Convergence analysis of CMA-ES

ISMP 2024
Stochastic DFO 1

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Advisors: Anne Auger & Nikolaus Hansen

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Covariance Matrix Adaptation-ES (CMA-ES)

Given $\theta_t = (m_t, \sigma_t, \mathbf{C}_t) \in \mathbb{R}^d \times \mathbb{R}_{>0} \times \mathcal{S}^d_{++}$:

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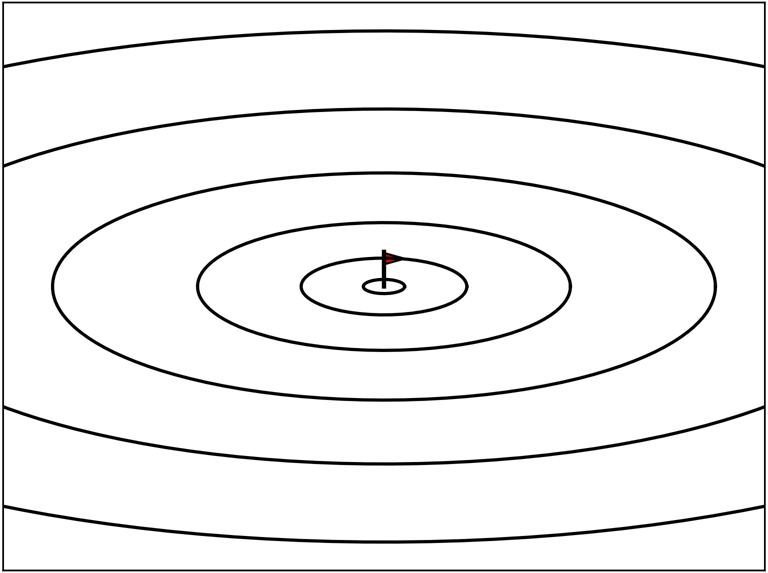

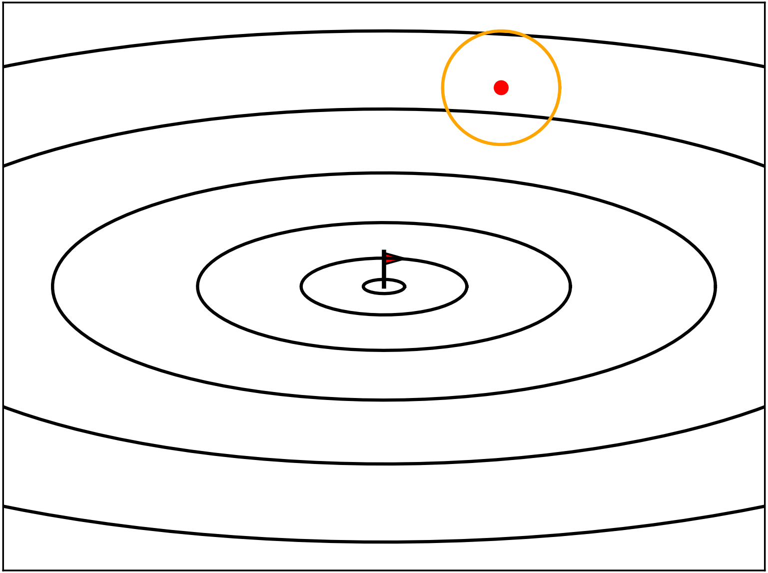

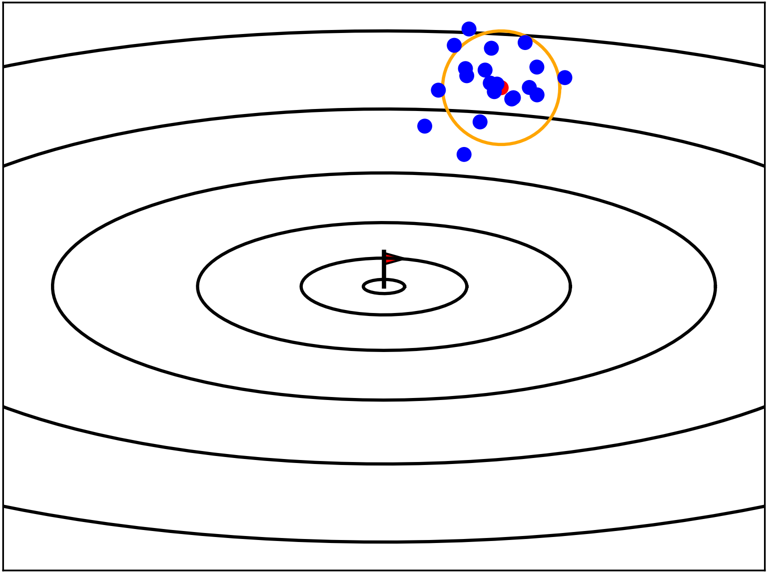

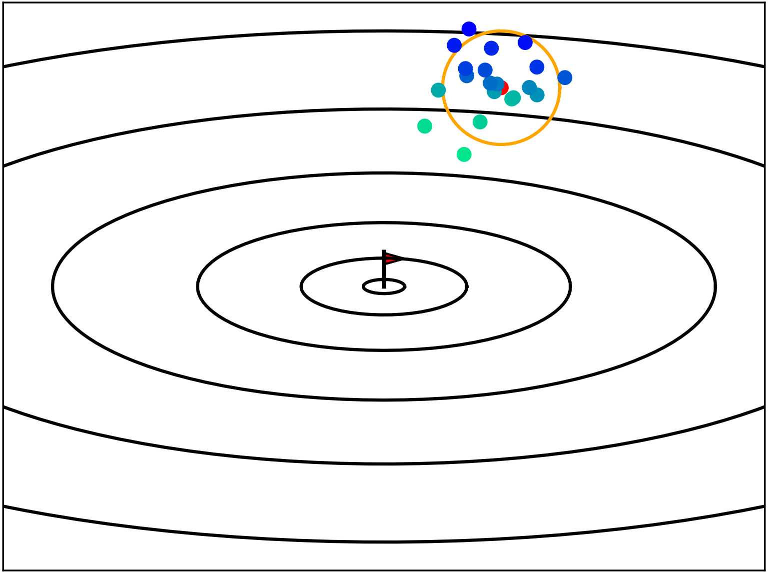

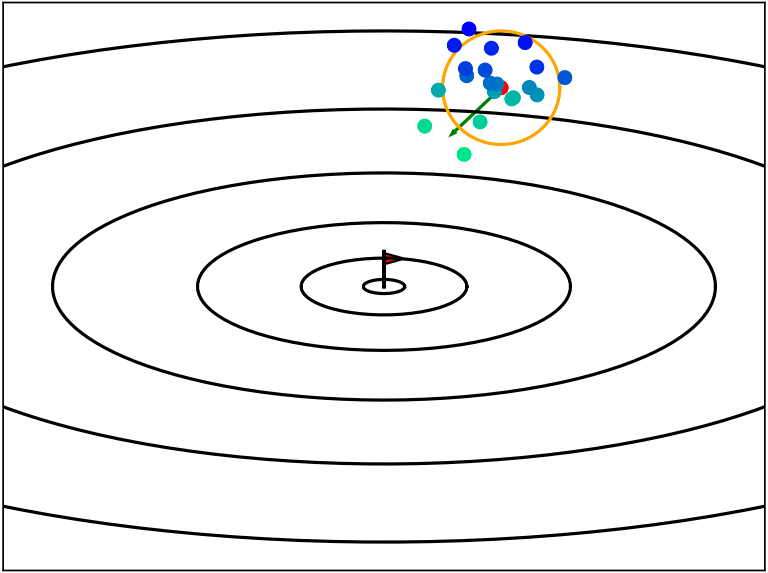

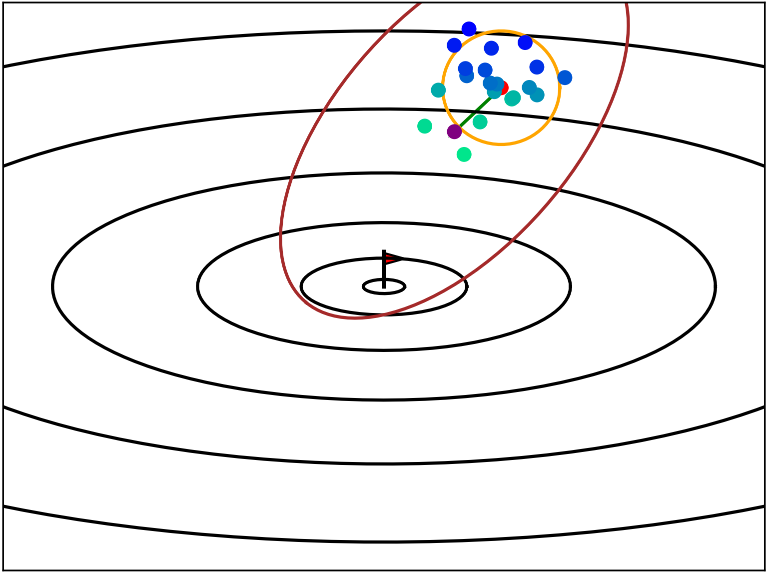

Mean update:

