Convergence proof of CMA-ES
Analysis of underlying Markov chains

Dagstuhl seminar

Theory of Randomized Optimization Heuristics

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Tuesday 2nd July, 2024

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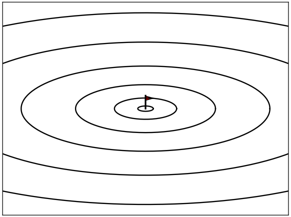

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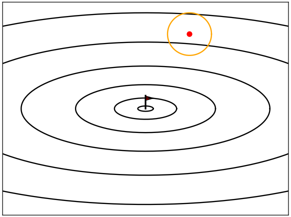

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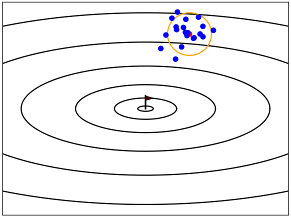

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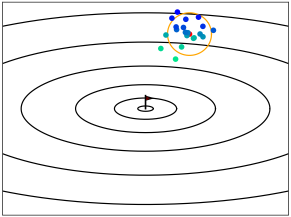

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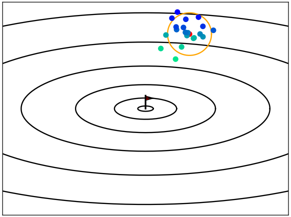

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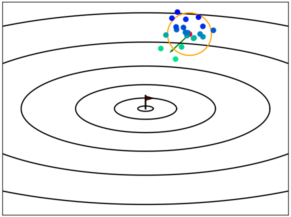

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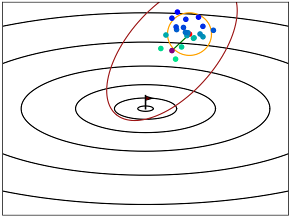

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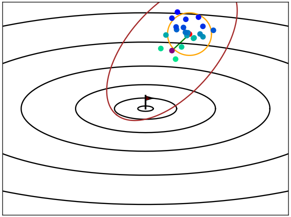

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5. $C_{t+1} = \text{Positive combination}\left(C_t, \overleftrightarrow{\mathrm{path}}, \text{Average}\left[\overleftrightarrow{(x^{i:\lambda}_{t+1} - m_t)}\right]\right)$

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Mean update:

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$$
\begin{aligned}
m_{t+1} &= \text{Average}(x_{t+1}^{1:\lambda}, \ldots, x_{t+1}^{\mu:\lambda}) \\
&= \sum_{i=1}^{\mu} \underbrace{\text{weight}_i}_{w_i} x_{t+1}^{i:\lambda}
\end{aligned}
$$

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

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$$\frac{1}{T}\log\frac{\|m_T - x^*\|}{\|m_0 - x^*\|} = \frac{1}{T}\sum_{t=0}^{T-1} \log\|z_{t+1}\| - \log\|z_t\| - \log\frac{\sigma_{t+1}}{\sigma_t}$$

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

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(and under which conditions?)

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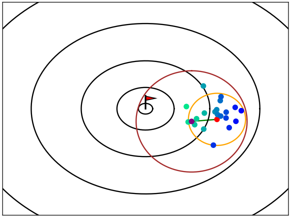

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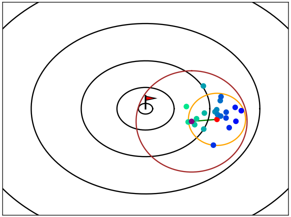

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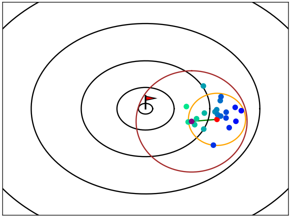

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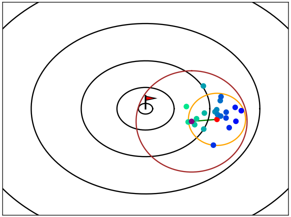

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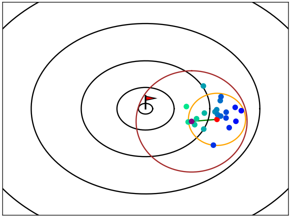

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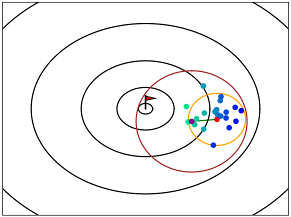

