

Derivative Free Optimization class

AMS & Optimization Masters

On the connection between affine-invariance, convergence and learning second order information

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Motivation

CMA-ES: a widely used randomized DFO algorithm [Hansen et al. 2001-2006]
for non-convex, non-smooth, difficult black-box problems
parameter-free
6.5 + 54 millions downloads for two main Python codes

does not even use function value

yet observed to learn “second-order” information in particular on
 $f(x) = g((x - x^*)^\top H(x - x^*))$, $H \succ 0$, $g : \mathbb{R} \rightarrow \mathbb{R}$ strict. increasing
sometimes presented as (randomized) quasi-Newton

How is that even possible??

Objectives

uncover the simple and nice mathematical arguments behind this learning

→ illustrate proofs on quasi-Newton algorithms (BFGS)
simpler and illustrates the generality of the ideas

Disclaimer: results on quasi-Newton presented are not new nor impressive *stronger results exists*
yet we show that they stem from simple fundamental properties

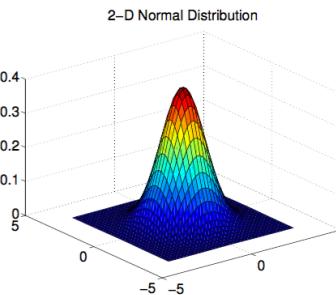
Adaptive Stochastic Optimization Algorithm

Given e.g. $\theta_t = (m_t, \sigma_t, C_t) \in \mathbb{R}^n \times \mathbb{R}_> \times \mathcal{S}_{++}^n$

- ① Sample candidate solutions $X_{t+1}^i \sim \mathcal{N}(m_t, \sigma_t^2 C_t)$, i.e.

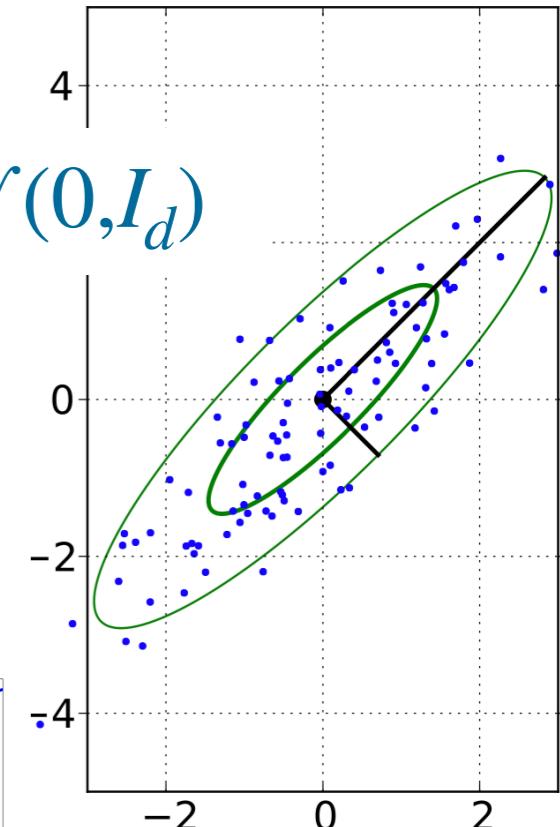
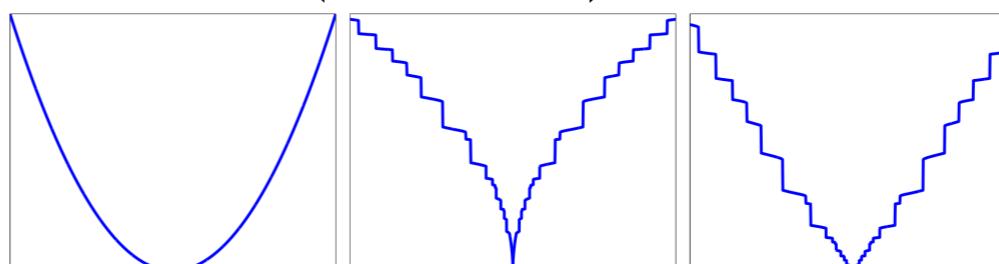
$$X_{t+1}^i = m_t + \sigma_t \sqrt{C_t} U_{t+1}^i, \quad i = 1, \dots, \lambda$$