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

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$$= \sigma_t \times \exp\left(\frac{1}{d_\sigma}\left(\frac{\|{\sigma_t}^{-1}{\mathbf{C}_t}^{-1/2}(m_{t+1} - m_t)\|}{\|\text{weights}\|\mathbb{E}\|\mathcal{N}\|} - 1\right)\right)$$

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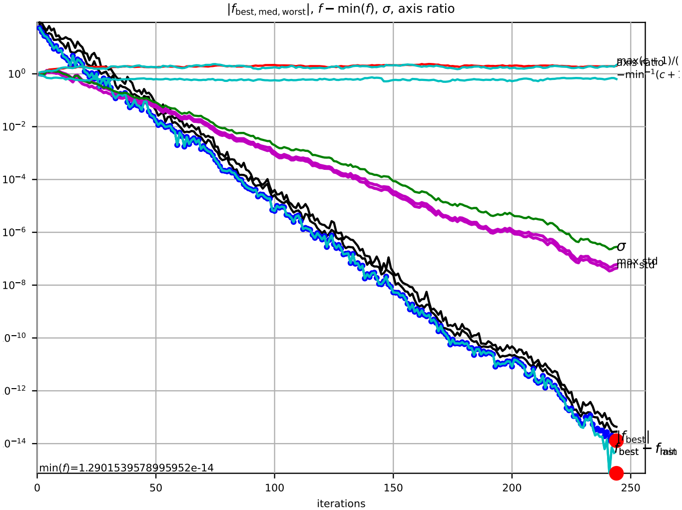
$$= (1 - c_\mu)\mathbf{C}_t + \frac{c_\mu}{\sigma_t^2} \underbrace{\sum_{i=1}^{\mu} w_i (x_{t+1}^{i:\lambda} - m_t)(x_{t+1}^{i:\lambda} - m_t)^\top}_{\text{rank-mu update}}$$

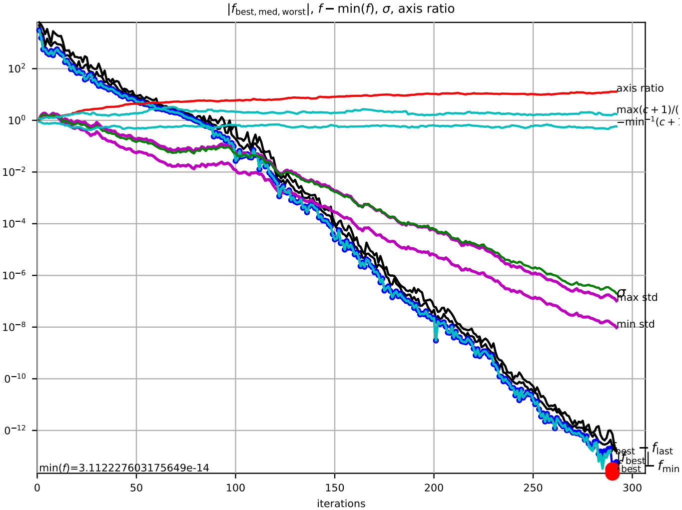
$$f(x) = \frac{1}{2} x^\top \mathbf{H} x$$

$$\mathrm{Cond}(\mathbf{H}) = 10^0$$



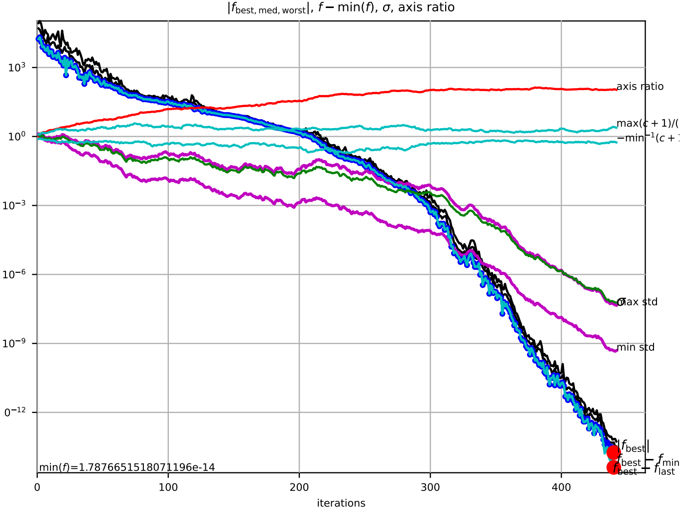
$$f(x) = \frac{1}{2} x^\top \mathbf{H} x$$

$$\mathrm{Cond}(\mathbf{H}) = 10^2$$



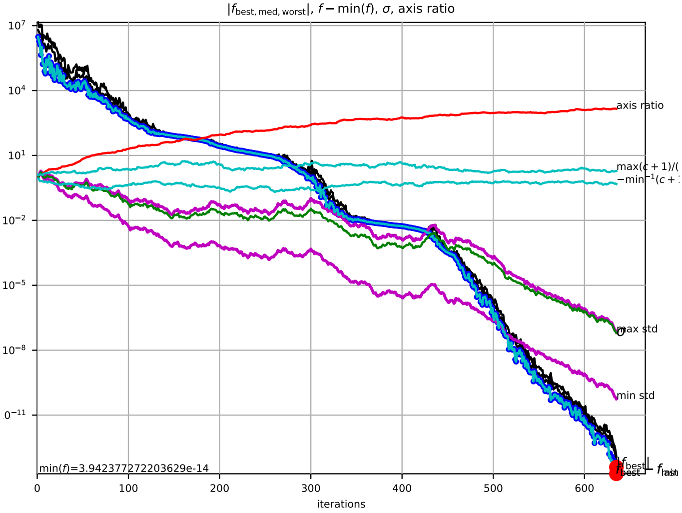
$$f(x) = \frac{1}{2} x^\top \mathbf{H} x$$

