Natural Evolution Strategies for Direct Search

PGMO-COPI 2014 Recent Advances on Continuous Randomized black-box optimization

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Tobias Glasmachers

Institut für Neuroinformatik Ruhr-Universität Bochum, Germany



Introduction

• Minimize $f : \mathbb{R}^d \to \mathbb{R}$.

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Don't ever rely on function values, only comparisons f(x) < f(x'), e.g., for ranking.</p>

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- 2 evaluate f(x) black box, most of the computation time
- So compare (rank) against other solutions: f(x) < f(x')?

Introduction: Challenges

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- black-box constraints (possibly non-smooth, ...)

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Evolution Strategies

input $m \in \mathbb{R}^d$, $\sigma > 0$, $C(= I) \in \mathbb{R}^{d \times d}$ loop sample "offspring" $x_1, \ldots, x_\lambda \sim \mathcal{N}(m, \sigma^2 C)$

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randomized

- population-based
- rank-based (function-value free)
- step size control
- metric learning (covariance matrix adaptation, CMA)

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Efficient optimization of ill-conditioned problems, similar to (quasi) Newton methods.

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- For multi-variate Gaussians:

$$\Theta = \mathbb{R}^{d} \times \mathcal{P}_{d}$$
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More flexible choice:

$$W_f(\theta) = \mathbb{E}_{x \sim P_{\theta}} \Big[w \big(f(x) \big) \Big]$$

with monotonic weight function $w : \mathbb{R} \to \mathbb{R}$.

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• "log-likelohood trick":

$$abla_{ heta} W_f(heta) =
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$$= \mathbb{E}_{x \sim P_{ heta}} \Big[
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- Optimization: follow inverse flow curves t → φ^{-t}(θ) from θ into (local) minimum of W_f.

• Black-box setting: expectation

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- Yields natural gradient MC approximation

$$ilde{G}(heta) = ig(\mathcal{I}(heta)ig)^{-1}\cdot G(heta)$$
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- SNGD algorithm invariant in first order approximation due to Euler steps.

• Stochastic Natural Gradient Descent (SNGD) update rule:

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Ollivier et al. Information-Geometric Optimization Algorithms: A Unifying Picture via Invariance Principles. *arXiv:1106.3708*, 2011.

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- NES approach: optimization of expected objective value with Gaussian distributions.
- Offspring x₁,..., x_λ act as MC sample for the estimation of G(θ).
- Closed form Fisher tensor for $\mathcal{N}(m, C)$:

$$\mathcal{I}_{i,j}(\theta) = \frac{\partial m^{T}}{\partial \theta_{i}} C^{-1} \frac{\partial m}{\partial \theta_{j}} + \frac{1}{2} \operatorname{tr} \left(C^{-1} \frac{\partial C}{\partial \theta_{i}} C^{-1} \frac{\partial C}{\partial \theta_{j}} \right)$$

NES algorithm

input
$$heta \in \Theta$$
, $\lambda \in \mathbb{N}$, $\eta > 0$
loop

sample
$$x_1, \ldots, x_\lambda \sim P_\theta$$

evaluate $f(x_1), \ldots, f(x_\lambda)$
 $G(\theta) \leftarrow \frac{1}{\lambda} \sum_{i=1}^{\lambda} \nabla_\theta \log (p_\theta(x_i)) \cdot f(x_i)$
 $\tilde{G}(\theta) \leftarrow (\mathcal{I}(\theta))^{-1} \cdot G(\theta)$
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Wierstra et al. Natural Evolution Strategies. CEC, 2008 and JMLR, 2014.
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- Sample ranks are *f*-quantile estimators, hence utility values can be represented as w(f(x_i)) with special weight function w = w_θ based on *f*-quantiles under current distribution P_θ.
- This turns NES into a function value free algorithm.
- Benefits:
 - invariance under monotonic transformations of objective values
 - linear convergence on scale invariant problems.

xNES (exponential NES) algorithm

input $(m, A) \in \Theta$, $\lambda \in \mathbb{N}$, $\eta_m, \eta_A > 0$ loop

sample
$$z_1, \ldots, z_{\lambda} \sim \mathcal{N}(0, I)$$

transform $x_k, \ldots, x_{\lambda} \leftarrow Az_k + m$
evaluate $f(x_1), \ldots, f(x_{\lambda})$
 $\tilde{G}_m(\theta) \leftarrow \frac{1}{\lambda} \sum_{i=1}^{\lambda} w(f(x_i)) \cdot z_i$
 $\tilde{G}_C(\theta) \leftarrow \frac{1}{\lambda} \sum_{i=1}^{\lambda} w(f(x_i)) \cdot \frac{1}{2}(z_i z_i^T - I)$
 $m \leftarrow m - \eta_m \cdot A \cdot \tilde{G}_m(\theta)$
 $A \leftarrow A \cdot \exp\left(-\eta_A \cdot \frac{1}{2}\tilde{G}_C(\theta)\right)$

until stopping criterion met

Glasmachers et al. Exponential Natural Evolution Strategies. GECCO, 2010.

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 - metric learning: adaptation of C.
- SNGD has only a single mechanism.
- Astonishing insight: all (most) parameters can be updated with a single mechanism.

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Akimoto et al. Bidirectional relation between CMA evolution strategies and natural evolution strategies. PPSN 2010.

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- This is insightful: it means that CMA-ES is (essentially) a SNGD algorithm.



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- The parameter space is equipped with the non-Euclidean information geometry of the corresponding statistical manifold of search distributions.
- SNGD on a stochastically relaxed problem results in a direct search algorithm: the Natural-gradient Evolution Strategy (NES) algorithm.
- The SNGD parameter update is by no means restricted to Gaussian distributions. It is a general construction template for update equations of continuous distribution parameters.

Thank you! Questions?