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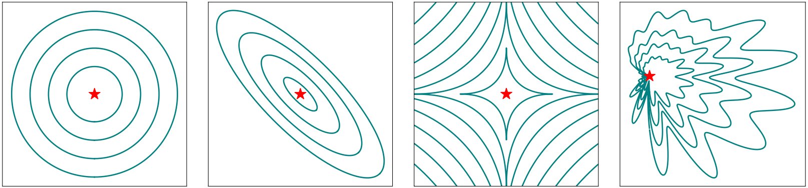
$$f\left(x_{t+1}^{1:\lambda}\right) \leqslant \cdots \leqslant f\left(x_{t+1}^{\lambda:\lambda}\right) \overset{?}{\Leftrightarrow} g\left(z_{t+1}^{1:\lambda}\right) \leqslant \cdots \leqslant g\left(z_{t+1}^{\lambda:\lambda}\right)$$

Scaling-invariant functions [TGAH21]



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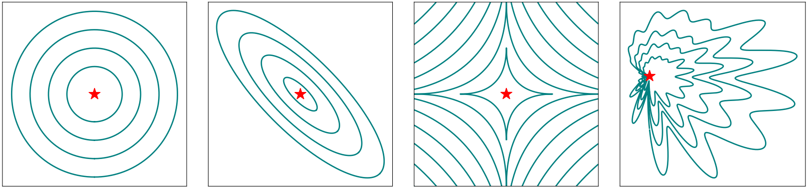

$$f\left(x_{t+1}^{i}\right) \leqslant f\left(x_{t+1}^{j}\right) \Leftrightarrow f\left({\color{red}\star} + \frac{x_{t+1}^{i} - {\color{red}\star}}{\sigma_t}\right) \leqslant f\left({\color{red}\star} + \frac{x_{t+1}^{j} - {\color{red}\star}}{\sigma_t}\right)$$

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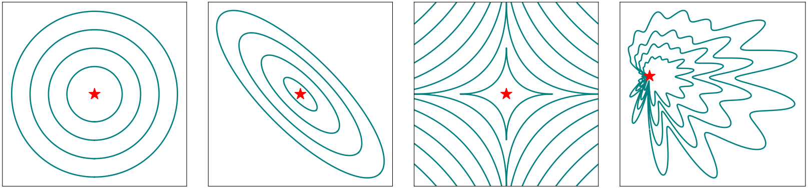

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Proposition ([AH16])

If $f \in$ { , , ,  } *, then $\{z_t\}_{t\in\mathbb{N}}$ is a Markov chain.*

How to prove that $\{z_t\}_{t\in\mathbb{N}}$ is stationary

1. Irreducibility and aperiodicity of $\{z_t\}$

2. Drift condition:

$$\mathbb{E}[V(z_1)] \leqslant (1-\varepsilon)V(z_0) \qquad \forall z_0 \notin \mathsf{K}$$

How to prove that $\{z_t\}_{t\in\mathbb{N}}$ is stationary

1. Irreducibility and aperiodicity of $\{z_t\}$
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$$\mathbb{E}[V(z_1)] \leqslant (1-\varepsilon)V(z_0) \qquad \forall z_0 \notin \mathsf{K}$$

Theorem ([MT09])
If 1. and 2. hold for a small set K*, then* $\{z_t\}$ *is stationary (*V*-geometrically ergodic).*

1. Irreducibility and aperiodicity

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

$$\forall z_{\mathrm{start}}, z_{\mathrm{end}} \in \mathcal{Z}, \underbrace{\exists k > 0,\ \mathbb{P}[z_k = z_{\mathrm{end}} \mid z_0 = z_{\mathrm{start}}] > 0}_{z_{\mathrm{start}} \rightsquigarrow z_{\mathrm{end}}}$$

1. Irreducibility and aperiodicity

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

$$\forall z_{\text{start}} \in \mathcal{Z}, \forall \mathcal{Z}_{\text{end}} \subset \mathcal{Z},\ \text{Volume}(\mathcal{Z}_{\text{end}}) > 0 \Rightarrow z_{\text{start}} \rightsquigarrow \mathcal{Z}_{\text{end}}$$

1. Irreducibility and aperiodicity

Theorem ([MC91], [MT09], [CA19], [GDA24])
The Markov chain

$$z_{t+1} = F(z_t, U_{t+1})$$

is irreducible and aperiodic when

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

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

Assumptions: F is loc. Lipschitz and $U_{t+1} \sim p_{z_t}$ where $(z, u) \mapsto p_z(u)$ is l.s.c.

