Convergence Analysis of Evolution Strategies with Covariance Matrix Adaptation (CMA-ES) via Markov Chain Stability Analysis

Blackbox Optimization and Derivative-Free Algorithms

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

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CMA-ES approximates the minimum x^* of f by a multivariate normal distribution $\mathcal{N}(m, \sigma^2 C)$ **by adapting** the mean $m \in \mathbb{R}^d$, the stepsize $\sigma > 0$ **and the covariance matrix** $C \in \mathcal{S}^d_{++}$.

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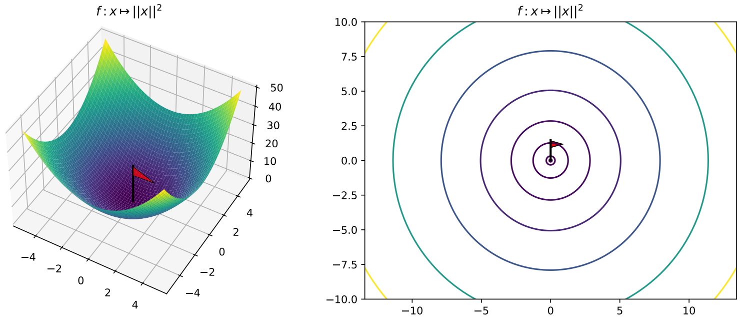
- **proofs of convergence require additional assumptions so far**

- Without covariance matrix adaptation: Touré et al, *Global linear convergence of Evolution Strategies with recombination on scaling-invariant functions* (2021)
- With a sufficient decrease condition: Diouane et al, *Globally convergent evolution strategies* (2015)
- Assuming that the covariance matrix is bounded: Akimoto et al, *Global linear convergence of evolution strategies on more than smooth strongly convex functions* (2022)
- Using a different update for the covariance matrix: Glasmachers et al, *Convergence analysis of the Hessian estimation evolution strategy* (2022)

CMA-ES: algorithm presentation

Level sets representation



CMA-ES : presentation

Principle of Evolution Strategies (ES) : approximate the minimum of the function by a distribution $\mathcal{N}(m, \sigma^2 C)$.

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At each iteration $t \in \mathbb{N}$, given a **mean** m_t, a **stepsize** σ_t and a **covariance matrix** C_t :

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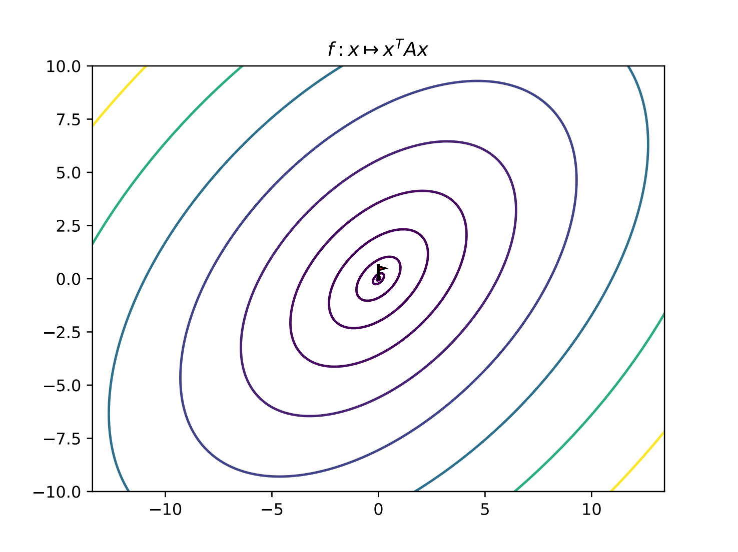

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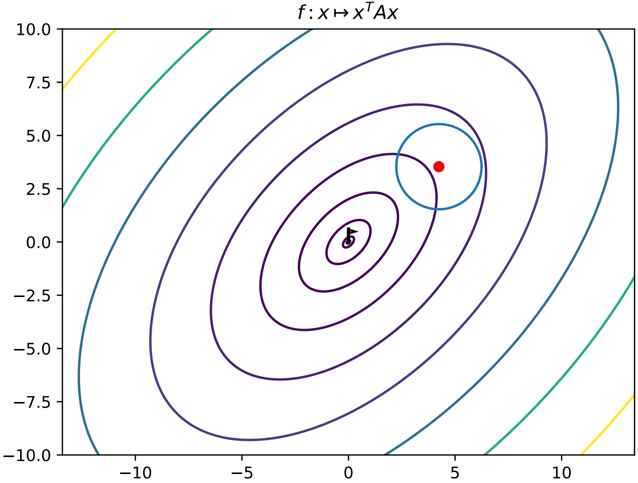

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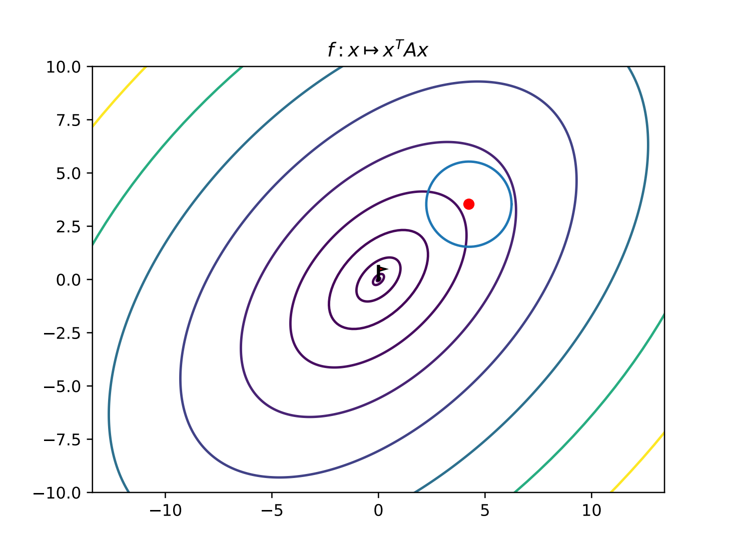

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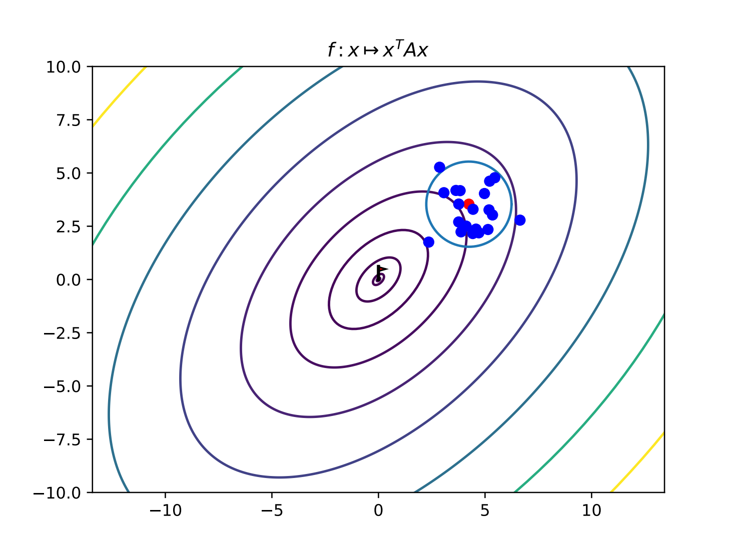

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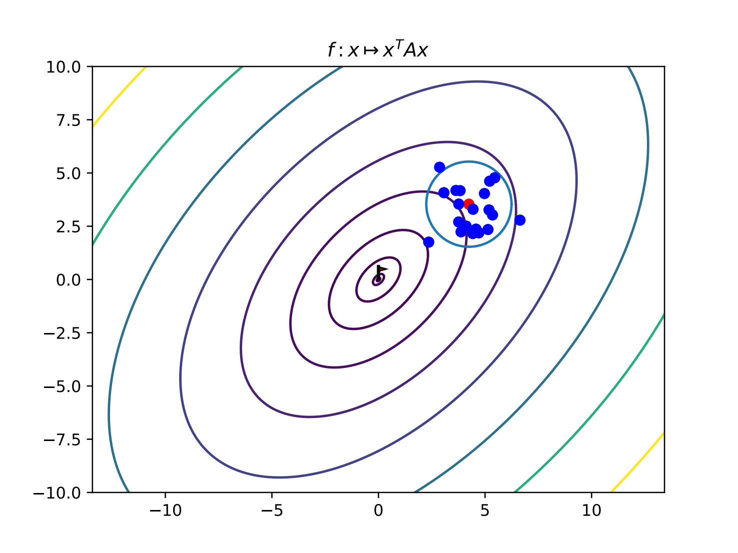

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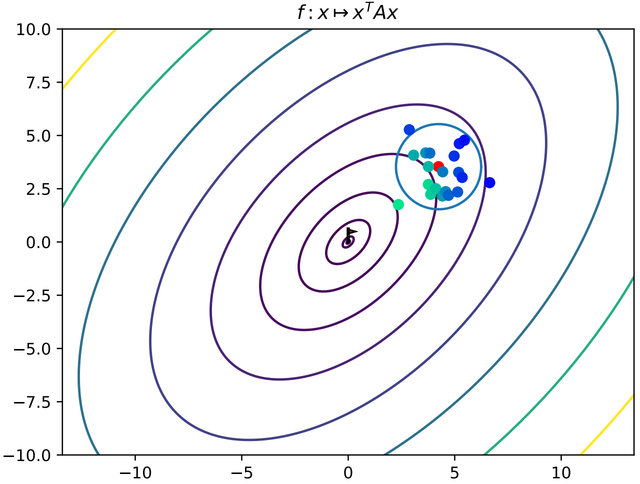

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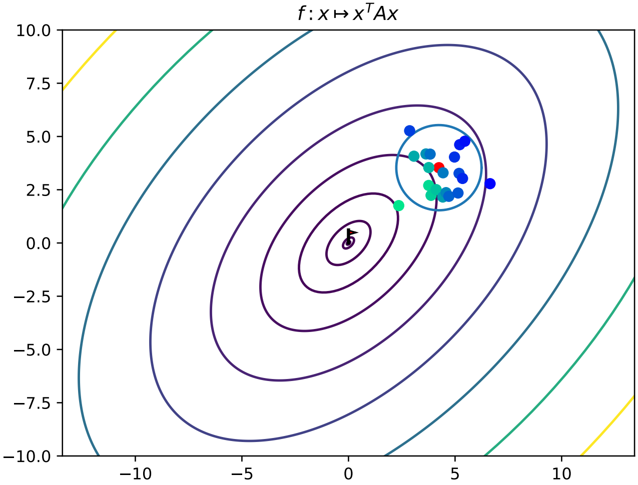