$$\{U_t, t \geq 1\} \text{ i.i.d., } U_{t+1}^i \sim \mathcal{N}(0, I_d)$$



- ② Evaluate and rank candidate solutions

$$f(X_{t+1}^{s_{t+1}(1)}) \leq \dots \leq f(X_{t+1}^{s_{t+1}(\lambda)})$$



- ③ Update θ_t :

$$\theta_{t+1} = F \left(\theta_t, [U_{t+1}^{s_{t+1}(1)}, \dots, U_{t+1}^{s_{t+1}(\lambda)}] \right)$$

should drive m_t towards the optimum

CMA-ES - simplified setting $\theta_t = (m_t, \sigma_t, C_t) \in \mathbb{R}^n \times \mathbb{R}_> \times \mathcal{S}_{++}^n$

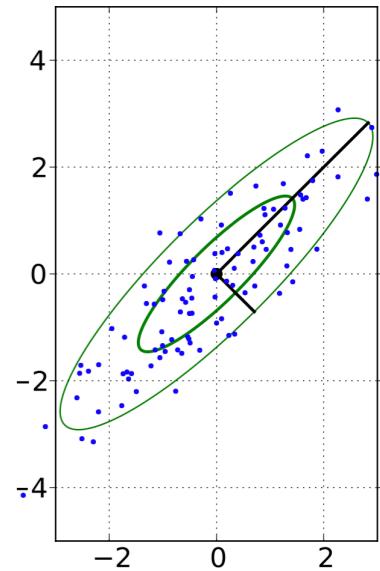
Sampling + ranking:

$$y_i \sim \mathcal{W}(0, C_t)$$

$$X_{t+1}^i = m_t + \sigma_t \sqrt{C_t} U_{t+1}^i \quad i = 1, \dots, \lambda$$

$$f\left(X_{t+1}^{s_{t+1}(1)}\right) \leq \dots \leq f\left(X_{t+1}^{s_{t+1}(\lambda)}\right)$$

$$\{U_t, t \geq 1\} \text{ i.i.d } U_{t+1}^i \sim \mathcal{N}(0, I_d)$$



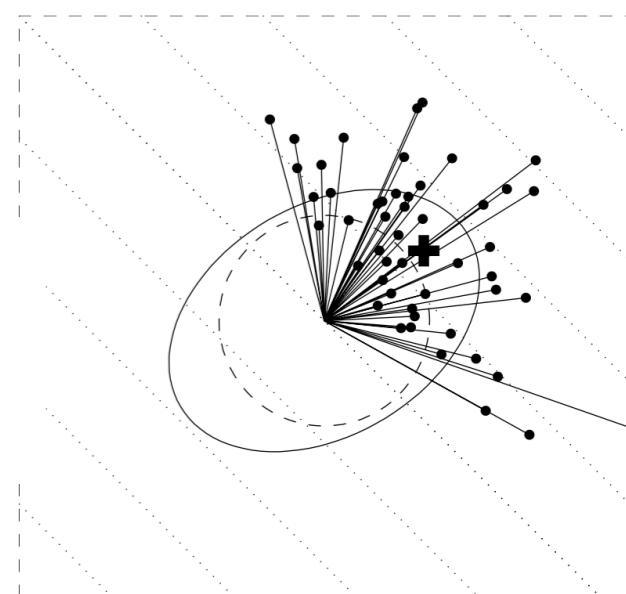
Update of θ_t :

$$m_{t+1} = \sum_{i=1}^{\mu} w_i X_{t+1}^{s_{t+1}(i)} = m_t + \sigma_t \sqrt{C_t} \sum_{i=1}^{\mu} w_i U_{t+1}^{s_{t+1}(i)}$$

$$\sigma_{t+1} = \sigma_t \exp \left(\frac{c_\sigma}{d_\sigma} \left[\frac{\sqrt{\mu_{\text{eff}}} \left\| \sum_{i=1}^{\mu} w_i U_{t+1}^{s_{t+1}(i)} \right\|}{E[\|\mathcal{N}(0, I_d)\|]} - 1 \right] \right)$$