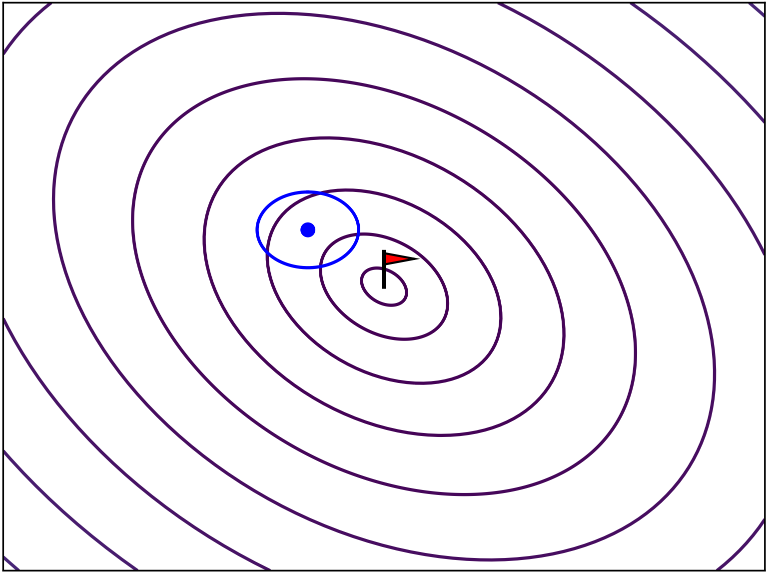
$$\mathrm{Cond}(\mathbf{H}) = 10^4$$

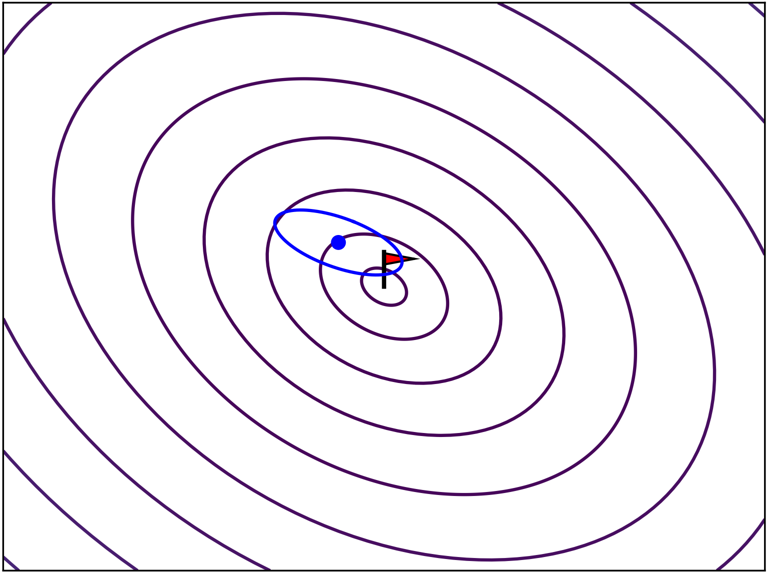


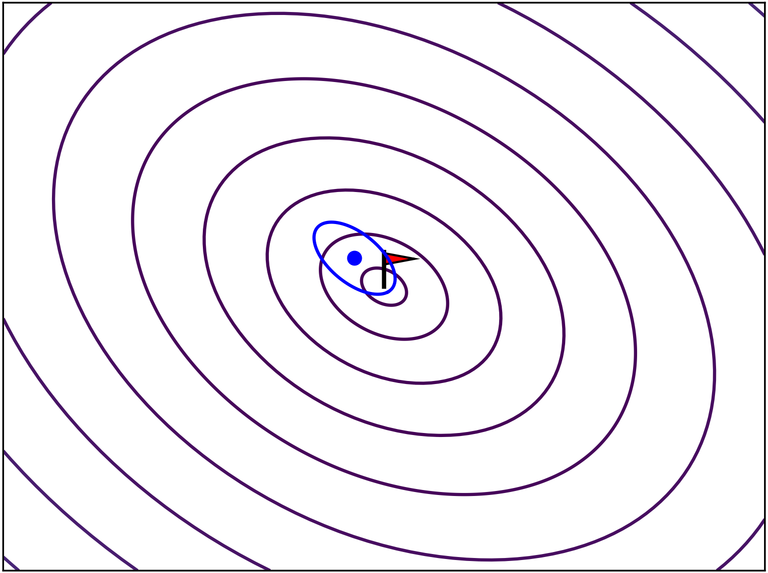
$$f(x) = \frac{1}{2} x^\top \mathbf{H} x$$