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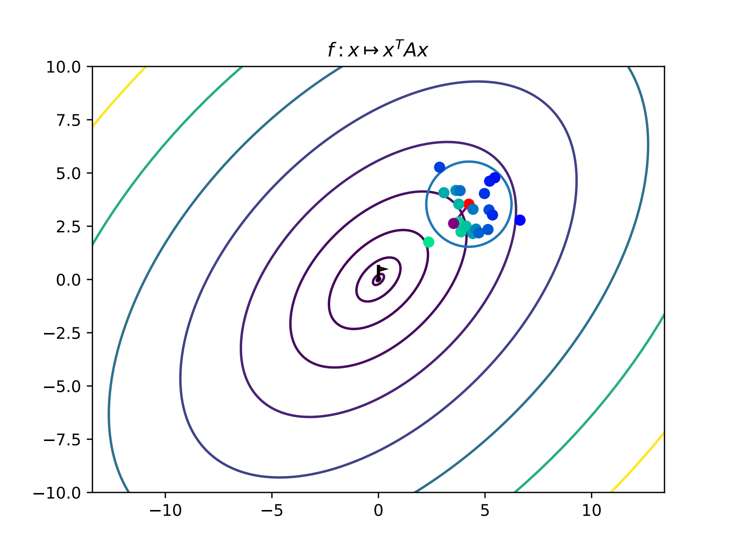

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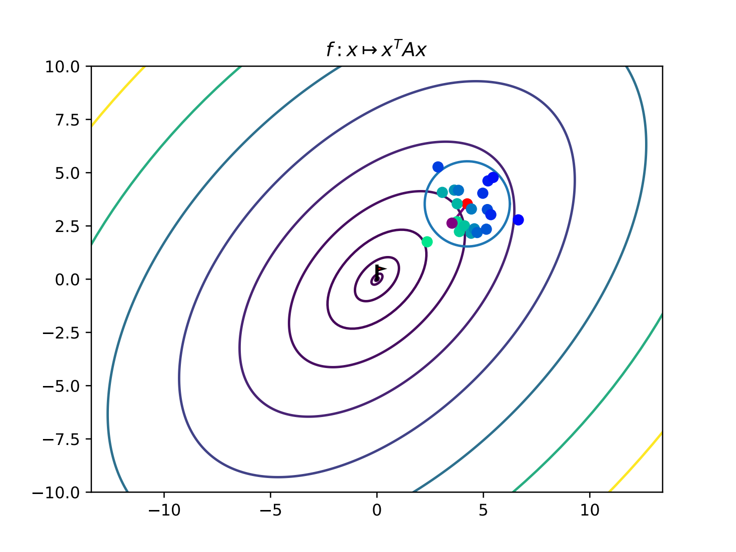

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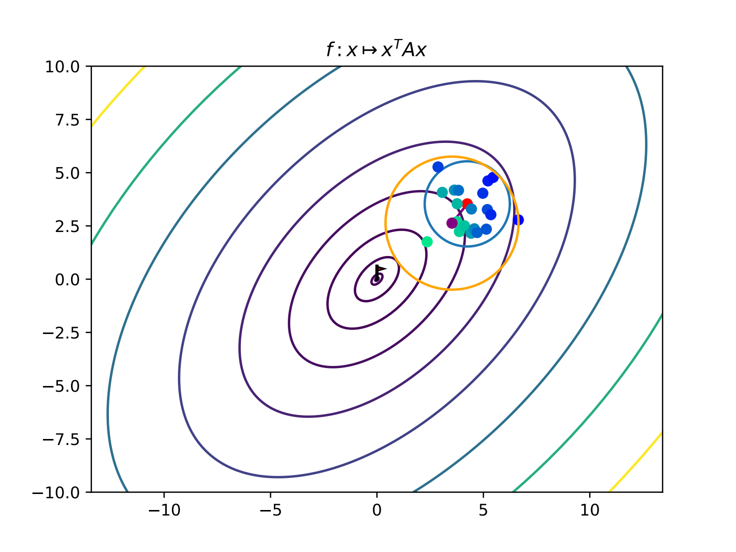

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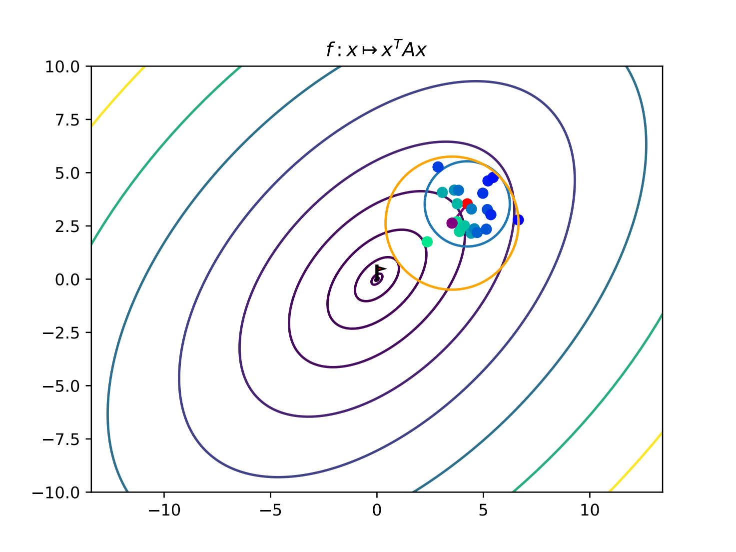

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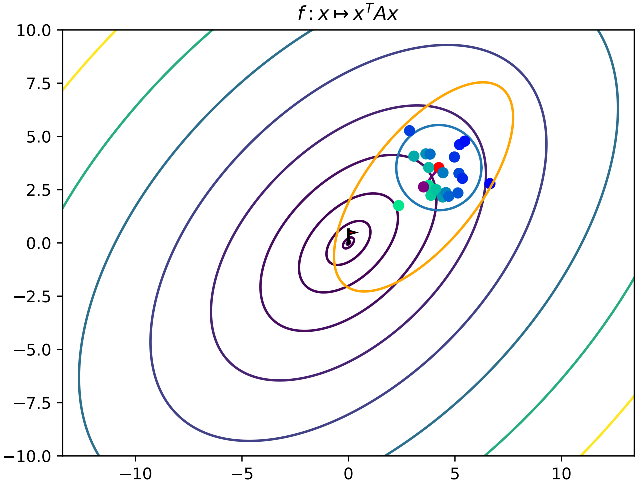

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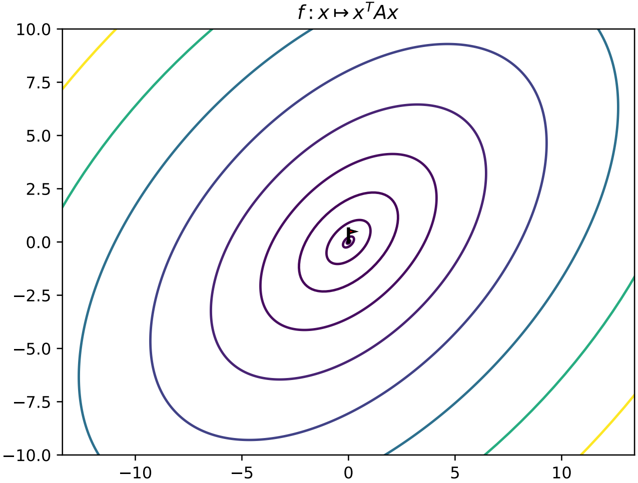

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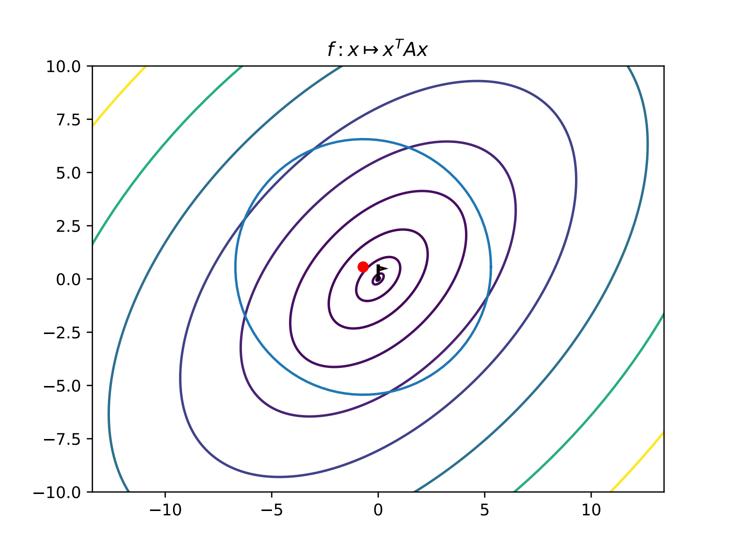

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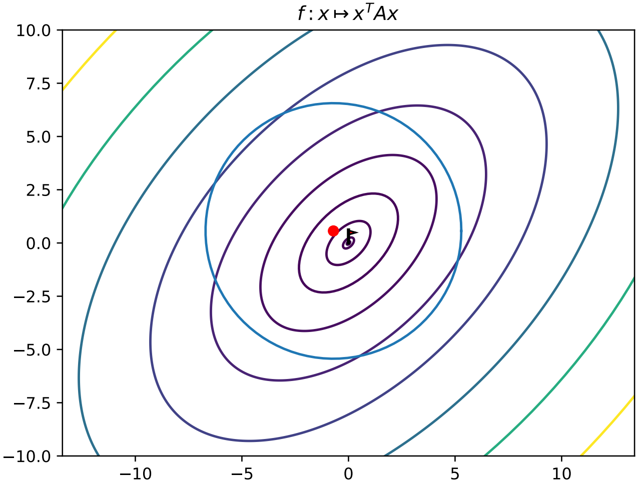