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For us:

$$z_{t+1} = F(z_t, z_{t+1}^{i:\lambda}) = \frac{\text{Average}(z_{t+1}^{1:\lambda}, \ldots, z_{t+1}^{\mu:\lambda})}{\text{normalization}}$$

Assumptions: F is loc. Lipschitz and $U_{t+1} \sim p_{z_t}$ where $(z, u) \mapsto p_z(u)$ is l.s.c.

(i) steadily attracting state

$$z_{t+1} = F(z_t, U_{t+1})$$

z^* is *steadily attracting* when

$$\forall z_0,\ \exists \{U_k\}_{k\in\mathbb{N}}, \quad \lim_{k\to\infty} F^k(z_0, U_1, \ldots, U_k) = z^*$$

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Proposition
0 *is steadily attracting*

Proof.
Choose $z_{t+1}^{i:\lambda} = 0$. Then

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

$\square$

(ii) submersion

$F(\cdot)$ is a submersion at x when $\mathcal{D}F(x)$ is surjective.

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Proposition
$F(0,\cdot)$ *is submersive at* 0

Proof.

$$F(0, 0 + h^i) = \frac{\text{Average}(h^1, \ldots, h^\mu)}{\text{normalization}} = \underbrace{\text{Average}(h^1, \ldots, h^\mu)}_{\text{surjective}} + o(h^i)$$

$\square$

Consequence

$\{z_t\}$ is an irreducible aperiodic Markov chain

2. Drift condition

$V(z) = \|z\|^2$

$$\mathbb{E}[\|z_1\|^2] \leqslant (1-\varepsilon)\|z_0\|^2$$

when $\|z_0\| \gg 1$ and $f \in \Big\{$ , ,  $\Big\}$

Theorem ([TAH23])

If $f \in \Big\{$ , ,  $\Big\}$, $\{z_t\}$ *is a stationary Markov chain.*

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If $f \in \Big\{$ , ,  $\Big\}$, $\{z_t\}$ *is a stationary Markov chain.*

Conclusion:

Theorem ([TAH23])
ES with step-size adaptation converges linearly

Back to CMA-ES

$$z_t = \frac{m_t}{\sigma_t \sqrt{\lambda_{\min}(C_t)}}$$

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

Proposition* ([GWAH])

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

How to prove that $\{(z_t, \Sigma_t)\}_{t\in\mathbb{N}}$ is stationary

1. Irreducibility and aperiodicity of $\{(z_t, \Sigma_t)\}$
2. Drift condition:

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

1. Irreducibility and aperiodicity

Theorem ([MC91], [MT09], [CA19], [GDA24])
The Markov chain

$$(z_{t+1}, \Sigma_{t+1}) = F(z_t, \Sigma_{t+1}, z_{t+1}^{i:\lambda})$$

is irreducible and aperiodic when

(i) *there exists a steadily attracting state* (z^*, Σ^*)*;*

(ii) *there exists a path* $z_1^{i:\lambda}, \ldots, z_k^{i:\lambda}$ *at which* $F^k(z^*, \Sigma^*, \cdot)$ *is submersive.*

Assumptions: F is loc. Lipschitz and $U_{t+1} \sim p_{z_t}$ where $(z, u) \mapsto p_z(u)$ is l.s.c.

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

Proof.
More complicated than before... $\square$

Proposition* ([GWAH])
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Proof.
More complicated than before... $\square$

Consequence:

$\{(z_t, \Sigma_t)\}$ is irreducible and aperiodic.

2. Drift condition

$$V(z, \Sigma) = \alpha \|z\|^2 + \beta |\!|\!|\Sigma|\!|\!|$$

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$$V(z, \Sigma) = \alpha \|z\|^2 + \beta |\!|\!| \Sigma |\!|\!|$$

(a) When $|\!|\!|\Sigma_0|\!|\!| \gg 1 + \|z_0\|^2$:

$$\mathbb{E}[|\!|\!|\Sigma_1|\!|\!|] \leqslant (1-\varepsilon)|\!|\!|\Sigma_1|\!|\!|$$