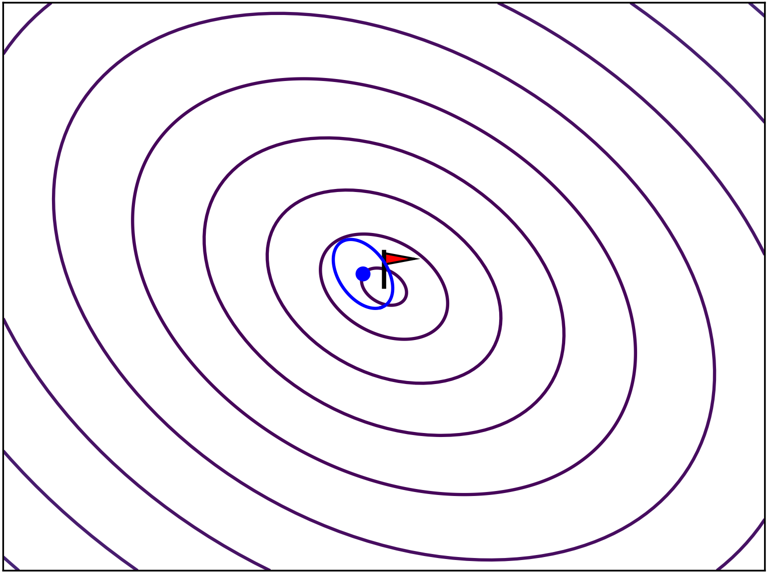
$$\mathrm{Cond}(\mathbf{H}) = 10^6$$

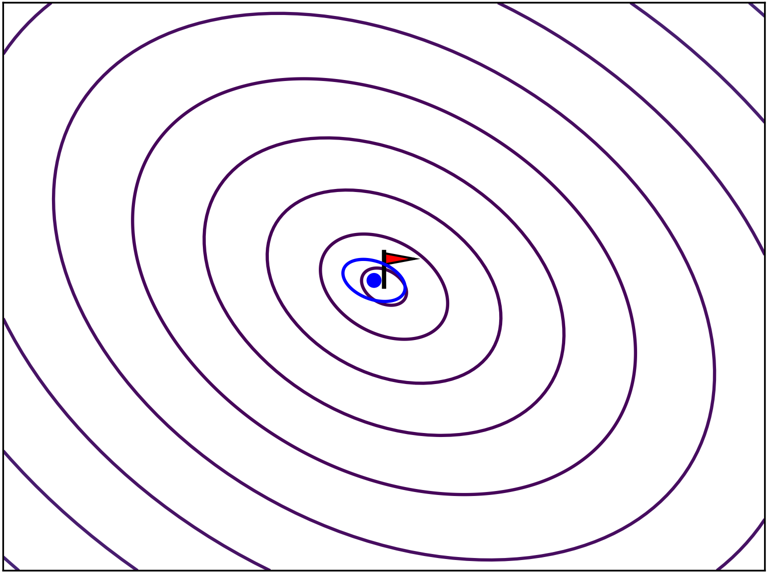


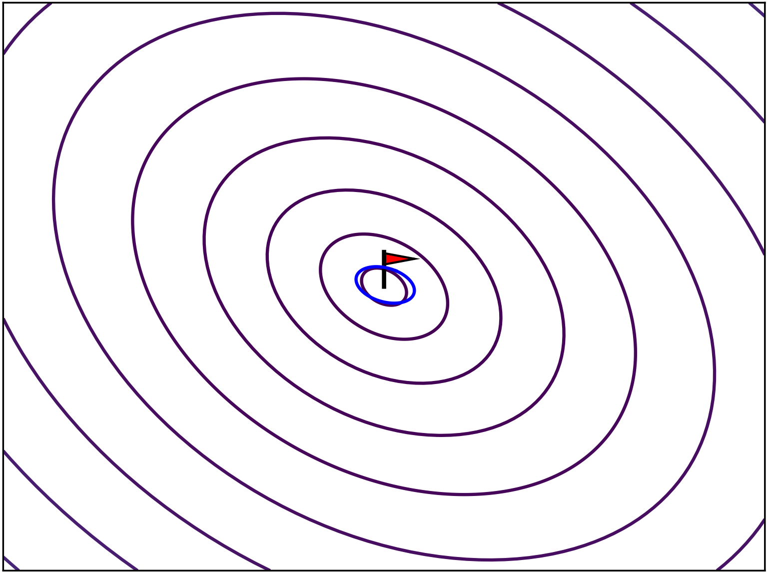


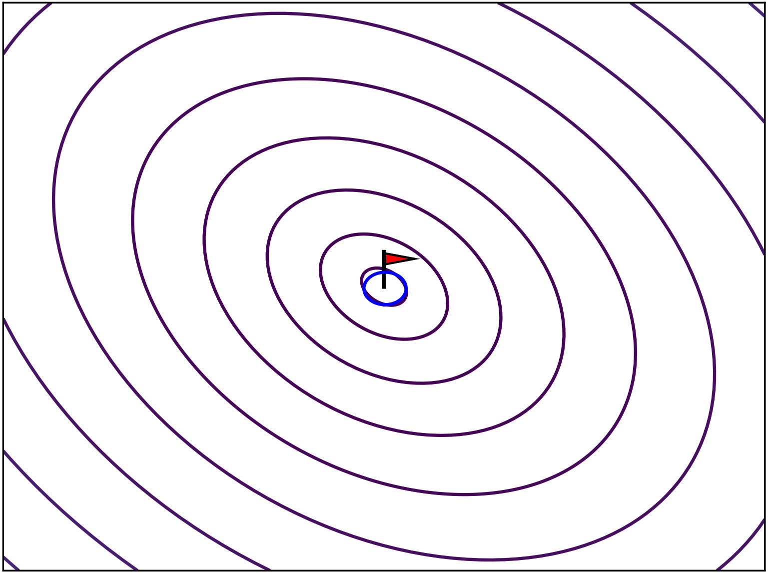


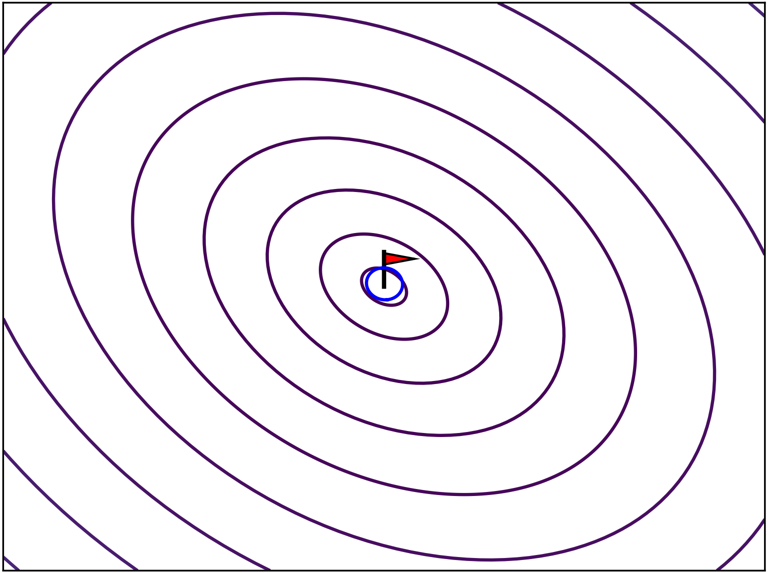


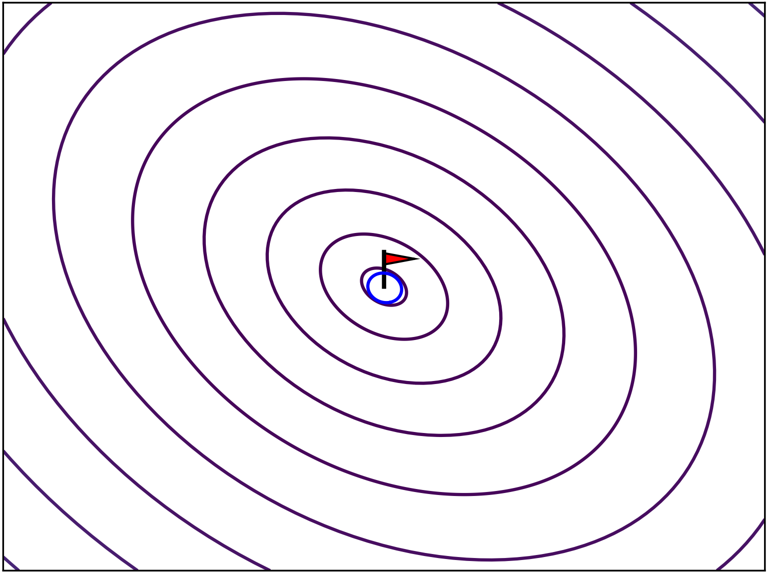


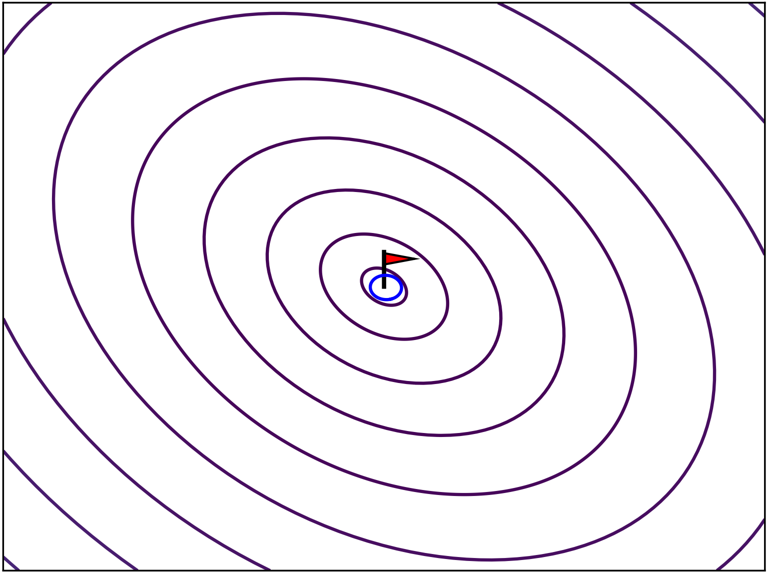


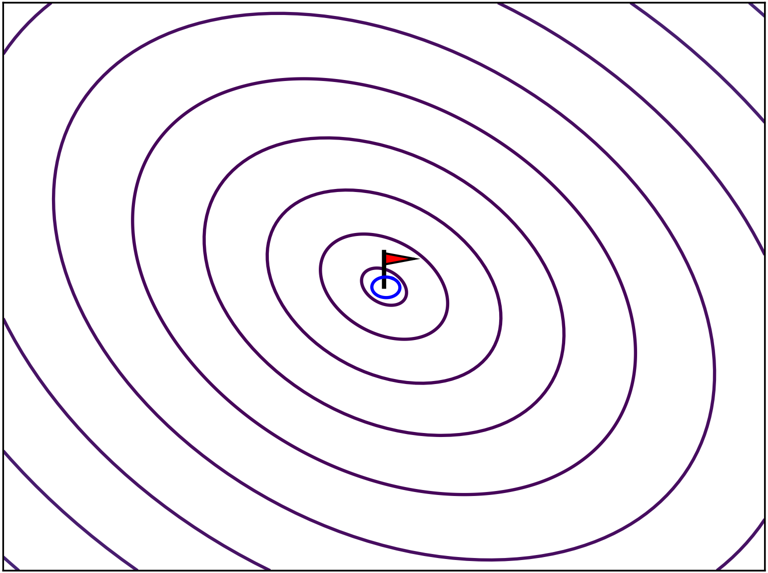


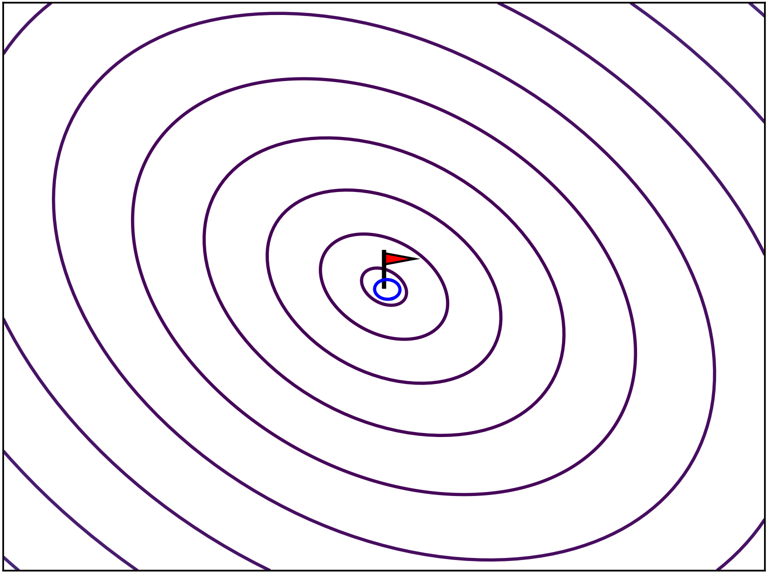


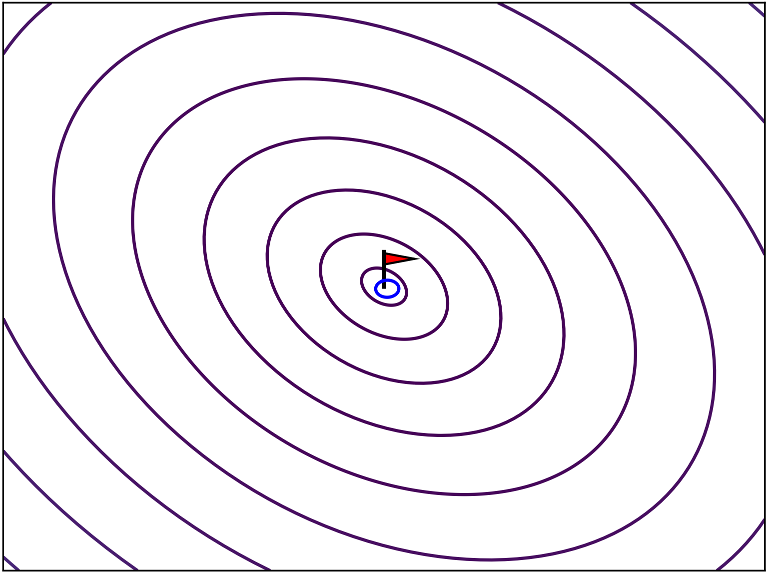


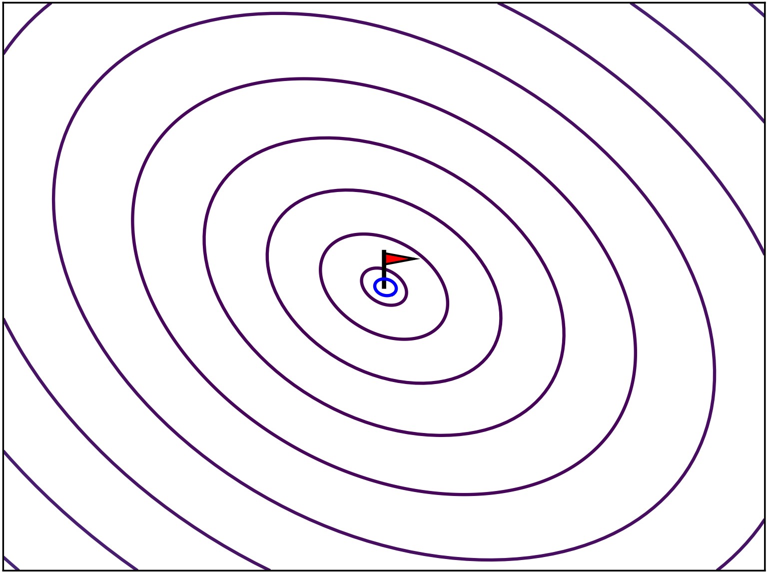