$$C_{t+1} = (1 - c_\mu) C_t + c_\mu \sqrt{C_t} \underbrace{\left(\sum_{i=1}^{\mu} w_i U_{t+1}^{s_{t+1}(i)} [U_{t+1}^{s_{t+1}(i)}]^\top \right)}_{\text{rank } \mu \text{ update}} \sqrt{C_t}$$

$$\sum_{i=1}^{\mu} w_i = 1, \mu_{\text{eff}} = 1 / \sum w_i^2$$



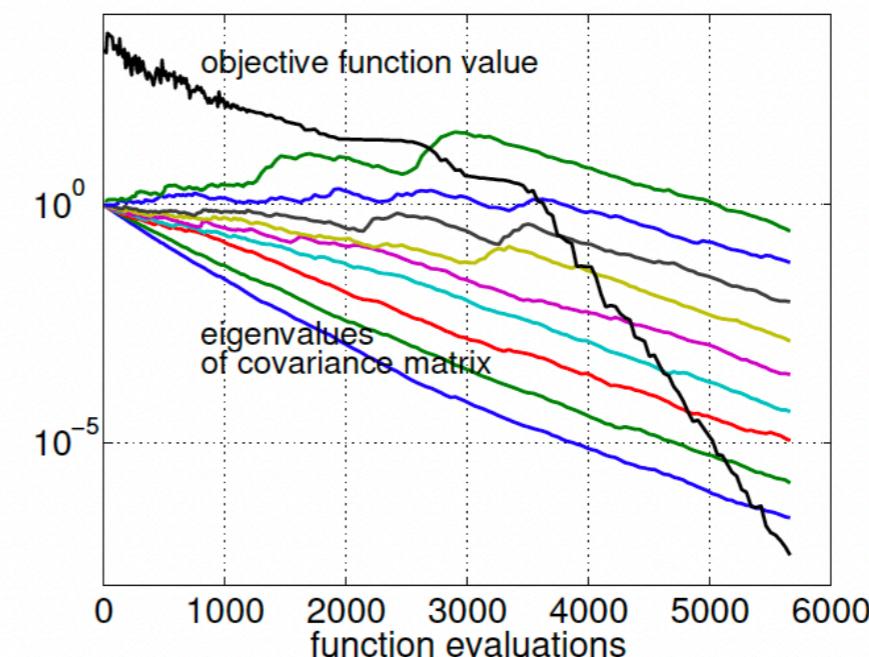
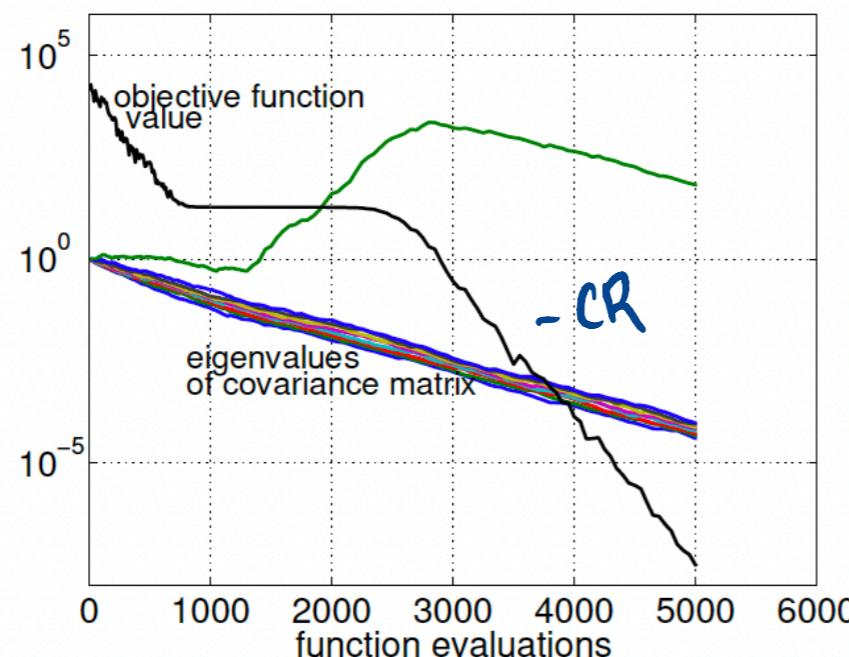
CMA-ES: Linear Convergence and Learning Inverse Hessian