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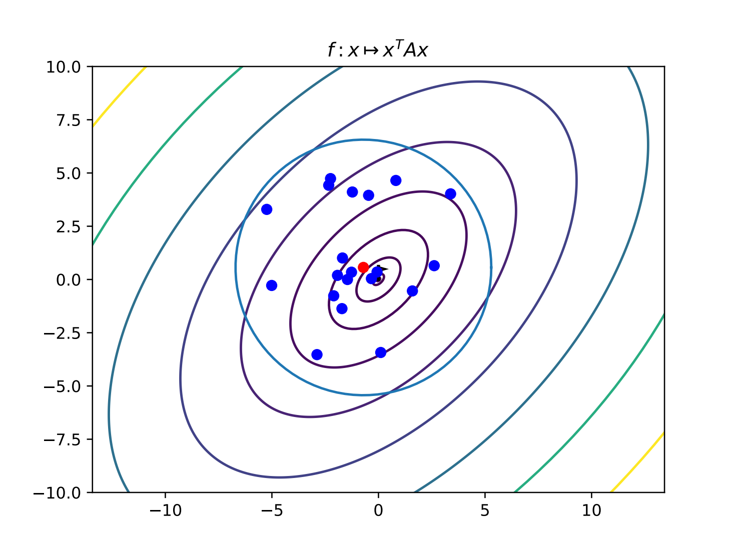

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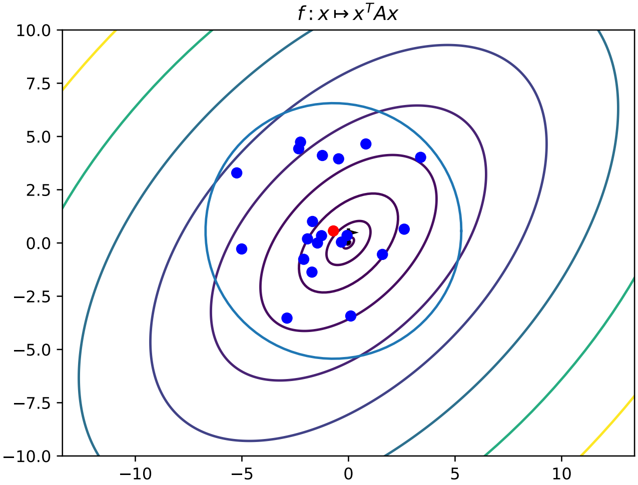

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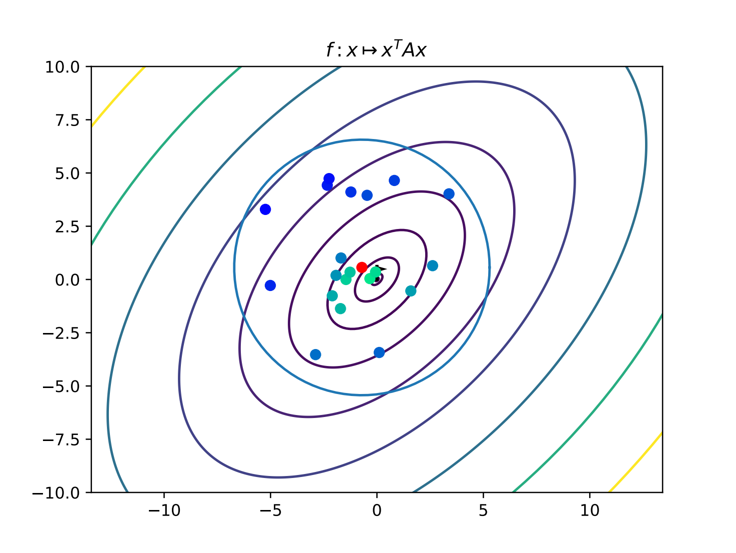

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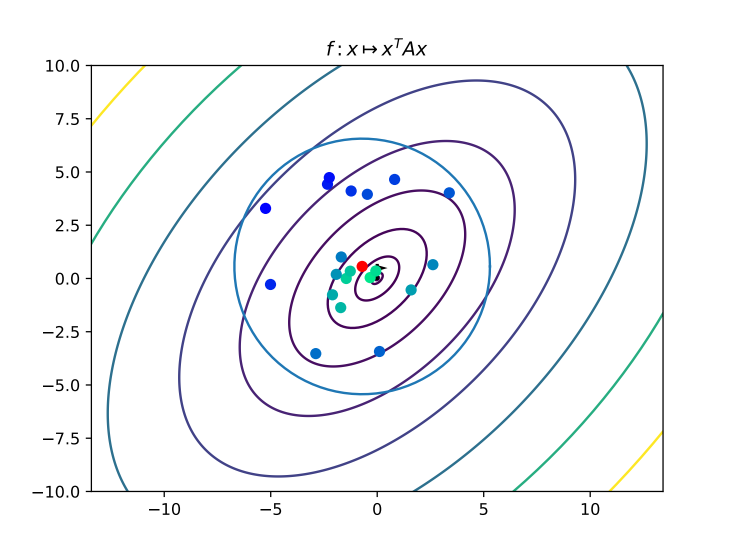

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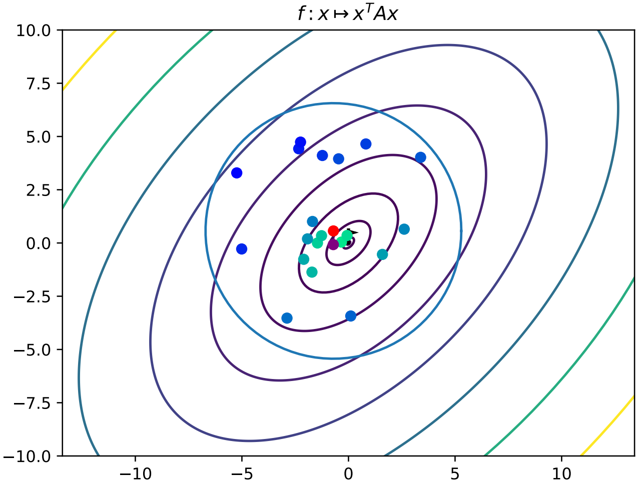
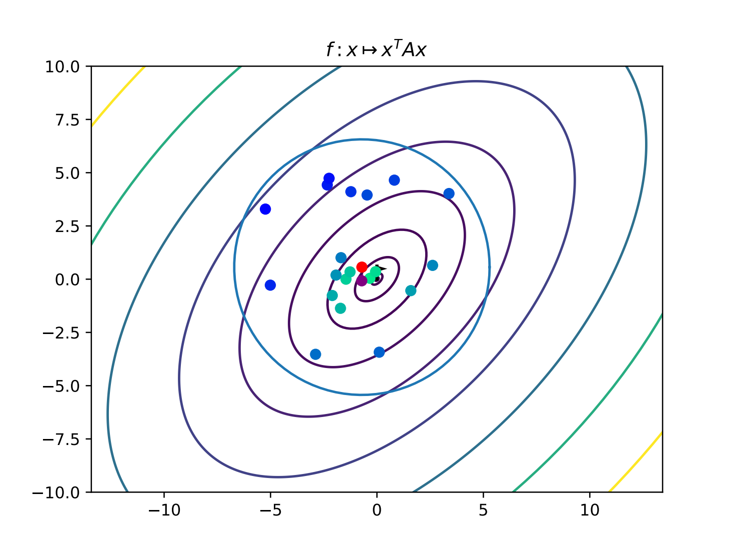


Adapt the stepsize



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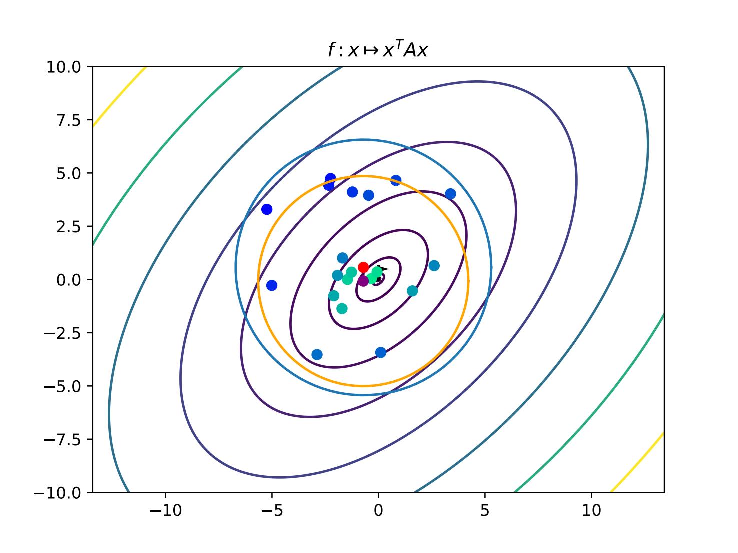
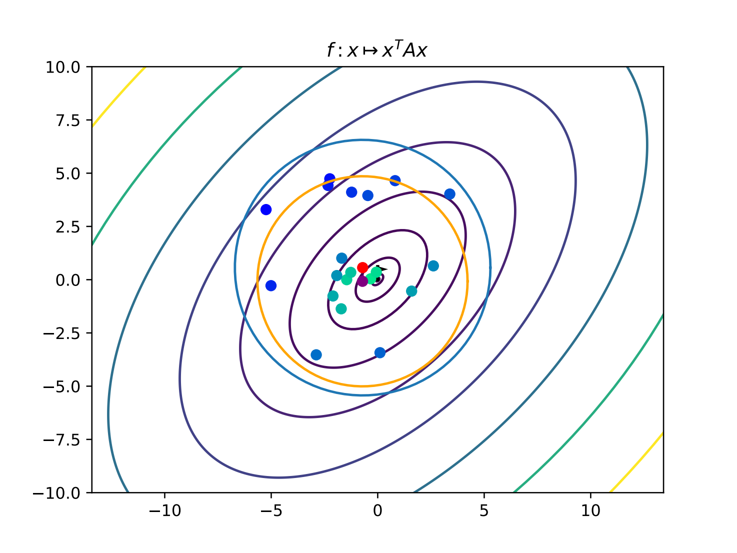