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(b) When $|||\Sigma_0||| \not\gg \|z_0\|^2$:

$$\mathbb{E}[\|z_1\|^2] \leqslant (1 - \varepsilon)\|z_0\|^2$$

2. Drift condition

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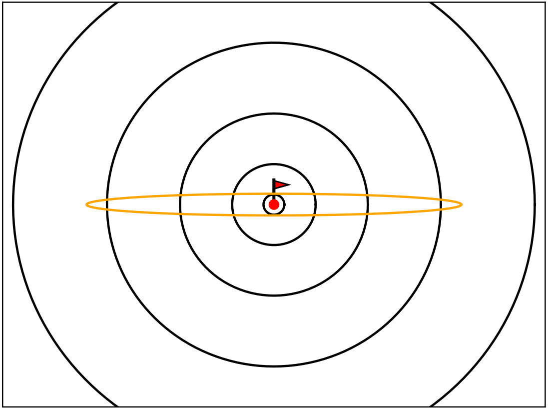
(b) When $|\!|\!|\Sigma_0|\!|\!| \not\gg \|z_0\|^2$:

$$\mathbb{E}[\|z_1\|^2] \leqslant (1 - \varepsilon)\|z_0\|^2$$

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

$$\exists \mathrm{K} \textit{ compact}, \; \mathbb{E}[V(z_1, \Sigma_1)] \leqslant (1 - \varepsilon) V(z_0, \Sigma_0) \quad \forall (z_0, \Sigma_0) \notin \mathrm{K}$$

(a) When $\|\Sigma_0\| \gg 1 + \|z_0\|^2$



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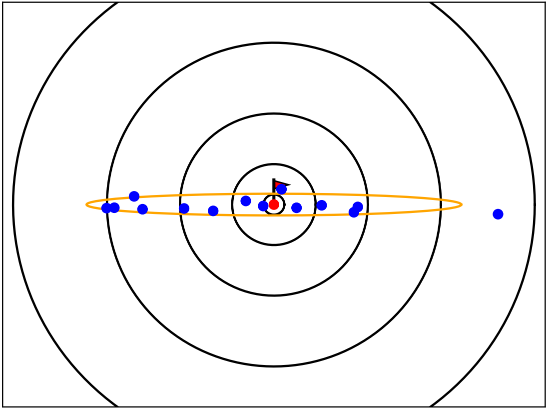

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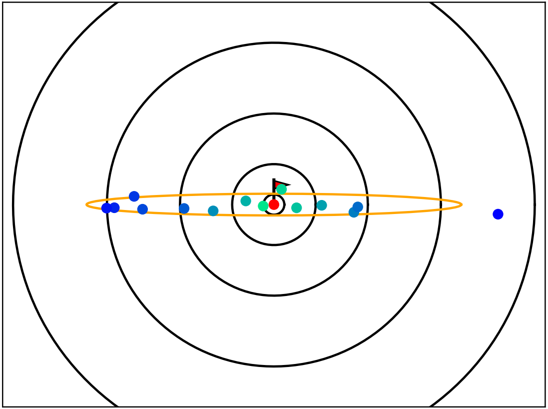

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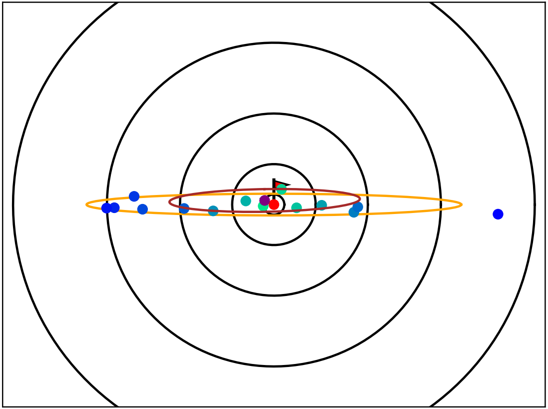
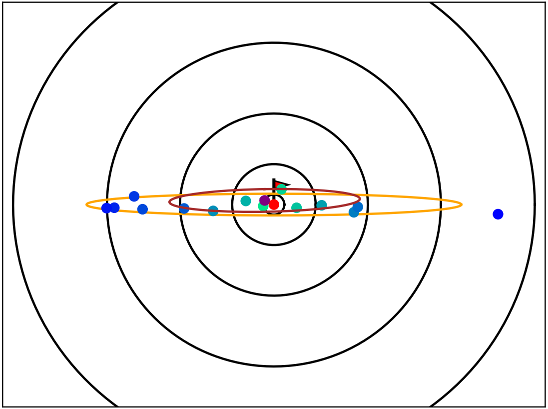


(a) **When** $|||\Sigma_0||| \gg 1 + \|z_0\|^2$



Proposition* ([GAH23], [GAHa])