For all $f(x) = g\left(\frac{1}{2}(x - x^*)^\top H(x - x^*)\right)$, with $g : \text{Im}(f) \rightarrow \mathbb{R}$ strict increasing, $H \succ 0$ (SDP)

$$\frac{1}{t} \ln \frac{\|m_t - x^*\|}{\|m_0 - x^*\|} \xrightarrow[t \rightarrow \infty]{} -\text{CR}$$

$$C_t \propto \alpha_t H^{-1} \text{ with } \alpha_t \rightarrow 0$$

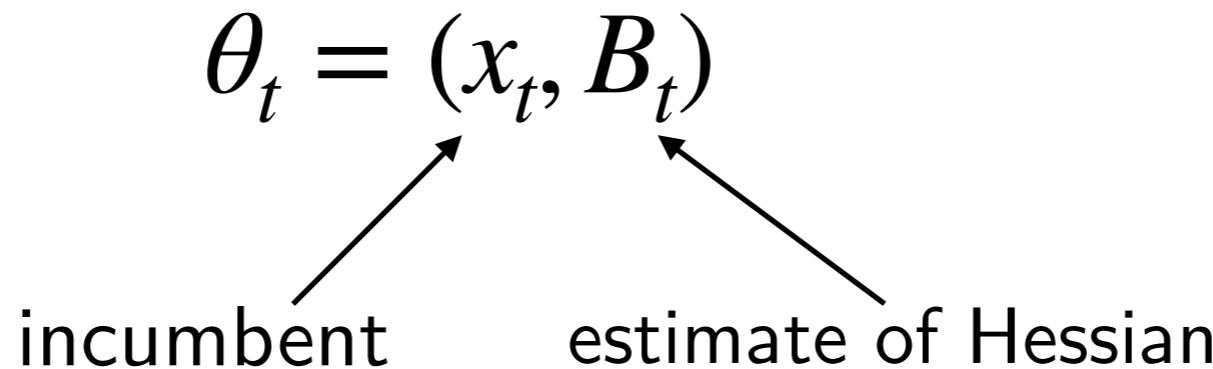
Empirical observations:



$$\text{Eig}(H) = (10^{-6}, 1, \dots, 1)$$

$$\text{Eig}(H) = (1, \dots, 10^{6\frac{i-1}{n-1}}, \dots, 10^6)$$

BFGS algorithm



- 1: initialize state $\theta_0 = (x_0, B_0) \in \mathbb{R}^n \times \mathcal{S}(n, \mathbb{R})$, $t = 0$
- 2: **while** stopping criterion not met **do**
- 3: compute $p_t = -B_t^{-1} \nabla f(x_t)$
- 4: compute step-size: $\alpha_t = \text{LineSearch}(x_t, p_t, f)$
- 5: move in the direction of p_t : $x_{t+1} = x_t + \alpha_t p_t = x_t - \alpha_t B_t^{-1} \nabla f(x_t)$
- 6: compute $s_t = \alpha_t p_t$
- 7: compute $y_t = \nabla f(x_{t+1}) - \nabla f(x_t)$
- 8: update estimate of Hessian: $B_{t+1} = B_t + \frac{y_t y_t^T}{y_t^T s_t} - \frac{B_t s_t s_t^T B_t}{s_t^T B_t s_t}$
- 9: $t = t + 1$
- 10: **end while**

On affine-invariance

Affine-invariance

on $x \mapsto f(x) \quad x_0 \quad x_1 \quad x_2 \quad \dots \quad x_t \quad \dots$

Affine-invariance

$$A \in \mathrm{GL}_n(\mathbb{R})$$

on $x \mapsto f(x)$ x_0 x_1 x_2 ... x_t ...

on $x' \mapsto f(Ax')$ x'_0 x'_1 x'_2 ... x'_t ...