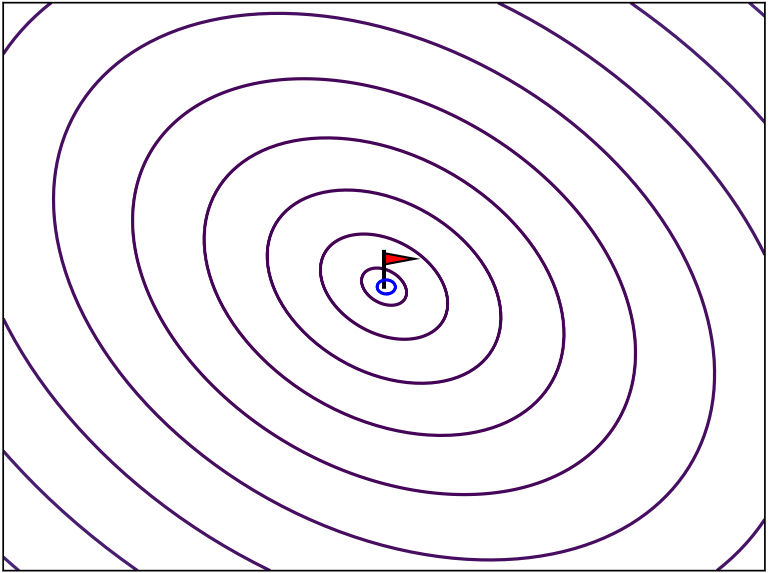


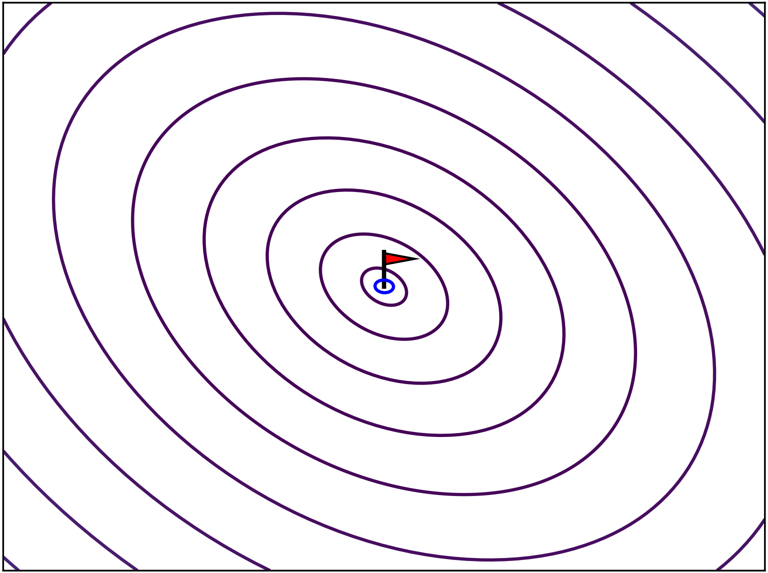


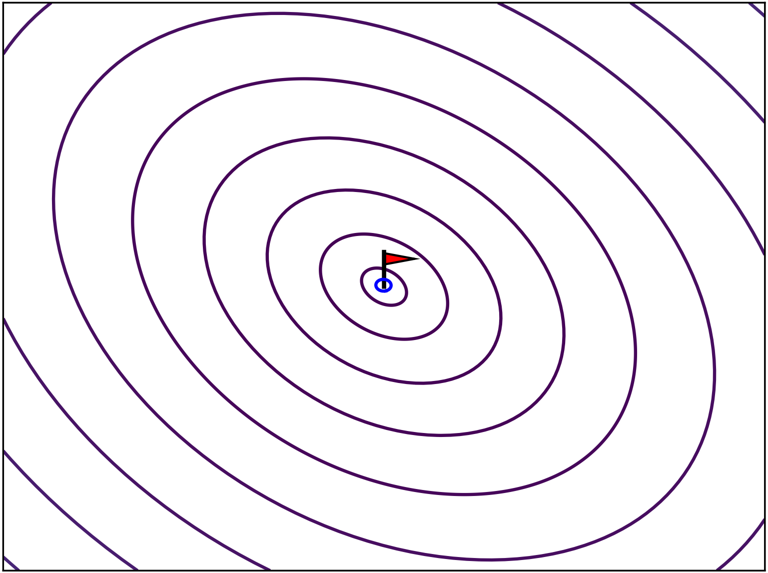


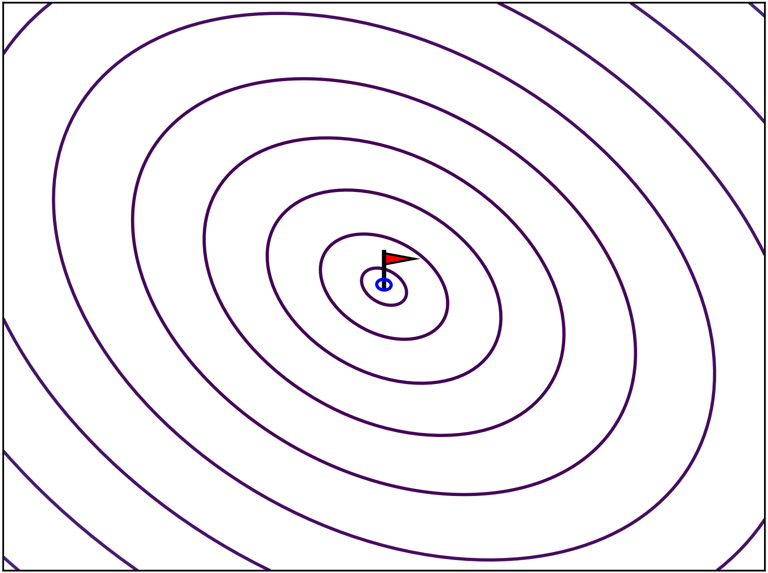












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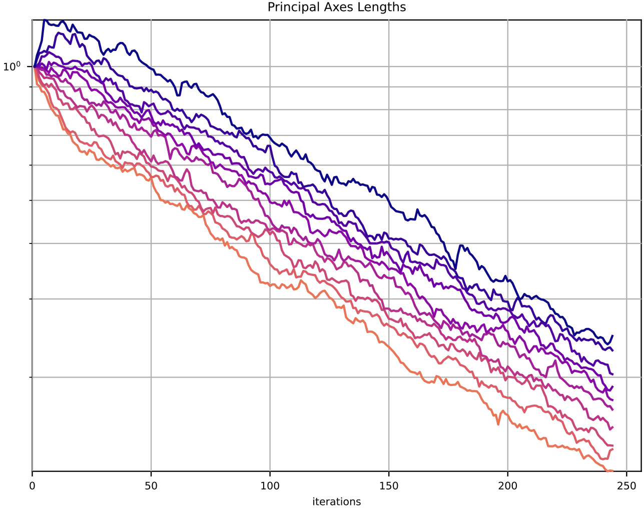

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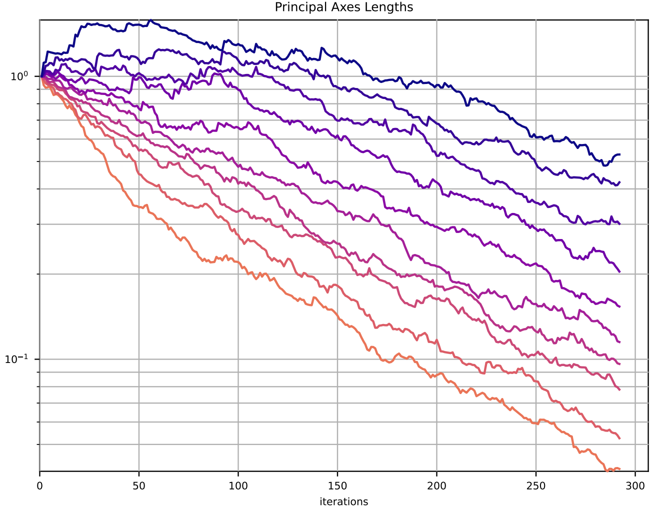

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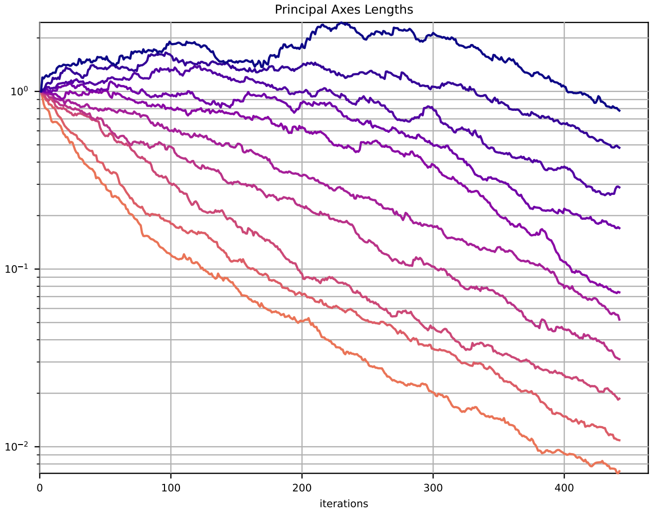