When $f =$  *and* $|||\Sigma_0||| \gg 1 + \|z_0\|^2$*:*

$$\mathbb{E}[|||\Sigma_1|||] \leqslant (1-\varepsilon)|||\Sigma_1|||$$

(b) When $\|\Sigma_0\| \not\gg \|z_0\|^2$

(b) When $\lVert\Sigma_0\rVert \not\gg \|z_0\|^2$

$$z_1 = \frac{\mathrm{Average}(z_1^{1:\lambda}, \ldots, z_1^{\mu:\lambda})}{\mathrm{normalization}}$$

(b) When $|||\Sigma_0||| \not\gg \|z_0\|^2$

$$z_1 = \frac{\text{Average}(z_1^{1:\lambda}, \dots, z_1^{\mu:\lambda})}{\text{normalization}}$$

with

$$\text{normalization} = \text{increasing function}(\|m_{t+1} - m_t\|) \times \sqrt{\lambda_{\min}(\Sigma_1)}$$

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Proposition* ([GAHa])

When $f =$  *and* $|||\Sigma_0||| \not\gg \|z_0\|^2$*:*

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

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If we choose the hyperparameters correctly:

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

(b) When $|||\Sigma_0||| \not\gg \|z_0\|^2$

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and

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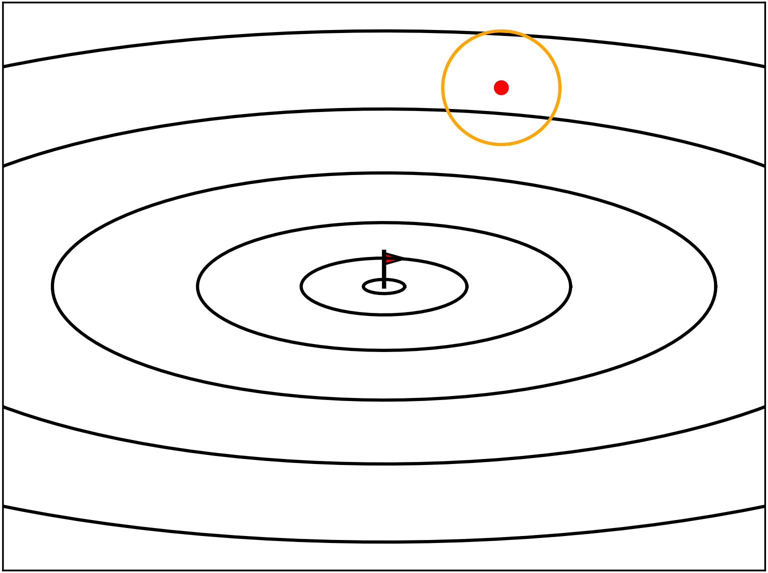