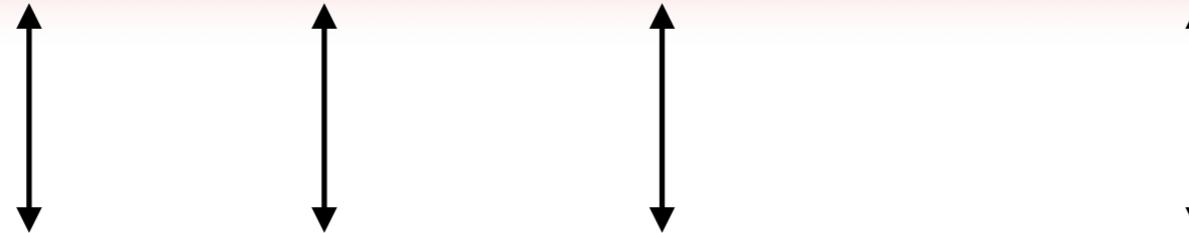
$f(Ax')$
because of translation
invariance

Affine-invariance

$$A \in \mathrm{GL}_n(\mathbb{R})$$

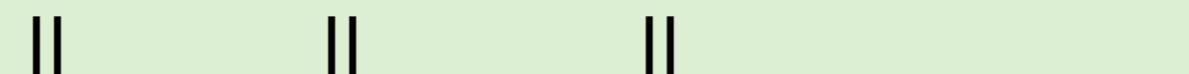
on $x \mapsto f(x)$

x_0 x_1 x_2 ... x_t ...



on $x' \mapsto f(Ax')$

x'_0 x'_1 x'_2 ... x'_t ...



$A^{-1}x_0$ $A^{-1}x_1$ $A^{-1}x_2$... $A^{-1}x_t$...

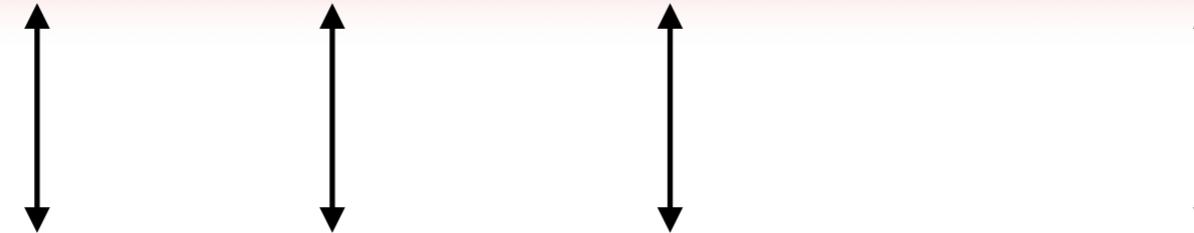
Affine-invariance

An algorithm is affine invariant if it produces the same trajectory when optimizing $f(x)$ or any $f(Ax')$ with $A \in \text{GL}_n(\mathbb{R})$

up to the change of variable: $x' = A^{-1}x$

on $x \mapsto f(x)$

$x_0 \quad x_1 \quad x_2 \quad \dots \quad x_t \quad \dots$



on $x' \mapsto f(Ax')$

$x'_0 \quad x'_1 \quad x'_2 \quad \dots \quad x'_t \quad \dots$

$\parallel \quad \parallel \quad \parallel \quad \parallel \quad \parallel$

$A^{-1}x_0 \quad A^{-1}x_1 \quad A^{-1}x_2 \quad \dots \quad A^{-1}x_t \quad \dots$

\parallel

$\Phi_A(x_0)$

Affine-invariance: commutative diagram

An algorithm is affine-invariant if for all $A \in \text{GL}_n(\mathbb{R})$, there exists Φ_A (a bijective change of state variables) s.t. the diagram commutes:

change of state variables

$$\begin{array}{ccc} x_t & \xrightarrow{x \mapsto f(x)} & x_{t+1} \\ \Phi_A \uparrow \downarrow \Phi_{A^{-1}} & & \Phi_A \uparrow \downarrow \Phi_{A^{-1}} \\ x'_t & \xrightarrow{x' \mapsto f(Ax')} & x'_{t+1} \end{array}$$

$$x'_t = \Phi_A(x_t) = A^{-1}x_t$$

Affine-invariance: commutative diagram

often state not reduced to incumbent solutions

example: BFGS where $\theta_t = (x_t, B_t)$

State for CMA-ES $\theta_t = (m_t, s_t, \mathbf{c}_t, \mathbf{p}_t^\sigma, \mathbf{p}_t^c)$