Adapt the covariance matrix



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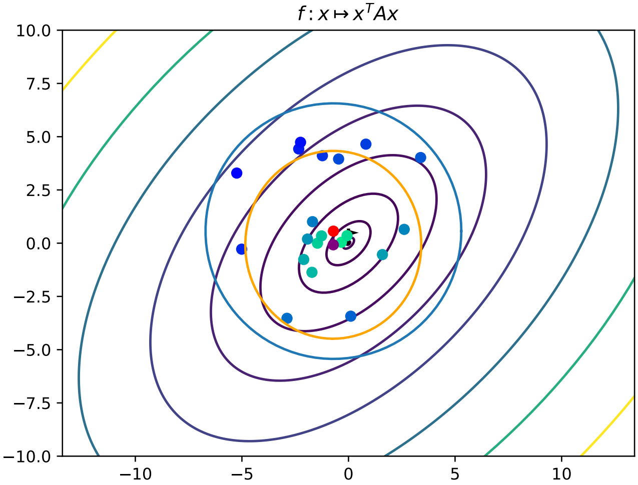
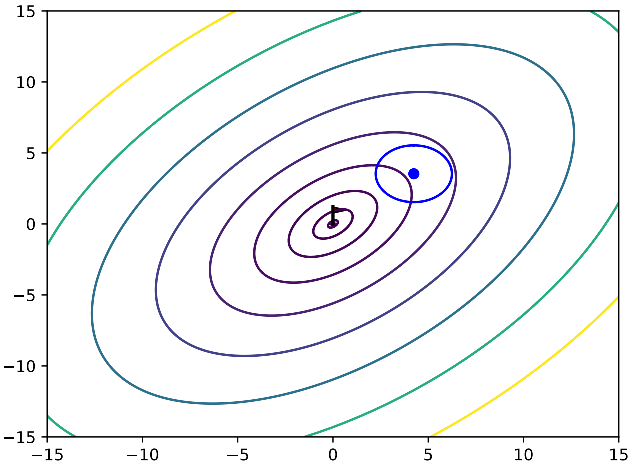


Linear convergence

Convergence



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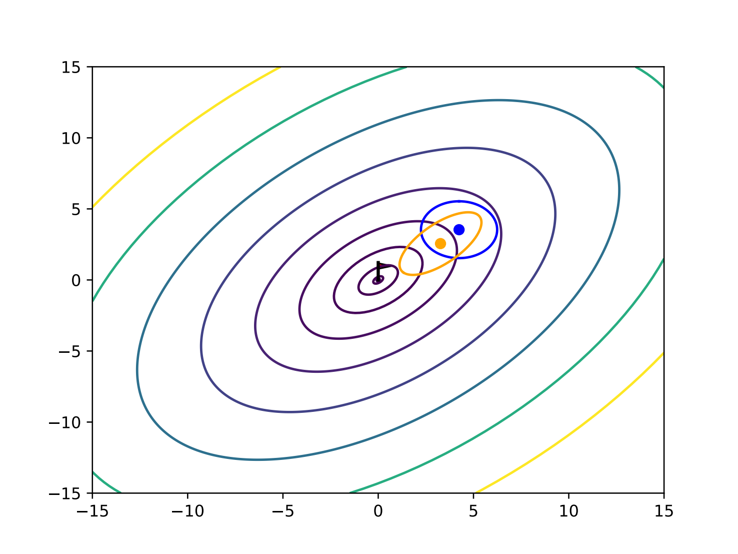

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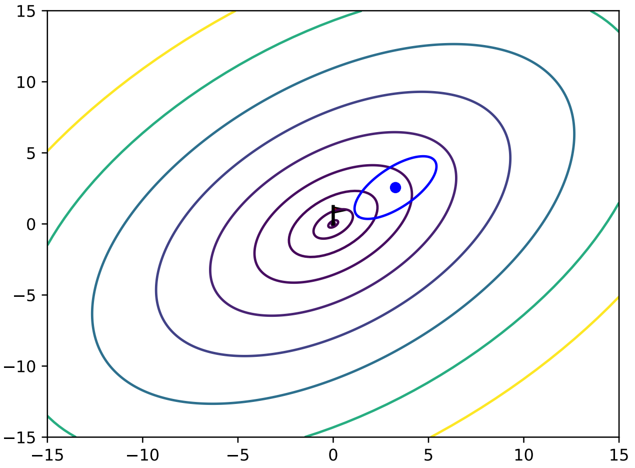

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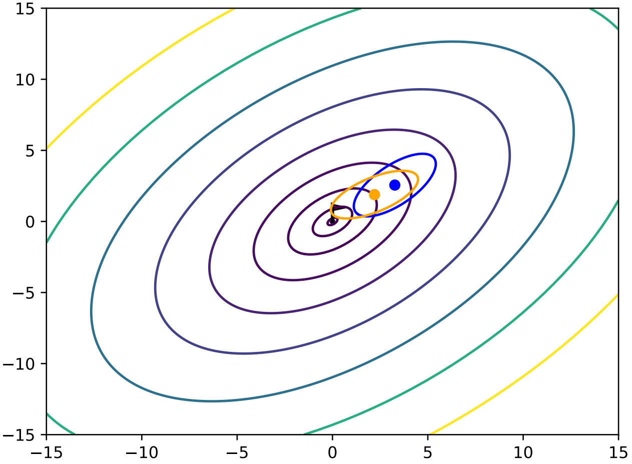

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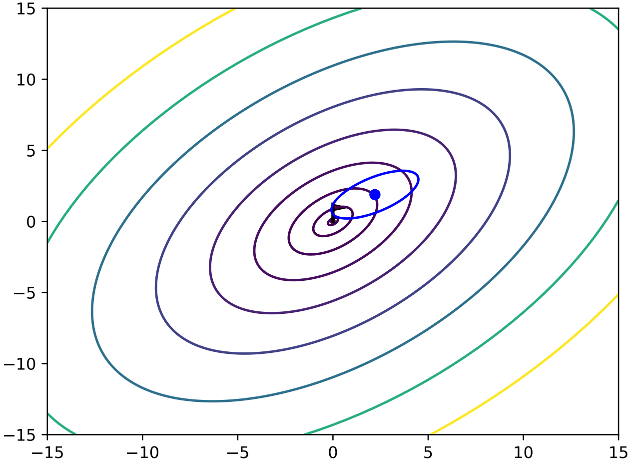

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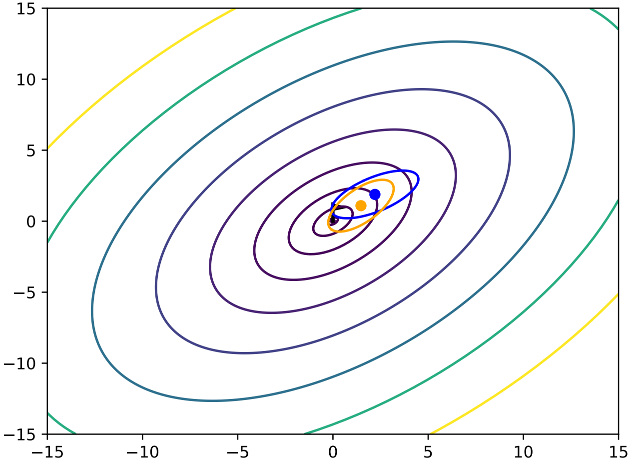

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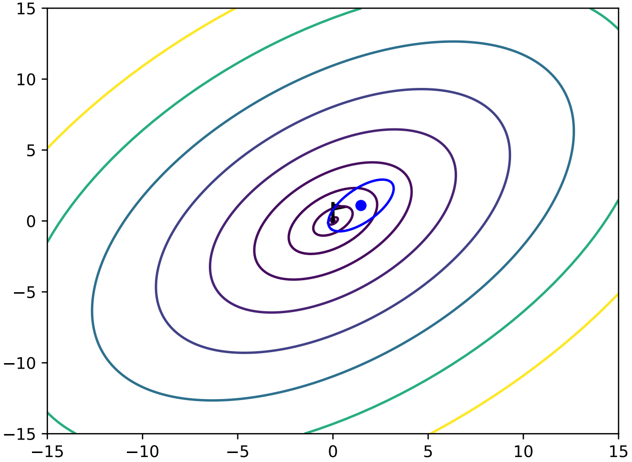

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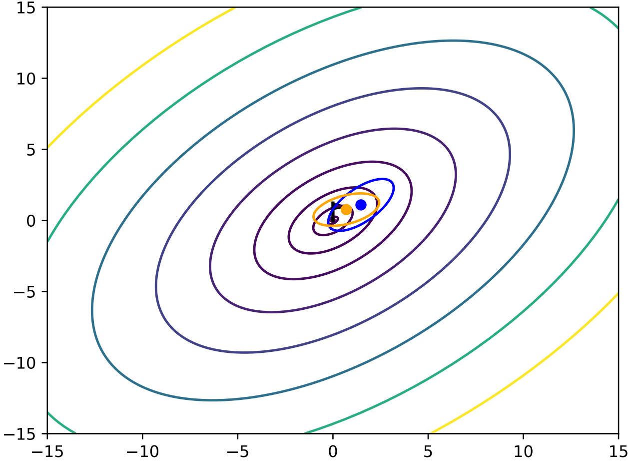

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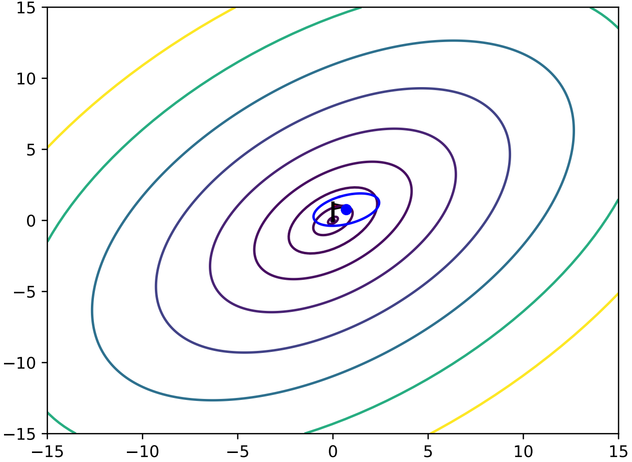