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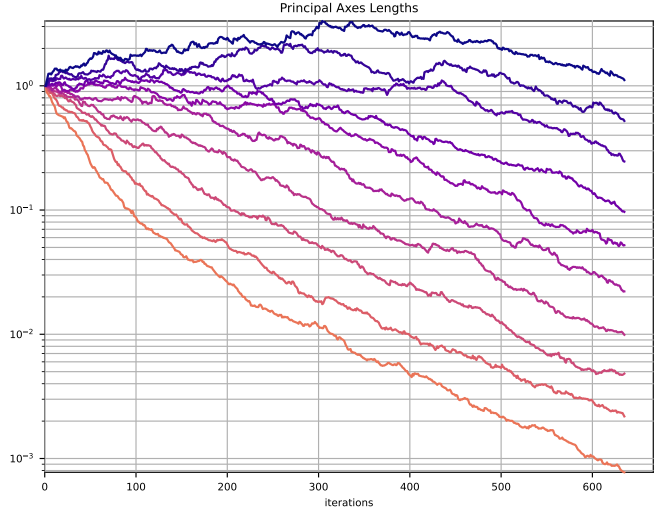

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$$\lim_{t\to\infty} \mathbb{E}\left[\frac{\mathbf{C}_t}{\text{normalization}}\right] \propto \mathbf{H}^{-1}$$

Markov chains and transition kernels

$P\colon \mathsf{X} \times \mathcal{B}(\mathsf{X}) \to \mathbb{R}$ is a **transition kernel** when

$$\forall x \in \mathsf{X}, \quad P(x, \cdot) \text{ is a probability measure.}$$

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

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

Ergodic Markov chain

If $\theta_0 \sim \nu_0$

After k steps:

$$\theta_k \sim \nu_k = \nu_0 P^k = \int \nu_0(\mathrm{d}x) P^k(x, \cdot)$$

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If

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

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

Limit theorems

If $\{\theta_t\}_{t\in\mathbb{N}}$ is ergodic with limit law π:

$$\lim_{t\to\infty} \mathbb{E}[f(\theta_t)] = \lim_{T\to\infty} \frac{1}{T}\sum_{t=0}^{T-1} f(\theta_t) = \mathbb{E}_{\theta\sim\pi}[f(\theta)]$$

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This approach was successful for stepsize adaptive-ES

Definition of a normalized Markov chain for CMA-ES

In order to obtain a stationary Markov chain:

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

$$\mathbf{\Sigma}_t = \frac{\mathbf{C}_t}{\lambda_{\min}(\mathbf{C}_t)}$$

Proposition

If $f \in \Big\{$ , , ,  $\Big\}$,[1] *then* $\{(z_t, \mathbf{\Sigma}_t)\}_{t\in\mathbb{N}}$ *is a Markov chain.*

[1] scaling-invariant functions

If $\{(z_t, \boldsymbol{\Sigma}_t)\}_{t \in \mathbb{N}}$ is ergodic:

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

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$$\|m_T - x^*\| \underset{T\to\infty}{\sim} e^{-T\mathbb{E}_\pi\left[\log\frac{\sigma_1\lambda_{\min}(\mathbf{C}_1)^{1/2}}{\sigma_0\lambda_{\min}(\mathbf{C}_0)^{1/2}}\right]}\|m_0 - x^*\|$$

$$\log \frac{\sigma_1}{\sigma_0} \propto \frac{\| \sum w_i z_1^{i:\lambda} \|}{\|\text{weights}\| \mathbb{E} \|\mathcal{N}\|} - 1$$

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We are able to prove

$$\mathbb{E}_\pi \left[\frac{\| \sum w_i z^{i:\lambda} \|^2}{\|\text{weights}\|^2 \mathbb{E} \|\mathcal{N}\|^2} - 1 \right] > 0$$

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(and under which conditions?)

How to prove that $\{\phi_t\}_{t\in\mathbb{N}}$ is ergodic

1. Irreducibility and aperiodicity of $\{\phi_t\}$
2. Drift condition:

$$\mathbb{E}[V(\phi_1)] \leqslant (1-\varepsilon)V(\phi_0) \qquad \forall \phi_0 \notin \mathsf{K}$$

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Theorem
If 1. and 2. hold for a small set K*, then* $\{\phi_t\}$ *is ergodic (*V*-geometrically ergodic).*

1. Irreducibility and aperiodicity

$\{\phi_t\}_{t\in\mathbb{N}}$ is irreducible when

$$\forall \phi_{\text{start}}, \phi_{\text{end}} \in \Phi, \underbrace{\exists k > 0,\ \mathbb{P}[\phi_k = \phi_{\text{end}} \mid \phi_0 = \phi_{\text{start}}] > 0}_{\phi_{\text{start}} \rightsquigarrow \phi_{\text{end}}}$$

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$\{\phi_t\}_{t\in\mathbb{N}}$ is irreducible when

$$\forall \phi_{\text{start}} \in \Phi, \forall \Phi_{\text{end}} \subset \Phi,\ \text{Volume}(\Phi_{\text{end}}) > 0 \Rightarrow \phi_{\text{start}} \rightsquigarrow \Phi_{\text{end}}$$

1. Irreducibility and aperiodicity

Theorem*
The Markov chain

$$\phi_{t+1} = F(\phi_t, U_{t+1})$$

is irreducible and aperiodic when

(i) *there exists a* **steadily attracting state** ϕ^**;*

(ii) *there exists a path* $U_1^*, \ldots, U_k^*$ *at which* $F^k(\phi^*, \cdot)$ *is* **submersive**.

Assumptions: F is loc. Lipschitz and $U_{t+1} \sim p_{\phi_t}$ where $(\phi, u) \mapsto p_\phi(u)$ is lsc

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For us:

$$(z_{t+1}, \mathbf{\Sigma}_{t+1}) = F((z_t, \mathbf{\Sigma}_t), z_{t+1}^{i:\lambda})$$

Assumptions: F is loc. Lipschitz and $U_{t+1} \sim p_{\phi_t}$ where $(\phi, u) \mapsto p_\phi(u)$ is lsc

Proposition*
$(z^*, \mathbf{\Sigma}^*) = (0, (1 - c_1 - c_\mu)\mathbf{I}_d)$ *is steadily attracting and there exists* $z_1^{i:\lambda}, \ldots, z_k^{i:\lambda}$ *at which* $F^k(z^*, \mathbf{\Sigma}^*, \cdot)$ *is submersive.*

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Consequence:

$\{(z_t, \mathbf{\Sigma}_t)\}$ is irreducible and aperiodic.

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$$V(z, \boldsymbol{\Sigma}) = \alpha \|z\|^2 + \beta |||\boldsymbol{\Sigma}|||$$

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$$\mathbb{E}[|||\mathbf{\Sigma}_1|||] \leqslant (1 - \varepsilon) |||\mathbf{\Sigma}_1|||$$

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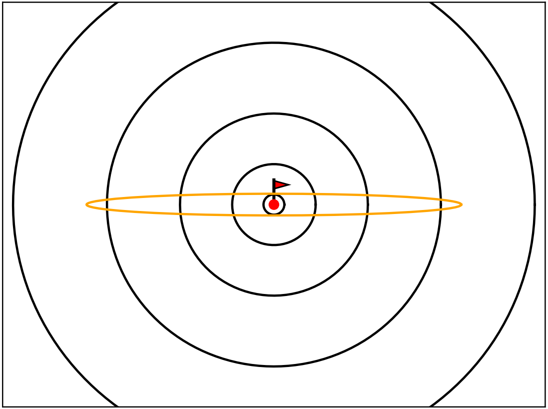
Proposition
If (a) and (b) are true:

$$\exists \mathsf{K} \text{ compact}, \; \mathbb{E}[V(z_1, \mathbf{\Sigma}_1)] \leqslant (1 - \varepsilon)V(z_0, \mathbf{\Sigma}_0) \quad \forall (z_0, \mathbf{\Sigma}_0) \notin \mathsf{K}$$

(a) When $\|\boldsymbol{\Sigma}_0\| \gg 1 + \|z_0\|^2$



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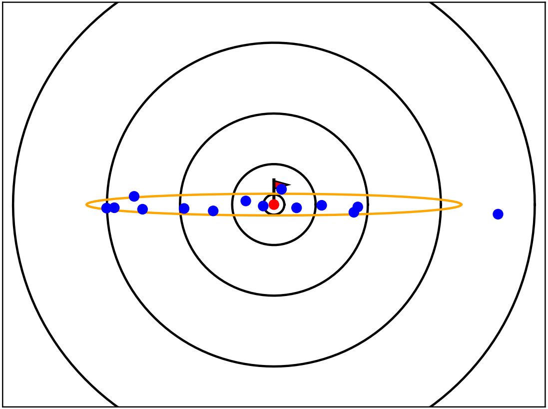

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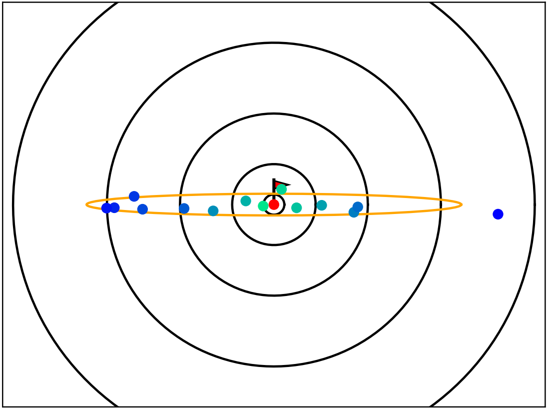