Affine-invariance: commutative diagram

often state not reduced to incumbent solutions

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$$\theta'_t = \Phi_A(\theta_t)$$

$$\theta_t = \Phi_{A^{-1}}(\theta'_t)$$

Affine-invariance: commutative diagram

Affine-invariance \Rightarrow rotational invariance

An algorithm is affine-invariant if for all $A \in \text{GL}_n(\mathbb{R})$, there exists a bijective change of state variables Φ_A s.t. the diagram commutes:

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Affine-invariance of BFGS

The BFGS algorithm (with affine-invariant step-size) satisfies for all $A \in GL(\mathbb{R}^n)$ the **commutative diagram**:

affine-invariant step-size: constant, exact line-search, ...

$$\begin{array}{ccc} (x_t, B_t) & \xrightarrow{x \mapsto f(x)} & (x_{t+1}, B_{t+1}) \\ \Phi_A \downarrow \quad \uparrow \Phi_{A^{-1}} & & \Phi_A \downarrow \quad \uparrow \Phi_{A^{-1}} \\ (x'_t, B'_t) & \xrightarrow{x' \mapsto f(Ax')} & (x'_{t+1}, B'_{t+1}) \end{array}$$

with $(x'_t, B'_t) = \Phi_A(x_t, B_t) := (A^{-1}x_t, A^\top B_t A)$

Exercice: prove that the BFGS algorithm is affine-invariant

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a Frechet differentiable objective function. Consider the BFGS algorithm defined as

- 1: initialize state $\theta_0 = (x_0, B_0) \in \mathbb{R}^n \times \mathcal{S}_{n,>}(\mathbb{R})$, $k = 0$
- 2: **while** stopping criterion not met **do**
- 3: compute $d_k = -B_k^{-1} \nabla f(x_k)$
- 4: compute step-size: $\alpha_k = \text{LineSearch}(x_k, d_k, f)$
- 5: move in the direction of d_k : $x_{k+1} = x_k + \alpha_k d_k$
- 6: compute $s_k = \alpha_k d_k$
- 7: compute $y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$
- 8: update estimate of Hessian: $B_{k+1} = B_k + \frac{y_k y_k^T}{y_k^T s_k} - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k}$
- 9: $k = k + 1$
- 10: **end while**

We will assume for the sake of simplicity that the step-size $\alpha_k = \alpha$ is constant.

Let $A \in \mathbb{R}^{n \times n}$ be an invertible matrix and let $x_0 \in \mathbb{R}^n$ and $B_0 \in \mathbb{R}^{n \times n}$ with $B_0 \succ 0$. Consider the sequence $(x_k, B_k)_{k \geq 1}$ generated by the BFGS algorithm optimizing $x \mapsto f(x)$. Let $(x'_0, B'_0) = (A^{-1}x_0, A^T B_0 A)$ and consider $(x'_k, B'_k)_{k \geq 1}$ the sequence of states of the BFGS algorithm optimizing $g(x') = f(Ax')$ and initialized in (x'_0, B'_0) .

Prove that for all $k \geq 1$, $(x'_k, B'_k) = (A^{-1}x_k, A^T B_k A)$, i.e. that the BFGS algorithm is affine-invariant.

(See separate correction)

Assume optimal step-size
 $\alpha_k = \arg \min \alpha f(x_k + \alpha d_k)$

Affine-invariance of CMA-ES

The CMA-ES algorithm is affine-invariant: for all $A \in GL(\mathbb{R}^n)$ the following commutative diagram holds:

$$\begin{array}{ccc} (m_t, C_t, \sigma_t) & \xrightarrow{x \mapsto f(x)} & (m_{t+1}, C_{t+1}, \sigma_{t+1}) \\ \Phi_A \uparrow \downarrow \Phi_{A^{-1}} & & \Phi_A \uparrow \downarrow \Phi_{A^{-1}} \\ (m'_t, C'_t, \sigma'_t) & \xrightarrow{x' \mapsto f(Ax')} & (m'_{t+1}, C'_{t+1}, \sigma'_{t+1}) \end{array}$$

$$\Phi_A(m_t, C_t, \sigma_t) = (A^{-1}m_t, A^{-1}C_t(A^{-1})^\top, \sigma_t)$$

How affine-invariance and stability imply
learning a matrix proportional to Hessian
on convex-quadratic functions