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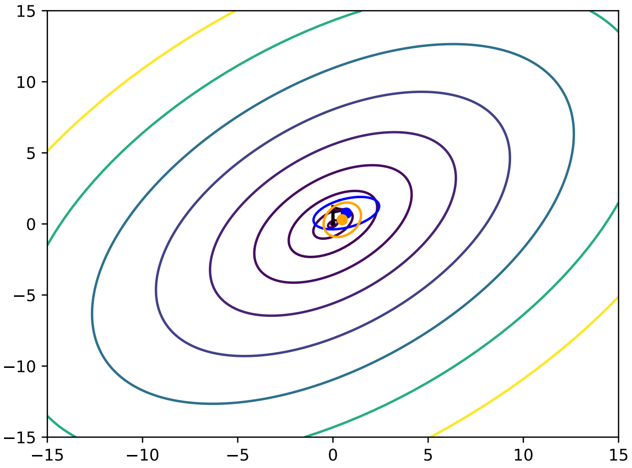

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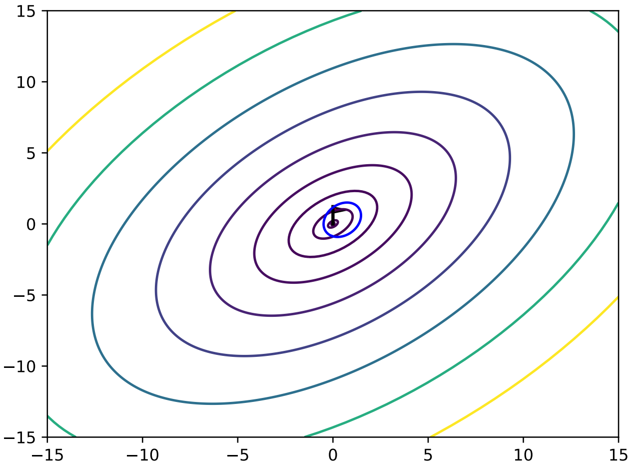

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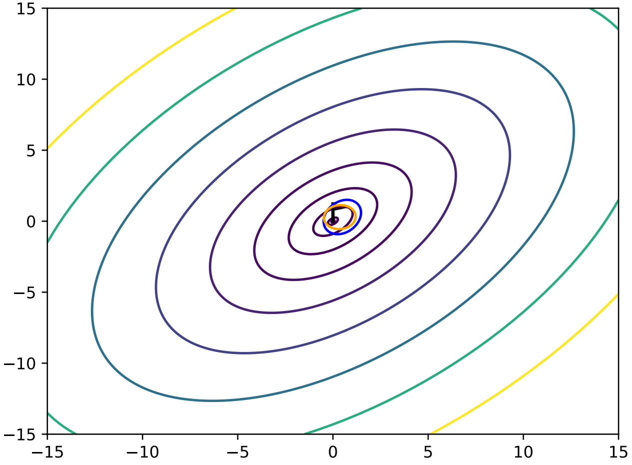

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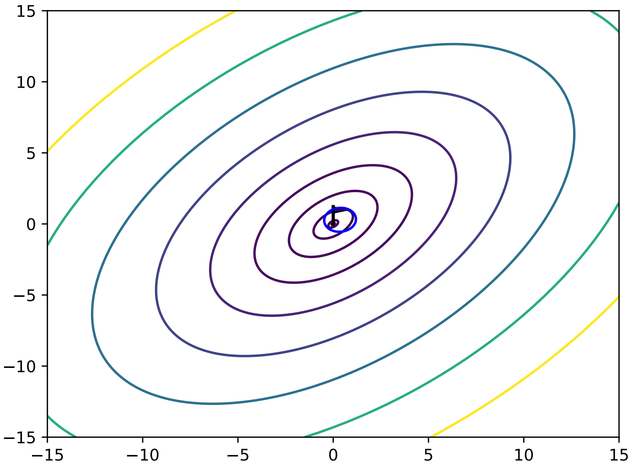

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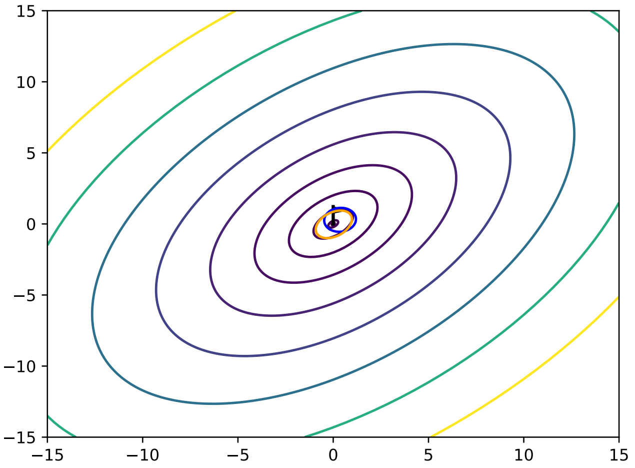

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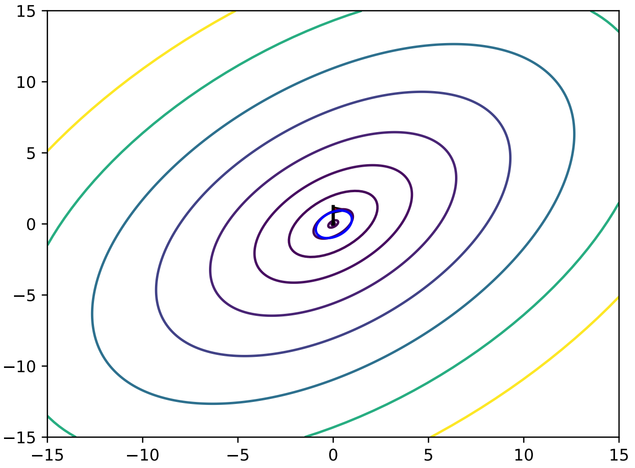

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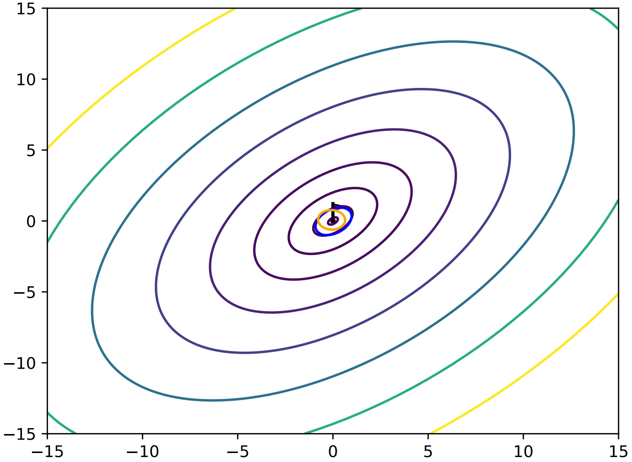

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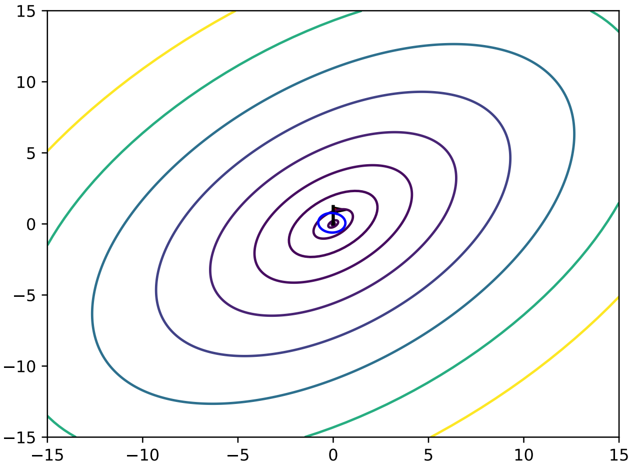

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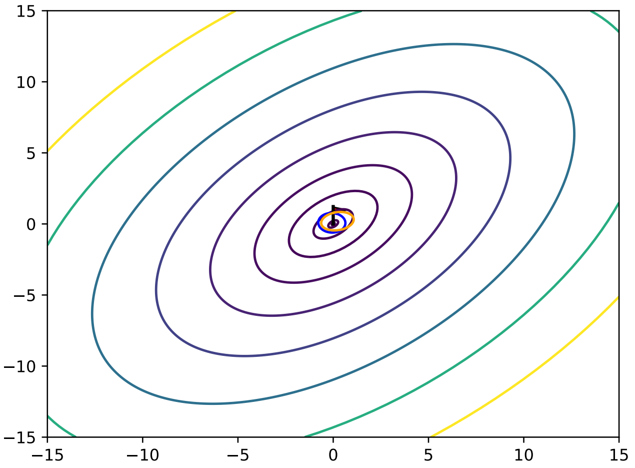

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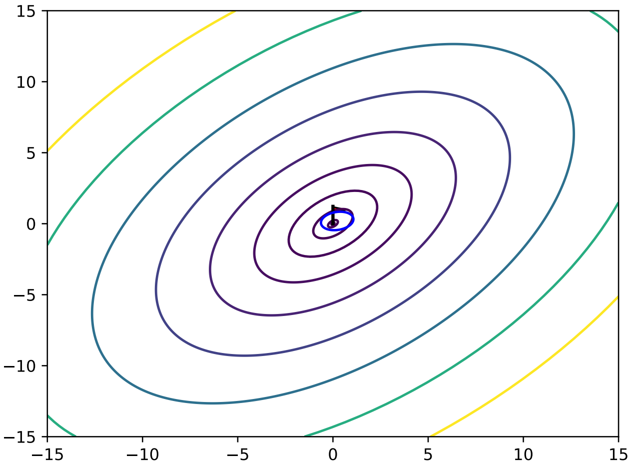

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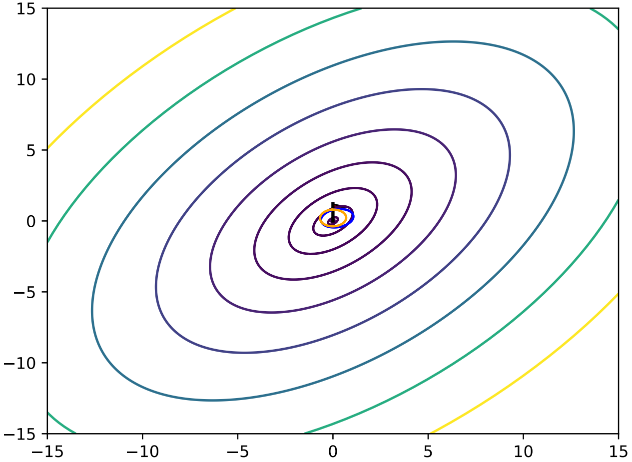