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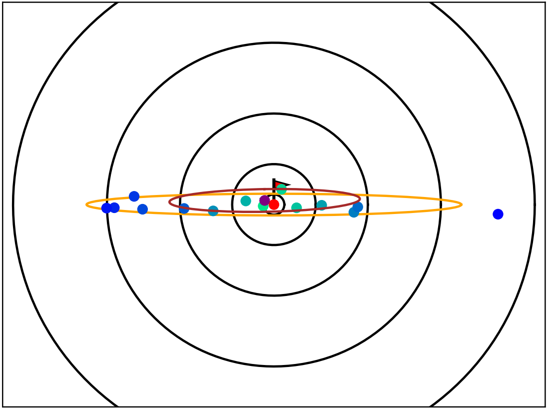

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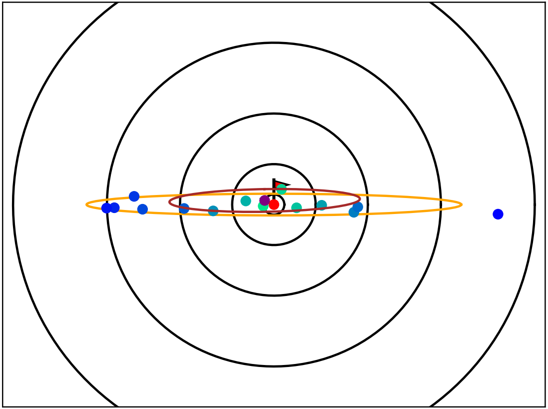

Proposition*

When $f =$  *and* $|||\boldsymbol{\Sigma}_0||| \gg 1 + \|z_0\|^2$*:*

$$\mathbb{E}[|||\boldsymbol{\Sigma}_1|||] \leqslant (1-\varepsilon)|||\boldsymbol{\Sigma}_1|||$$

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When $f =$  *and* $\|\|\|\boldsymbol{\Sigma}_0\|\|\| \not\gg \|z_0\|^2$*:*

$$\mathbb{E}[\|m_{t+1} - m_t\|] > \mathbb{E}\|\mathcal{N}\|$$

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If we choose the hyperparameters correctly:

$$\mathbb{E}[\textit{normalization}] > 1$$

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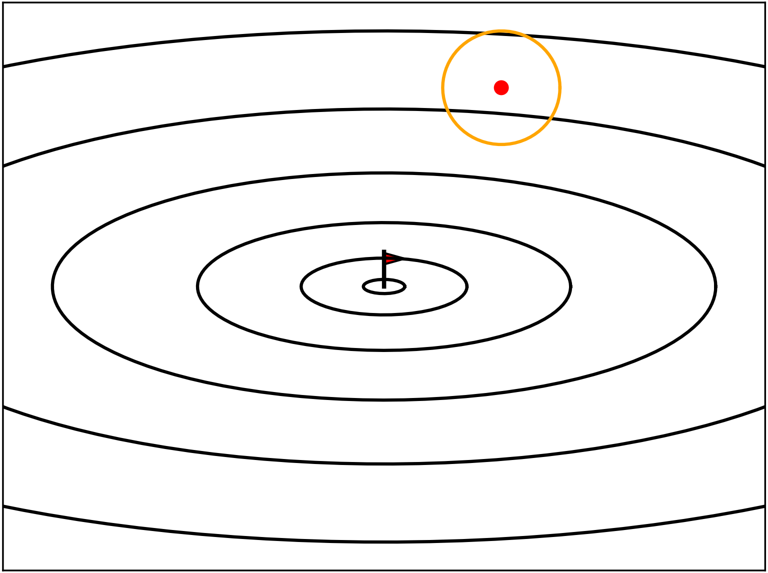

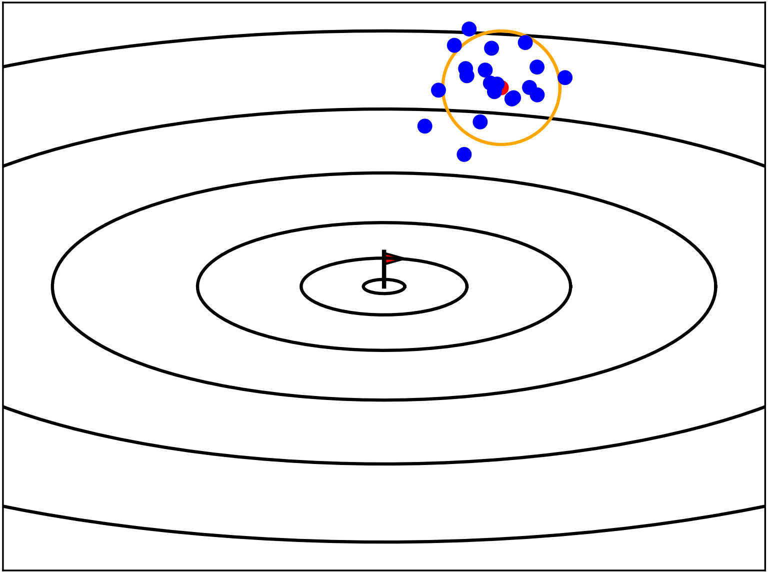

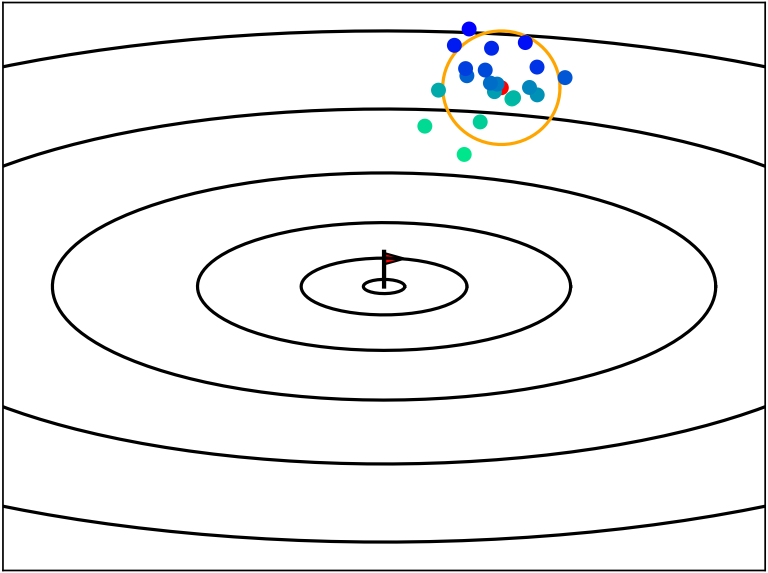

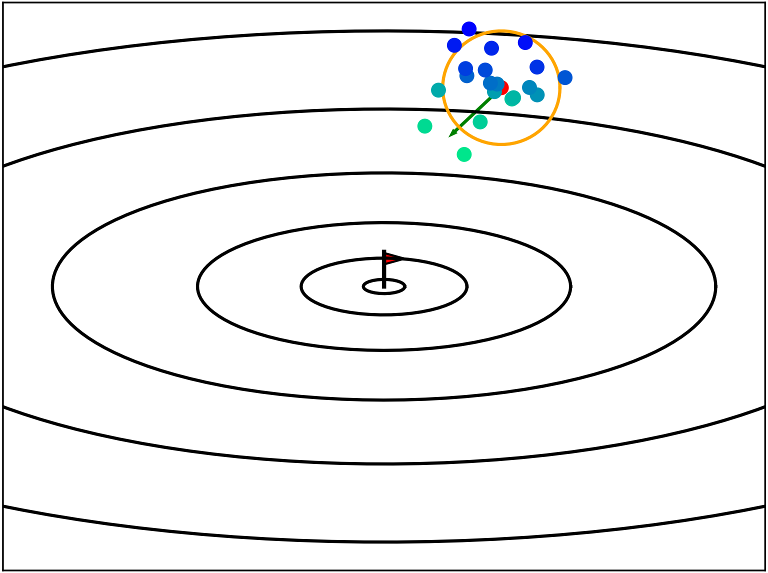

Theorem*

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Consequence:

$\{(z_t, \mathbf{\Sigma}_t)\}_t$ is ergodic

Theorem*

When $f =$ *, CMA-ES converges linearly.*

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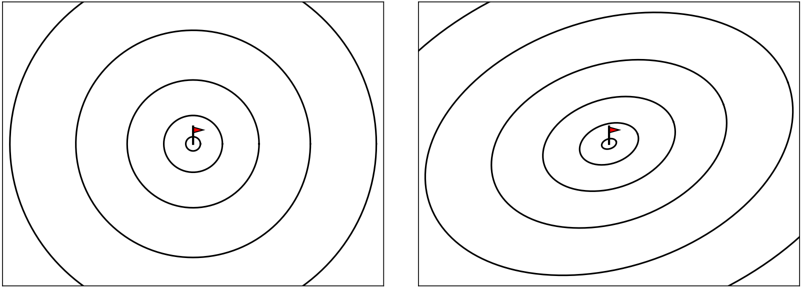
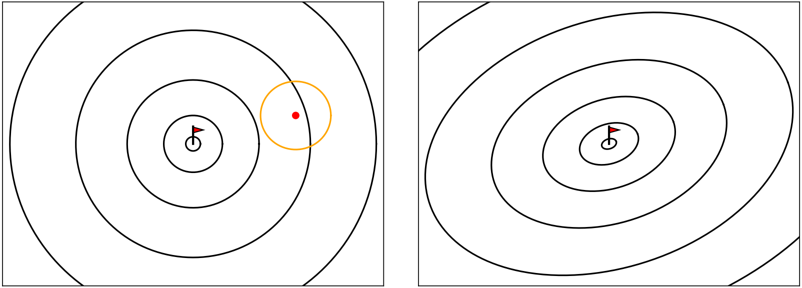
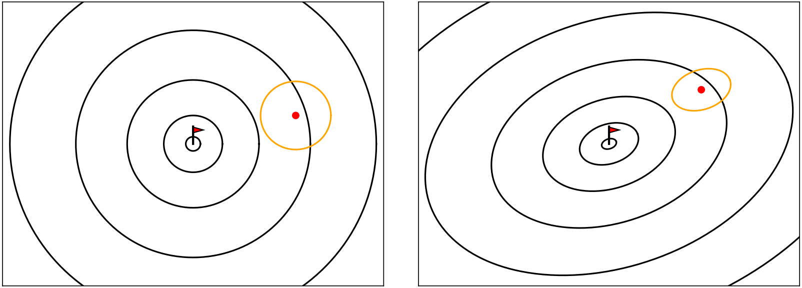
How to extend to $f =$ **?**

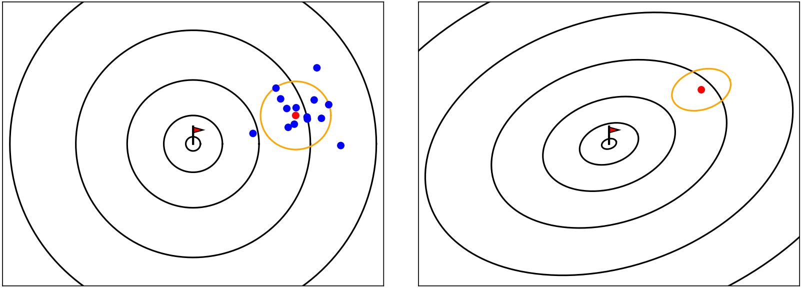
Affine-invariance

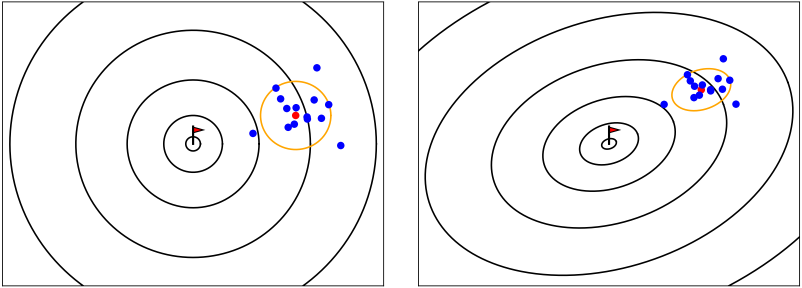
$$
\begin{array}{ccc}
(m_0, \mathbf{C}_0) & \xrightarrow{\min f(x)} & (m_1, \mathbf{C}_1) \\
\Psi \big\downarrow & & \big\uparrow \Psi^{-1} \\
(m_0', \mathbf{C}_0') & \xrightarrow{\min f(Bx+b)} & (m_1', \mathbf{C}_1')
\end{array}
$$

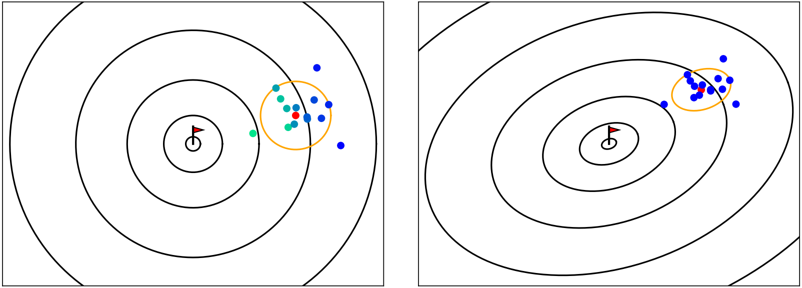


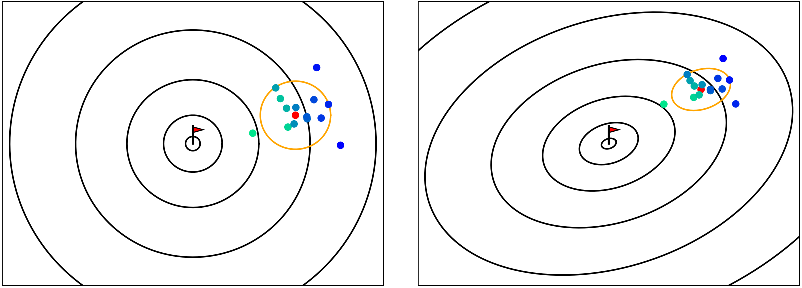


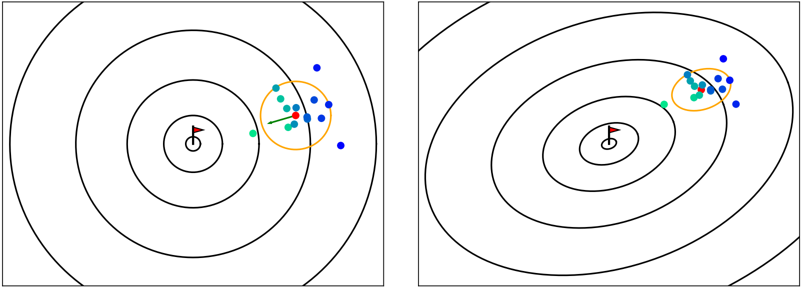


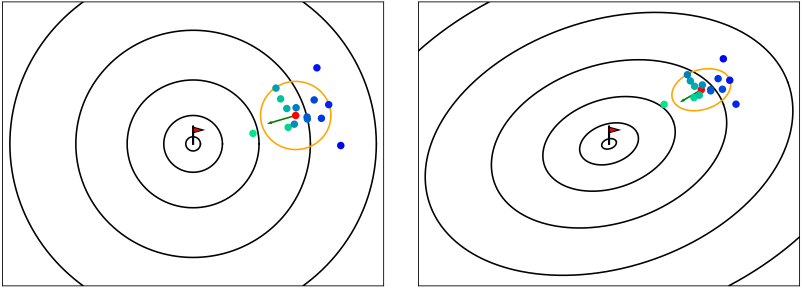


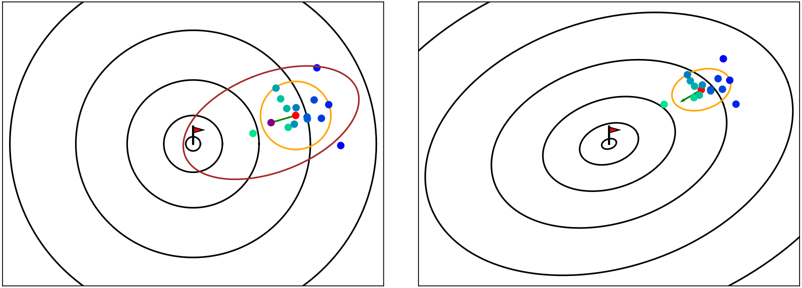


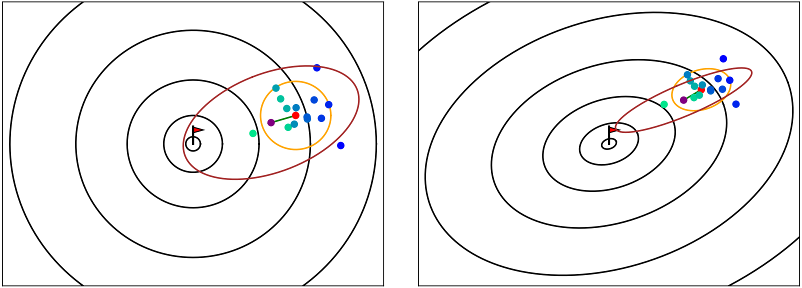












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(with the same convergence rate than *)*

Learning of the inverse Hessian

When $f =$ , we find

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Theorem*

CMA-ES learns the inverse Hessian of .

Conclusions

- CMA-ES converges linearly when $f =$ 
- The convergence rate does not depend on 
- The covariance matrix approximates the inverse Hessian

Thank you