Consequence of rotational invariance + stability

Lemma: Consider a rotational invariant function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ [such that $f(Rx) = f(x)$ for all $R \in O_n(\mathbb{R})$]

f is a radial function: $f(x) = g(\|x\|)$

example: $f(x) = \gamma x^\top x = \gamma \|x\|^2$

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[stability] Suppose that $\exists! (x^*, B^*) \in \mathbb{R}^n \times \mathcal{S}_>$ such that BFGS converges globally to (x^*, B^*) .

for all (x_0, B_0) , $\lim_{t \rightarrow \infty} (x_t, B_t) = (x^, B^*)$*

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Then for all R

$$\begin{aligned} Rx^* = x^* &\Rightarrow x^* = 0 \\ R^\top B^* R = B^* &\Rightarrow B^* = \alpha I_d \end{aligned}$$

Corollary: If $f(x) = \frac{1}{2} \|x\|^2$, $\lim_{t \rightarrow \infty} B_t = \alpha \nabla^2 f$.

Proof: uses only rotational invariance and stability

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Let $(x_t, B_t) \rightarrow (x^*, B^*)$. Let $R \in O_n(\mathbb{R})$

$$(x_t, B_t) \xrightarrow{x \mapsto f(x)} (x_{t+1}, B_{t+1}) \xrightarrow{t \rightarrow \infty} (x^*, B^*)$$

Proof: uses only rotational invariance and stability

Let $(x_t, B_t) \rightarrow (x^*, B^*)$. Let $R \in O_n(\mathbb{R})$

$$\begin{array}{ccccc} (x_t, B_t) & \xrightarrow{x \mapsto f(x)} & (x_{t+1}, B_{t+1}) & \xrightarrow{t \rightarrow \infty} & (x^*, B^*) \\ \downarrow \Phi_R & & \downarrow & & \\ (x'_t, B'_t) & \xrightarrow{x' \mapsto f(Rx')} & (x'_{t+1}, B'_{t+1}) & & \end{array}$$

The diagram commutes with: $(x'_t, B'_t) = \Phi_R(x_t, B_t) = (R^\top x_t, R^\top B_t R)$

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Since f is rotational invariant $f(Rx') = f(x')$ so (x'_t, B'_t) optimizes f also.

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Hence by stability $(x'_t, B'_t) = (R^\top x_t, R^\top B_t R) \rightarrow (x^*, B^*)$

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$$\begin{array}{ccc}
 & \downarrow & \\
 (R^\top x^*, R^\top B^* R) & \not\equiv & \text{by unicity}
 \end{array}$$

Proof: uses only rotational invariance and stability

Let $(x_t, B_t) \rightarrow (x^*, B^*)$. Let $R \in O_n(\mathbb{R})$

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 (x_t, B_t) & \xrightarrow{x \mapsto f(x)} & (x_{t+1}, B_{t+1}) & \xrightarrow{t \rightarrow \infty} & (x^*, B^*) \\
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$$\begin{array}{ccc}
 & \downarrow & \\
 (R^\top x^*, R^\top B^* R) & \xrightarrow[\text{by unicity}]{} &
 \end{array}$$

Then for all R

$$Rx^* = x^*$$

$$R^\top B^* R = B^*$$

Proof: uses only rotational invariance and stability

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 \end{array}$$

Then for all R

$$Rx^* = x^* \Rightarrow x^* = 0$$

$$R^\top B^* R = B^* \Rightarrow B^* = \alpha I_d$$

Consequence of affine-invariance + stability

Lemma: Consider $h(x') = f(H^{1/2}x')$ with f rotational invariant, $H \succ 0$.

example: $h(x) = \frac{1}{2}\gamma x^\top H x, H \succ 0$

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Then on h :

$$\lim_{t \rightarrow \infty} x'_t = 0$$

$$\lim_{t \rightarrow \infty} B'_t = \alpha H.$$

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Then on h :

$$\lim_{t \rightarrow \infty} x'_t = 0$$

$$\lim_{t \rightarrow \infty} B'_t = \alpha H.$$

Corollary: If $h(x') = \frac{1}{2}x'^\top H x', H \succ 0$, $\lim_{t \rightarrow \infty} B'_t = \alpha \nabla^2 f(x)$.