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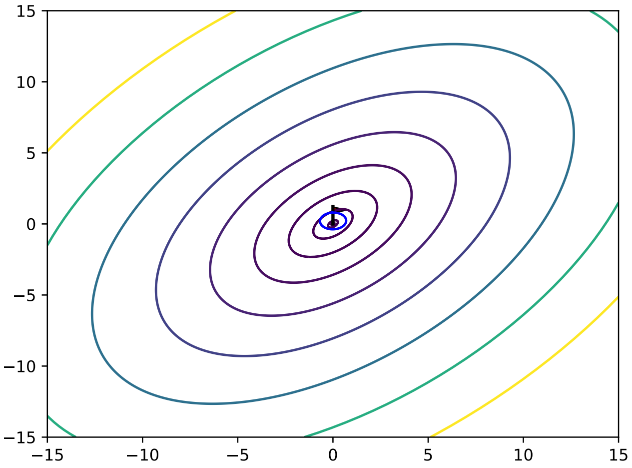

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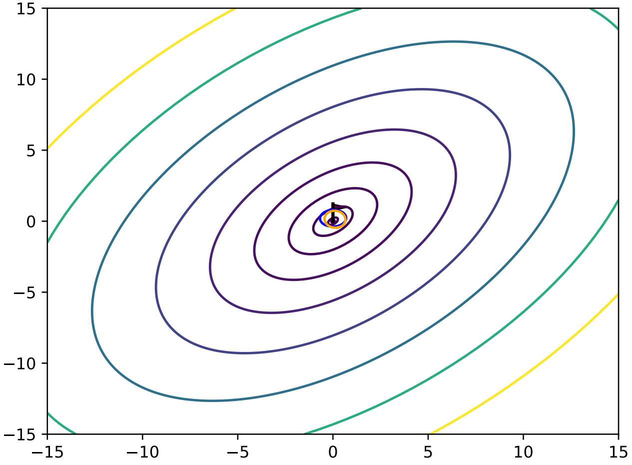

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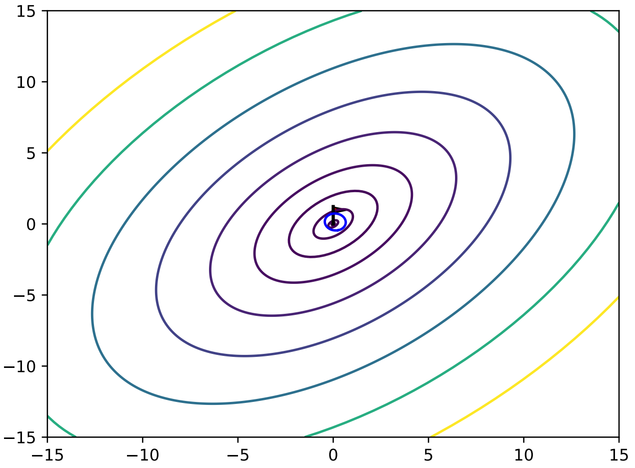

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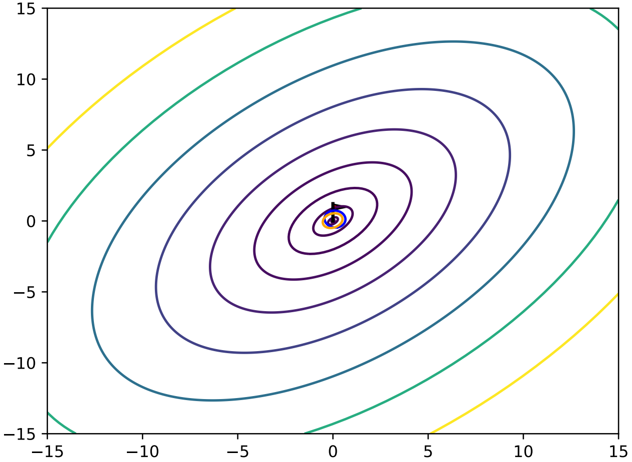

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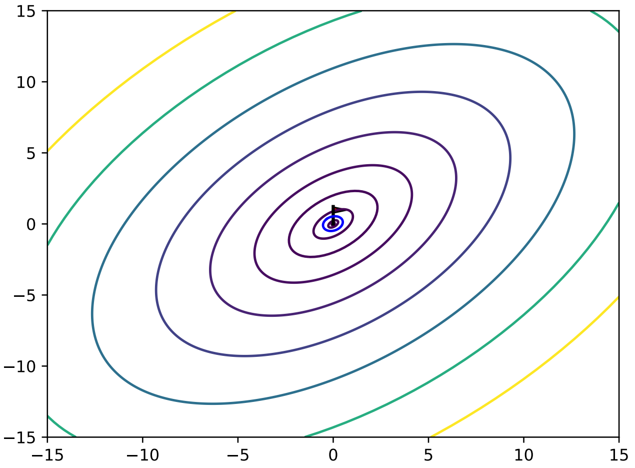

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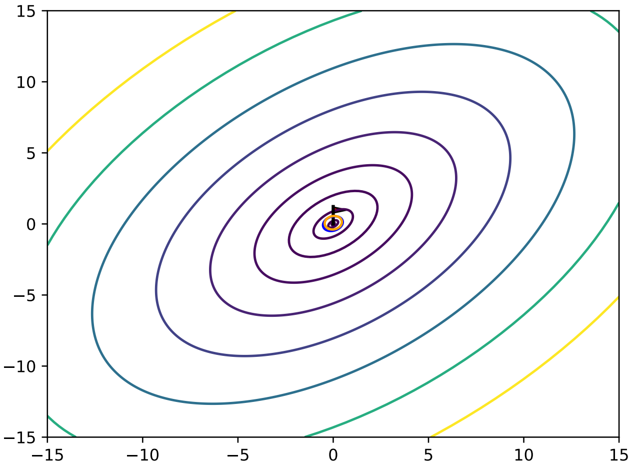

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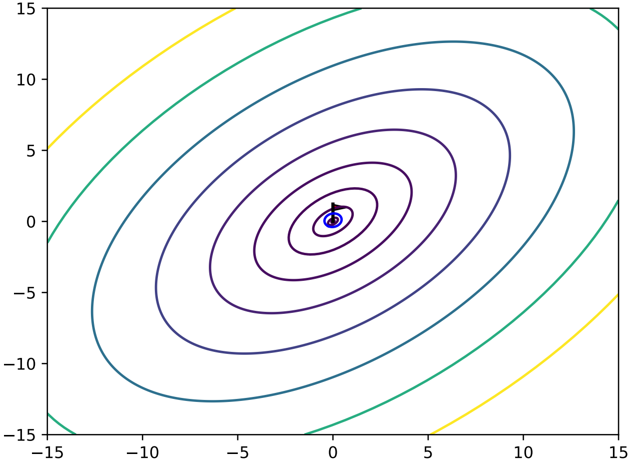

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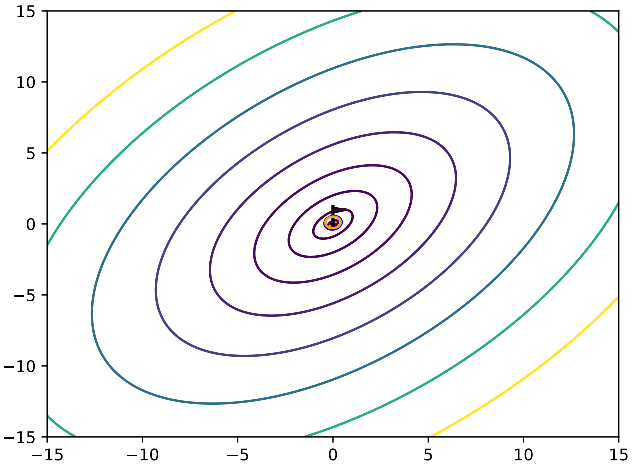

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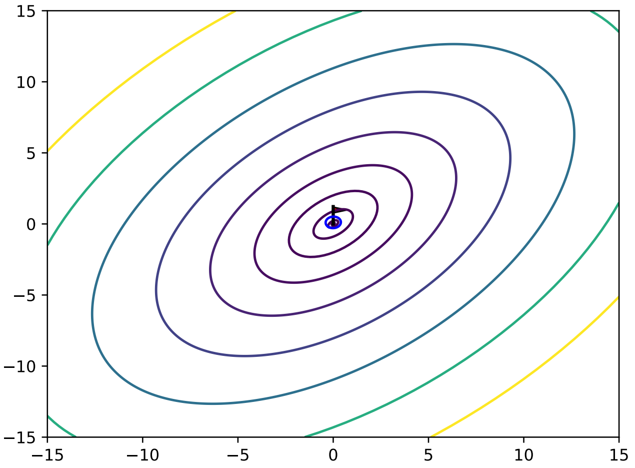

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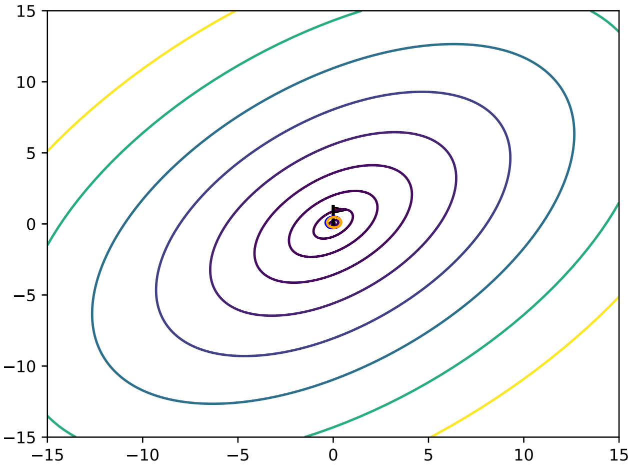

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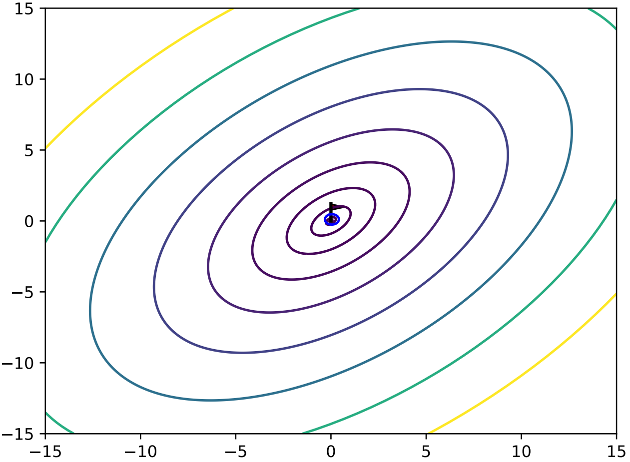

