed{\sigma_{t+1} = \sigma_t \times \text{increasing function}(\|\text{path}_{t+1}^\sigma\|)}$$

$\text{path}_{t+1}^c = \text{linear function}(\text{path}_t^c, m_{t+1} - m_t)$

$$\text{path}_{t+1}^c = \text{linear function}(\text{path}_t^c, m_{t+1} - m_t)$$

$$C_{t+1} = \text{Linear combination} \left(C_t, \text{Average}[x_{t+1}^{i:\lambda} - m_t], \overleftarrow{\text{path}}_{t+1}^c \right)$$

Algorithm 5 CMA-ES

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

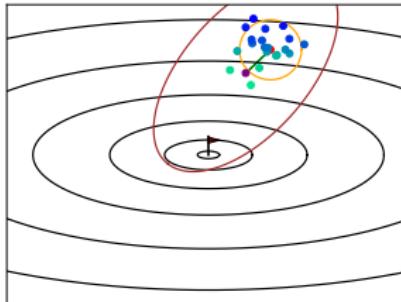
Repeat ($m_t \in \mathbb{R}^d$, $\sigma_t > 0$, $C_t \succ 0$)

1. $x_{t+1}^1, \dots, x_{t+1}^\lambda \sim \mathcal{N}(m_t, \sigma_t^2 C_t)$
2. sort $f(x_{t+1}^i)$:
 $f(x_{t+1}^{1:\lambda}) \leq \dots \leq f(x_{t+1}^{\lambda:\lambda})$
3. $m_{t+1} = \text{Average}(x_{t+1}^{1:\lambda}, \dots, x_{t+1}^{\mu:\lambda})$
- 4.

$$\sigma_{t+1} = \sigma_t \times \text{increasing function}(\|m_{t+1} - m_t\|)$$

- 5.

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λ = population size

μ = parent number

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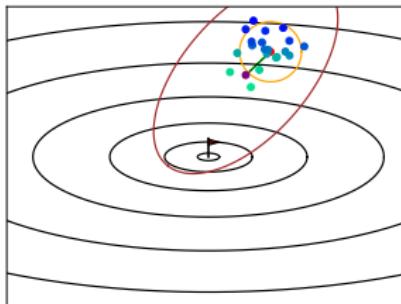
3. $m_{t+1} = \text{Average}(x_{t+1}^{1:\lambda}, \dots, x_{t+1}^{\mu:\lambda})$

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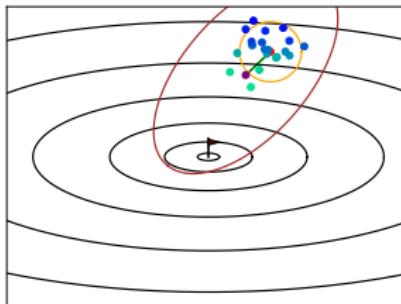
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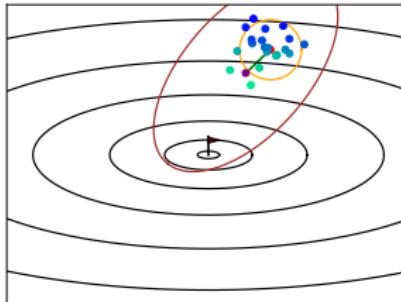
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Algorithm 5 CMA-ES

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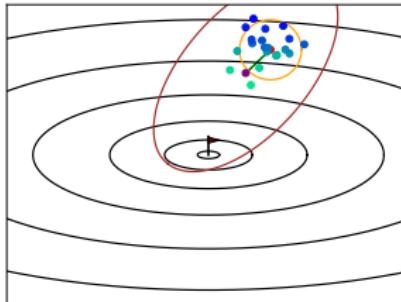
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μ = parent number

$$z_t = \frac{m_t - x^*}{\sigma_t \sqrt{\lambda_{\min}(C_t)}}$$

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$$\text{normalized path}_t^{c,\sigma} = \frac{\text{path}_t^{c,\sigma}}{\text{normalization}}$$

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$$\Sigma_t = \frac{C_t}{\lambda_{\min}(C_t)}$$

normalized path $_t^{c,\sigma} = \frac{\text{path}_t^{c,\sigma}}{\text{normalization}}$

Proposition

If $f \in \left\{ \begin{array}{c} \text{[contour plot]} \\ \text{[square with red dot]} \\ \text{[wavy lines]} \\ \text{[fractal]} \end{array} \right\}$, then $\{(z_t, \Sigma_t, n. \text{ path}_t^c, n. \text{ path}_t^\sigma)\}_{t \in \mathbb{N}}$
is a Markov chain.

When X is infinite:

Theorem

If $\{\theta_t\}_{t \in \mathbb{N}}$ is an irreducible, aperiodic Markov chain, then it is ergodic if

$$\mathbb{E}[V(\theta_{t+1}) \mid \theta_t] \leq (1 - \varepsilon)V(\theta_t) \quad \text{if } \theta_t \notin \text{compact set}$$

for some $V : X \rightarrow [1, +\infty]$.

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Theorem

If $\{\theta_t\}_{t \in \mathbb{N}}$ is an irreducible, aperiodic Markov chain, then it is ergodic if

$$\mathbb{E}[V(\theta_{t+n(\theta_t)}) \mid \theta_t] \leq (1 - \varepsilon)^{n(\theta_t)} V(\theta_t) \quad \text{if } \theta_t \notin \text{compact set}$$

for some $V : X \rightarrow [1, +\infty]$.

$$V(z, \Sigma, \text{n. path}^c, \text{n. path}^\sigma) = \text{linear combination}(\|z\|^2, \|\Sigma\|, \|\text{n. paths}\|^2)$$

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Proposition

If $f = \boxed{\text{?}}$, then:

$$\mathbb{E}[V(\text{iteration}_{t+k}) \mid \text{iteration}_t] \leq (1 - \varepsilon) \times V(\text{iteration}_t)$$

when $\|z_t\| \gg 1$ or $\|\Sigma_t\| \gg 1$ or $\|\text{n. path}_t^c\| \gg 1$ or $\|\text{n. path}_t^\sigma\| \gg 1$.

Theorem

If $f \in \left\{ \begin{array}{c} \text{Diagram A} \\ \text{Diagram B} \end{array} \right\}$:

$$\lim_{t \rightarrow \infty} m_t = x^* \quad \text{geometrically}$$

and

$$\lim_{t \rightarrow \infty} \mathbb{E} \left[\frac{C_t}{\text{normalization}} \right] = H^{-1}$$

Thank you!