Proof: uses only affine-invariance and stability

Consider (x'_t, B'_t) optimizing h .

$$(x'_t, B'_t) \xrightarrow{x' \mapsto h(x') = f(H^{1/2}x')} (x'_{t+1}, B'_{t+1})$$

Proof: uses only affine-invariance and stability

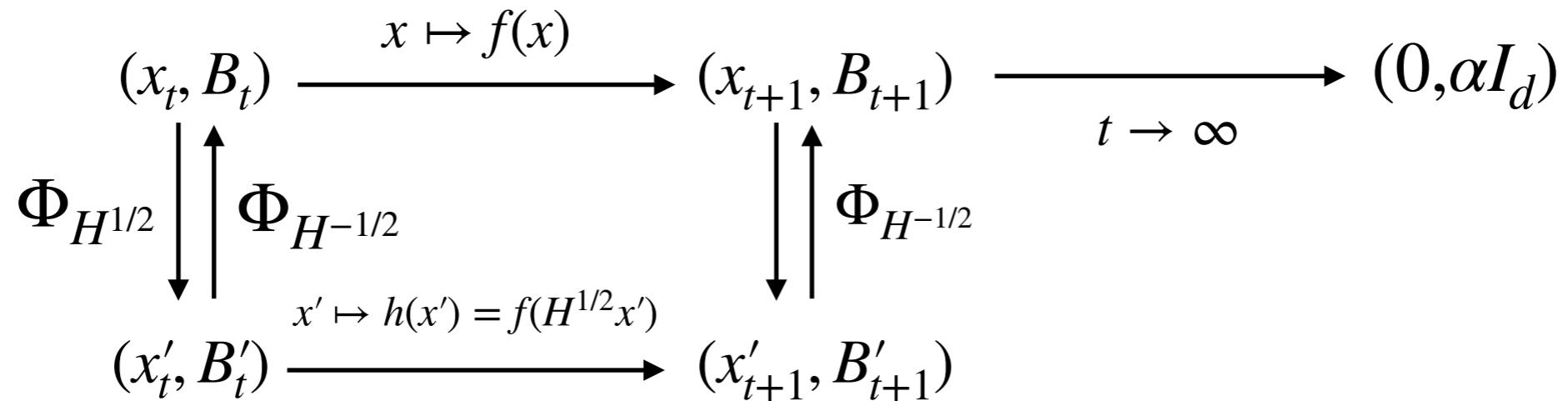
Consider (x'_t, B'_t) optimizing h .

$$\begin{array}{ccc} (x_t, B_t) & \xrightarrow{x \mapsto f(x)} & (x_{t+1}, B_{t+1}) \\ \Phi_{H^{1/2}} \downarrow \uparrow \Phi_{H^{-1/2}} & & \downarrow \uparrow \Phi_{H^{-1/2}} \\ (x'_t, B'_t) & \xrightarrow{x' \mapsto h(x') = f(H^{1/2}x')} & (x'_{t+1}, B'_{t+1}) \end{array}$$

By affine-invariance $(x_t, B_t) = \Phi_{H^{-1/2}}(x'_t, B'_t) = (H^{1/2}x'_t, H^{-1/2}B'_t H^{-1/2})$ optimizes f .

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By stability on f , then $(x_t, B_t) \rightarrow (0, \alpha I_d)$, such that:

$$\lim_{t \rightarrow \infty} x'_t = H^{-1/2}0 = 0$$

$$\lim_{t \rightarrow \infty} B'_t = \alpha H^{1/2} I_d H^{1/2} = \alpha H.$$

Recap

learning Hessian and convergence to the optimum on convex-quadratic implied from:

- ① affine-invariance
- ② stability (convergence to unique point from any starting point)

The same two ingredients and proof ideas applies to CMA-ES to imply:

learning of inverse-Hessian by the covariance matrix on
 $g((x - x^{\star})^{\top} H(x - x^{\star})), H \succ 0$

*quite tricky to prove stability in the CMA-ES case
[see PhD thesis Armand Gissler]*

Thank you !