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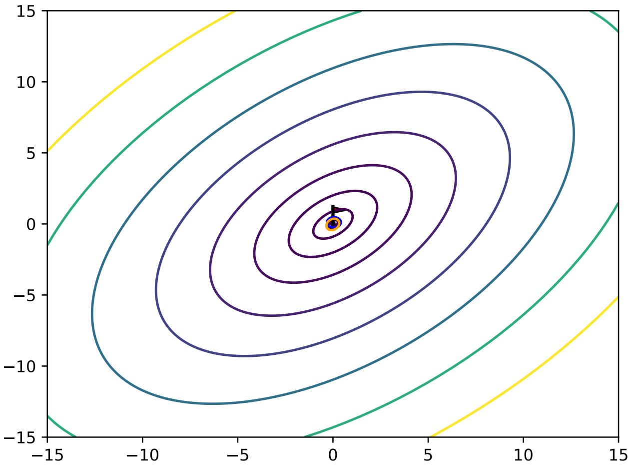

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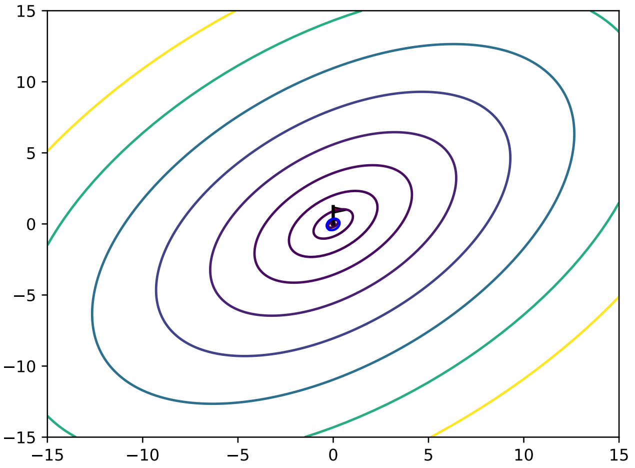

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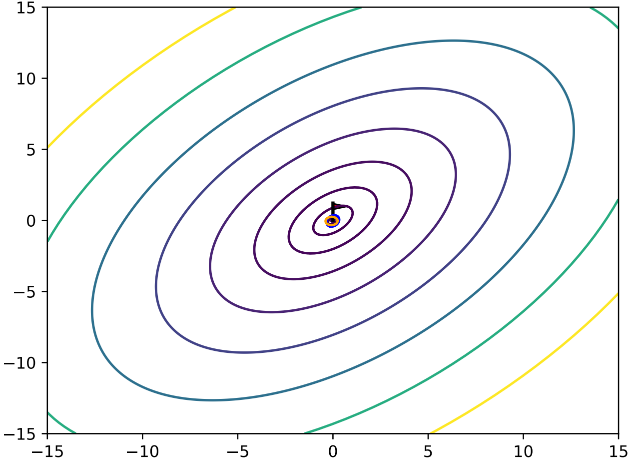
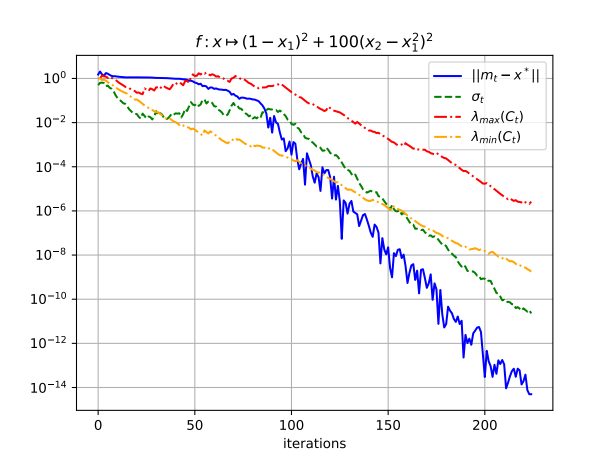
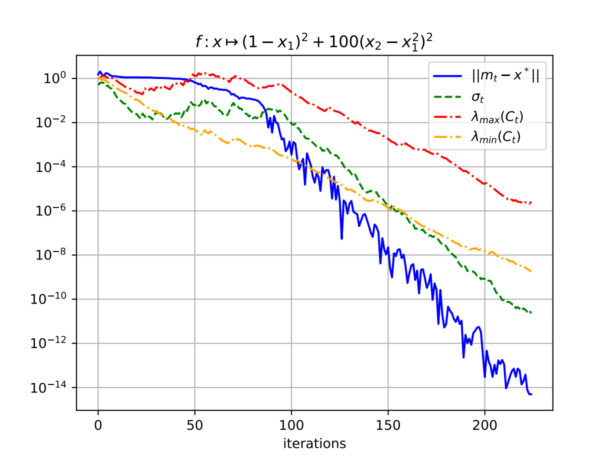


Linear convergence



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

Linear convergence



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

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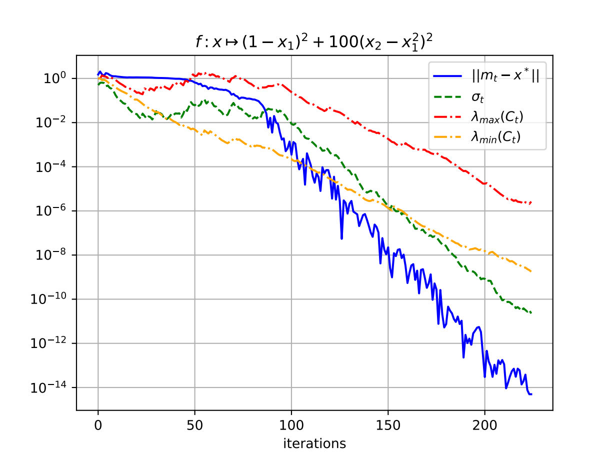

$$\log \frac{\|m_t - x^*\|}{\|m_0 - x^*\|} = -\mathrm{CR} \times t$$

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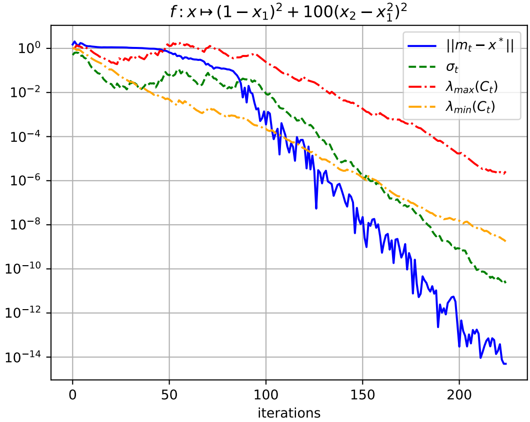

$$\frac{1}{t}\log\frac{\|m_t - x^*\|}{\|m_0 - x^*\|} = -\mathrm{CR}$$

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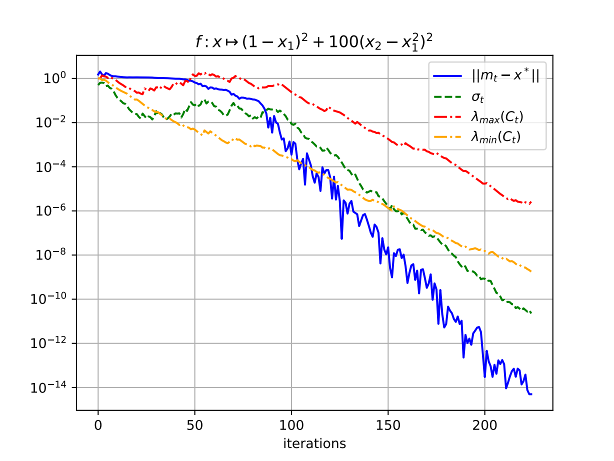

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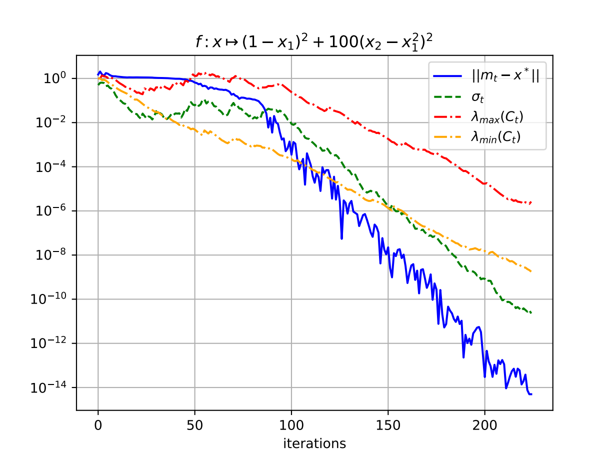

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CMA-ES : presentation

At each iteration $t \in \mathbb{N}$, given a **mean** m_t, a **stepsize** σ_t and a **covariance matrix** C_t :

1. Generate λ offspring $x_{t+1}^i \sim \mathcal{N}(m_t, \sigma_t^2 C_t)$ *independently*
2. Rank the x_{t+1}^i w.r.t. their f-values: $f\left(x_{t+1}^{1:\lambda}\right) \leqslant \cdots \leqslant f\left(x_{t+1}^{\lambda:\lambda}\right)$
3. Update the mean: $m_{t+1} = \sum w_i x_{t+1}^{i:\lambda}$

   The best offspring have the largest weights: $w_1 \geqslant w_2 \ldots$
4. Update the stepsize:
   Increase the stepsize if the path taken by the mean is larger than expected (assuming no selection)
5. Update the covariance matrix

$$C_{t+1} = (1-c)C_t + c\sum w_i \frac{(x_{t+1}^{i:\lambda} - m_t)(x_{t+1}^{i:\lambda} - m_t)^T}{\sigma_t^2}$$