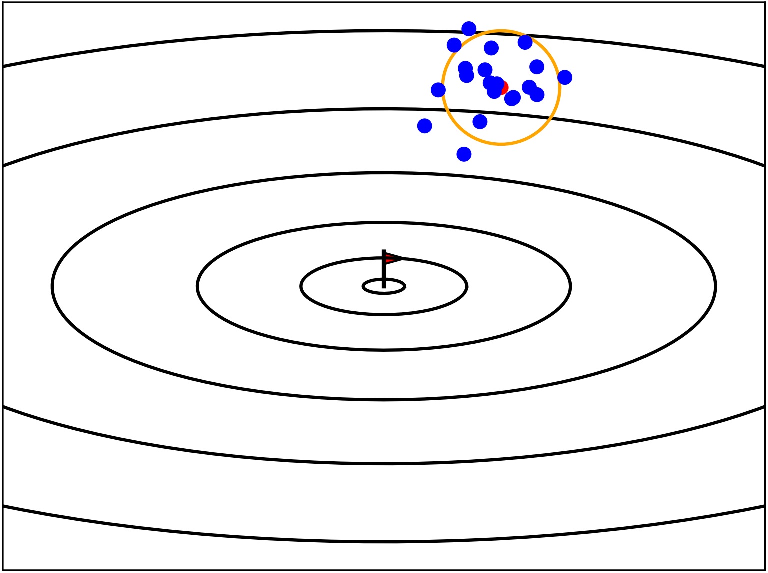

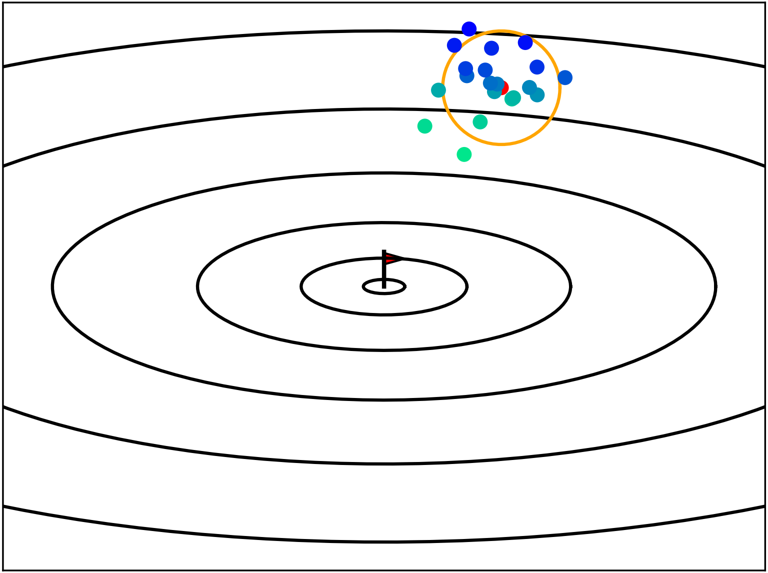

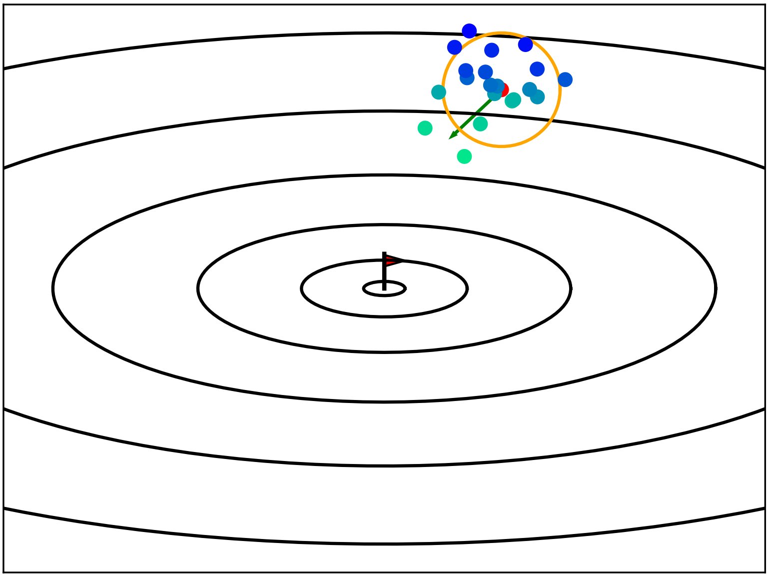

Theorem* ([GAHa])

When $f =$ 

$$\exists \mathsf{K} \text{ compact}, \; \mathbb{E}[V(z_1, \Sigma_1)] \leqslant (1-\varepsilon) V(z_0, \Sigma_0) \quad \forall (z_0, \Sigma_0) \notin \mathsf{K}$$

Theorem* ([GAHb])

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

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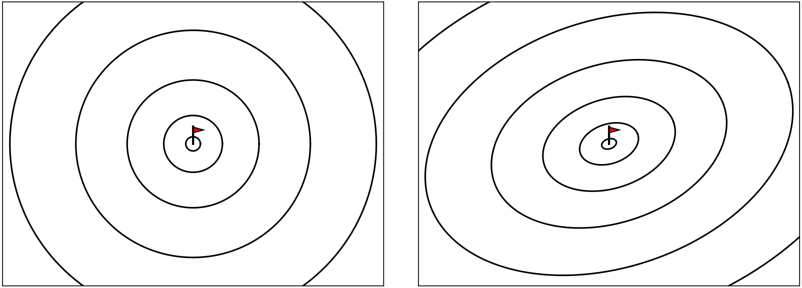
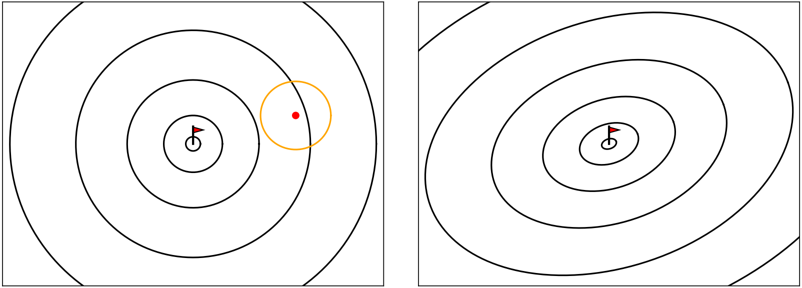
When $f =$ *, CMA-ES converges linearly.*

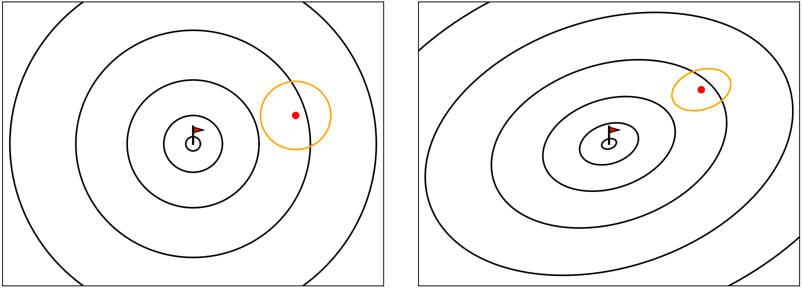
How to extend to $f =$ **?**

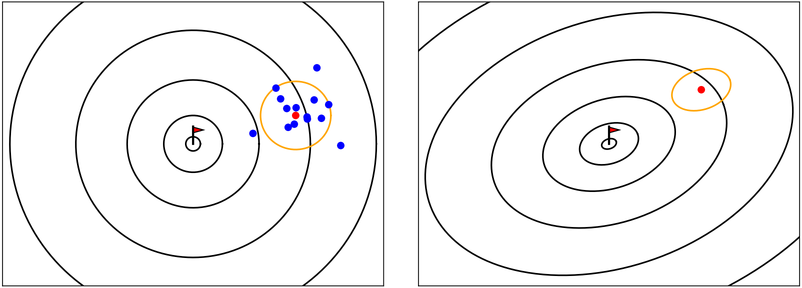
Affine-invariance

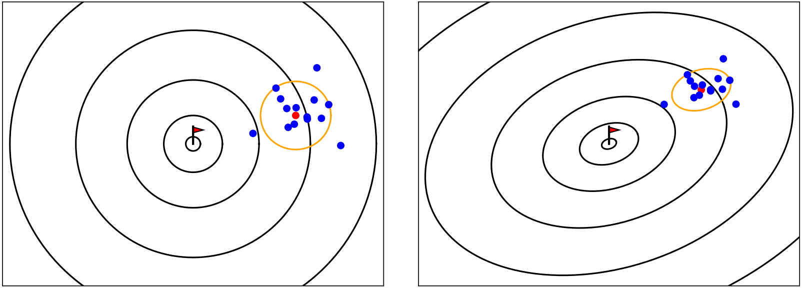
$$
\begin{tikzcd}
(m_0, C_0) \arrow[rrr, "\min f(x)"] \arrow[d, "\Psi"'] & & & (m_1, C_1) \\
(m_0', C_0') \arrow[rrr, "\min f(Bx+b)"] & & & (m_1', C_1') \arrow[u, "\Psi^{-1}"']
\end{tikzcd}
$$