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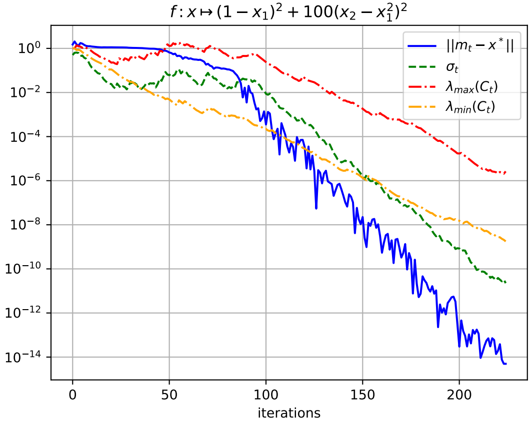

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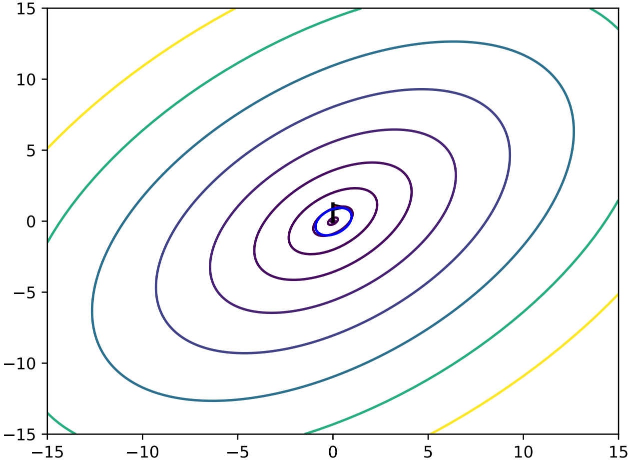

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Goal: proof of linear convergence and of the learning of the inverse Hessian

Analysis via Markov chains

Markov chains

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

$$\mathrm{Distribution}\left(\phi_{t+1} \mid \phi_0, \ldots, \phi_t\right) = \mathrm{Distribution}\left(\phi_{t+1} \mid \phi_t\right)$$

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  (π is a "fixed point" for $(\phi_t)_{t\in\mathbb{N}}$)
- The Markov chain is **ergodic** when it satisfies the following LLN

$$\lim_{T\to\infty} \frac{1}{T} \sum_{t=0}^{T-1} f\left(\phi_t\right) = \int f(x)\pi(dx).$$

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CMA-ES as a Markov chain

Consider the random sequence

$$(\underbrace{m_t}_{\text{mean}}, \overbrace{\sigma_t}^{\text{stepsize}}, \underbrace{C_t}_{\text{covariance matrix}})$$

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

Invariant measure for CMA-ES?

Suppose that $(m_t, \sigma_t, C_t)_{t\in\mathbb{N}}$ has an invariant measure π.

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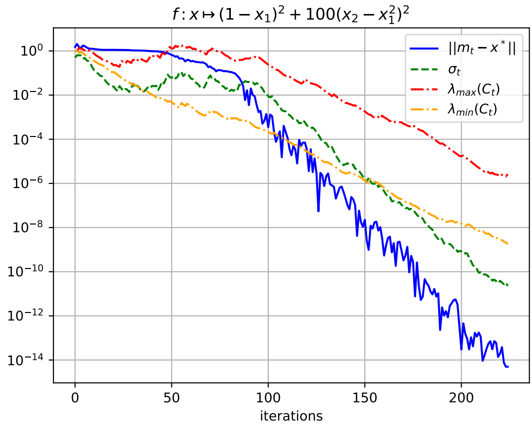
We do not progress towards the optimum anymore! The **existence of an invariant measure** seems to be **incompatible** with the **convergence** to the optimum.

Linear convergence



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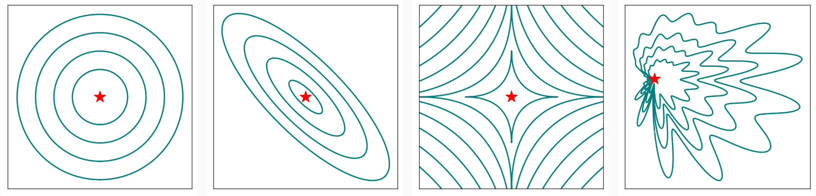
Scaling-invariant functions



Irreducibility of CMA-ES

A Markov chain $(\phi_t)_{t\in\mathbb{N}}$ is **irreducible** if all states are reachable in finite time with positive probability.

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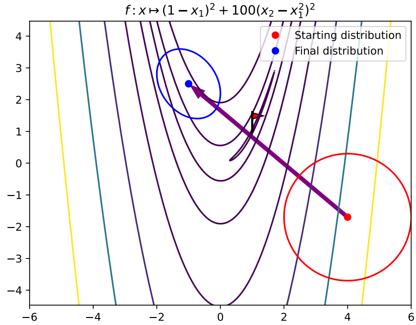

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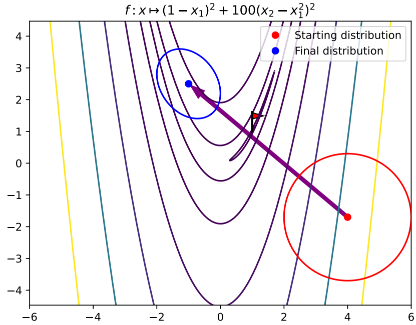

Given a starting and a final distributions, **can we reach the final distribution in finite time with positive probability?**

Theorem (Irreducibility of the normalized chain)

When minimizing a scaling-invariant function f with Lebesgue-negligible level sets, the sequence

$$\left(Z_t, \frac{C_t}{\lambda_{\min}(C_t)}\right)_{t\in\mathbb{N}}$$

defines a irreducible, aperiodic Markov chain, and compact sets are small sets.

Ergodicity of the normalized chain[2]

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is **ergodic** if

[2]Sean P. Meyn and Richard L. Tweedie. **Markov Chains and Stochastic Stability.** Springer Science & Business Media, Dec. 2012. ISBN: 978-1-4471-3267-7.

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The function V is called the **potential function** or the **drift function** or the **Lyapunov function**.

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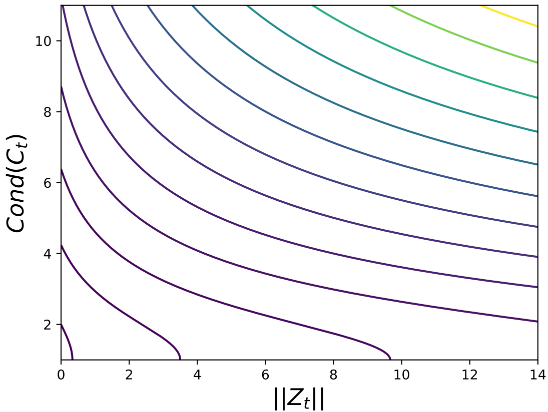

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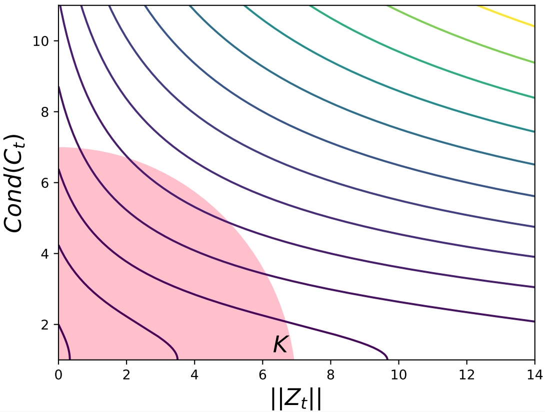

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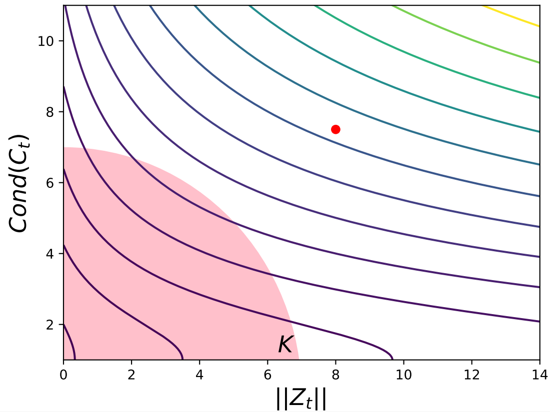

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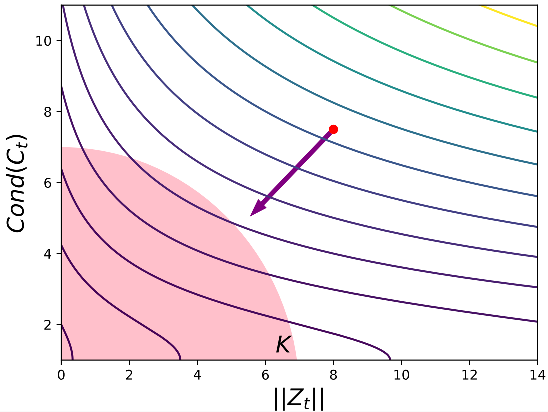

Theorem (Drift condition for the normalized chain)

When minimizing a spherical function $f: x \mapsto g\left(x^T x\right)$ $(g: \mathbb{R} \to \mathbb{R}$ *increasing), then the irreducible, aperiodic Markov chain* $(Z_t, C_t/\lambda_{\min}(C_t))_{t\in\mathbb{N}}$ *satisfies a Foster-Lyapunov condition with the potential defined by*

$$V(Z,C) = \sum_{k=1}^{d} \left\{ \frac{\lambda_k(C)}{\lambda_1(C)} |\langle v_k(C), Z\rangle|^2 \right\} + \beta \times \mathrm{Cond}(C)$$

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

Affine-Invariance

$$
\begin{array}{ccc}
(m_0, \sigma_0, C_0) & \xrightarrow{\min f(x)} & (m_1, \sigma_1, C_1) \\
\Psi \downarrow & & \uparrow \Psi^{-1} \\
(m_0', \sigma_0', C_0') & \xrightarrow{\min f(Bx + b)} & (m_1', \sigma_1', C_1')
\end{array}
$$

Proof of linear convergence

$$\frac{1}{T}\log\frac{\|m_T - x^*\|}{\|m_0 - x^*\|} \to -\mathrm{CR}?$$

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

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$$+ \frac{1}{2}\log\lambda_{\min}(C_{t+1}) - \log\|m_t - x^*\|$$

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$$\mathbb{E}\left[\frac{C_t}{\text{normalization}}\right] \underset{t\to\infty}{\longrightarrow} \text{constant} \times H^{-1}$$

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Thank you!