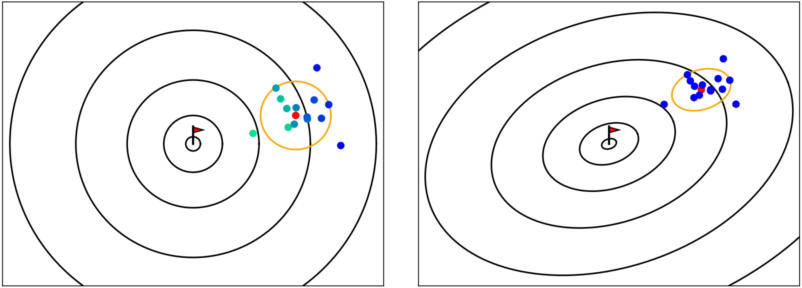


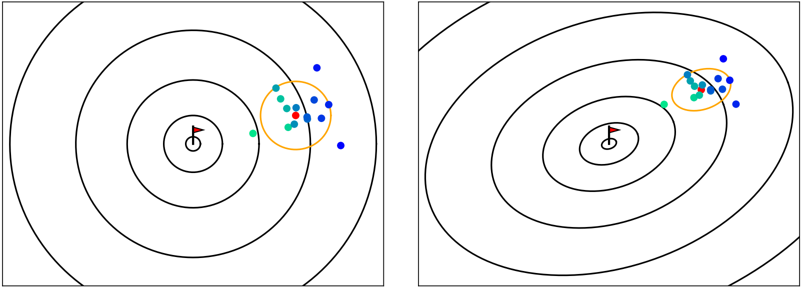


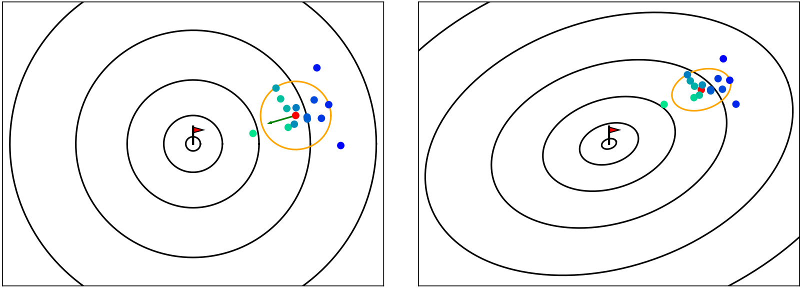


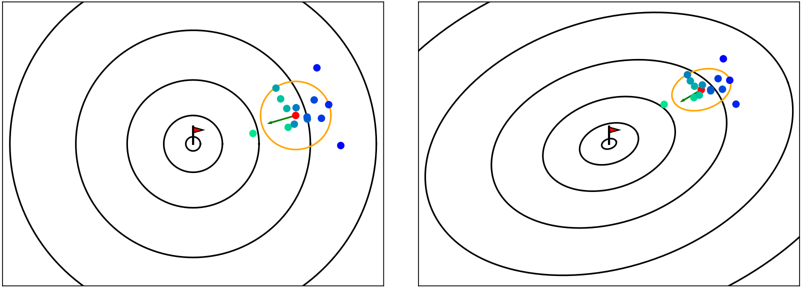


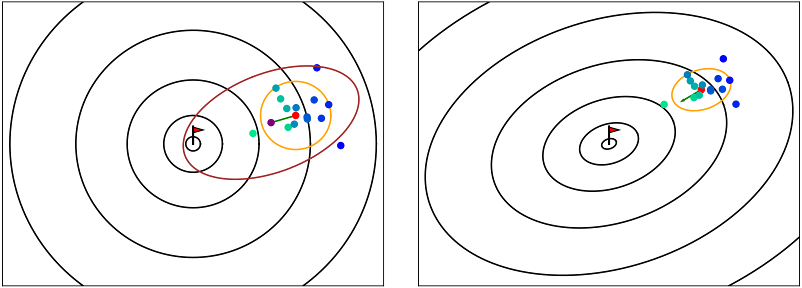


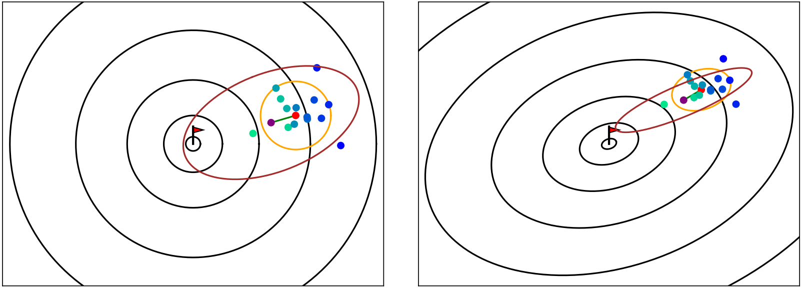












Theorem ([HA14], [A16])
CMA-ES is affine-invariant

Theorem* ([GAHb])

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

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

(with the same convergence rate than *)*

Learning of the inverse Hessian

When $f =$ , we find

$$\lim_{t\to\infty} \mathbb{E}\left[\frac{C_t}{\text{normalization}}\right] = I_d$$

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Since  $= \text{Hessian}^{-1/2} \times$ :

$f =$ 
$$\Rightarrow \lim_{t\to\infty} \mathbb{E}\left[\frac{C_t}{\text{normalization}}\right] = \text{Hessian}^{-1/2} \times I_d \times \text{Hessian}^{-1/2}$$
$$= \text{Hessian}^{-1}$$

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Theorem* ([GAHb])
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

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