Stochastic Search using the Natural Gradient

Efficient Natural Evolution Strategies (eNES)

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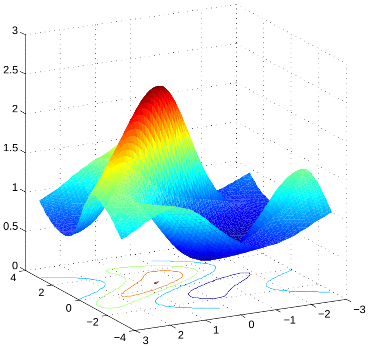
June 17th, 2009

Blackbox Optimization

Goal: Maximizing some unknown 'fitness' function $f(\mathbf{z})$, $\mathbf{z} \in \mathbb{R}^d$.



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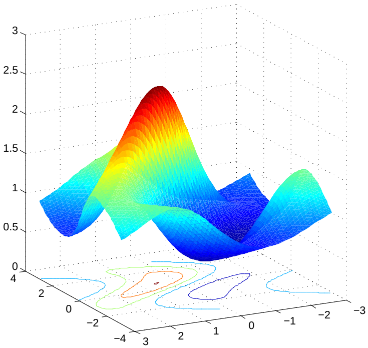

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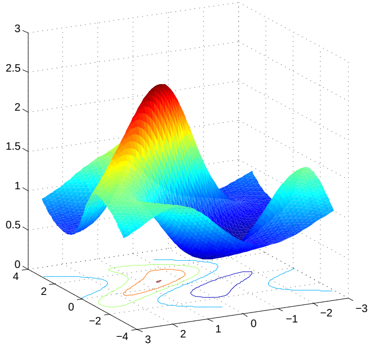

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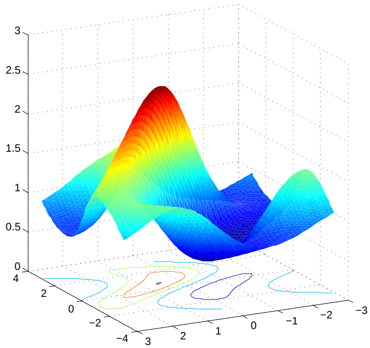

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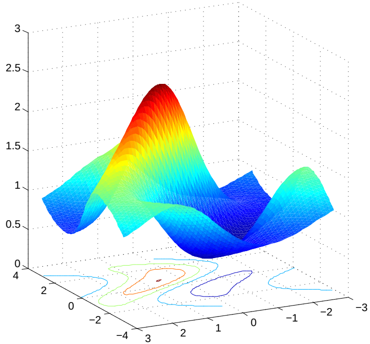

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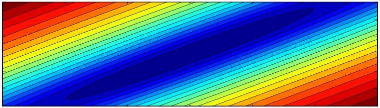

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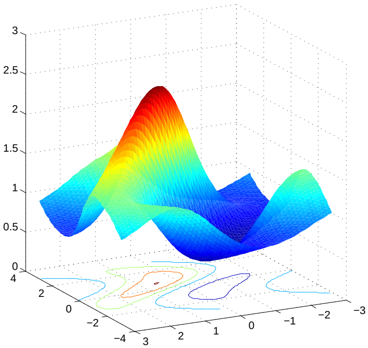

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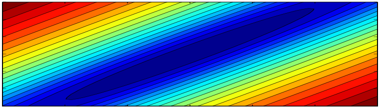

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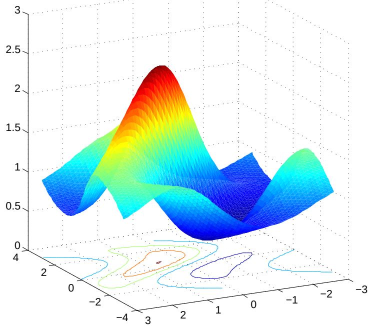

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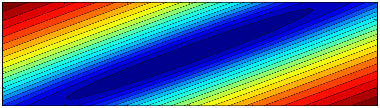

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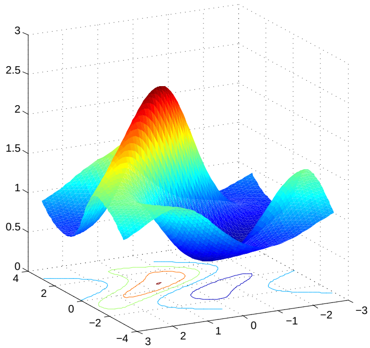

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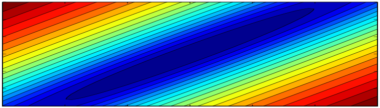

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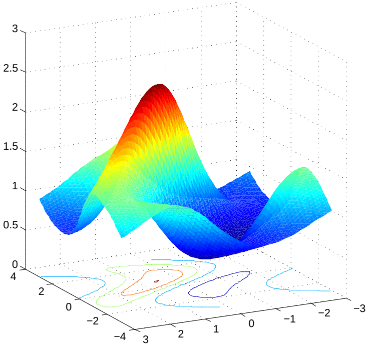

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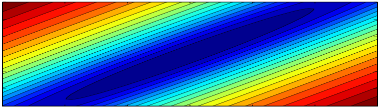

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Powerful methods are required to solve such problems.

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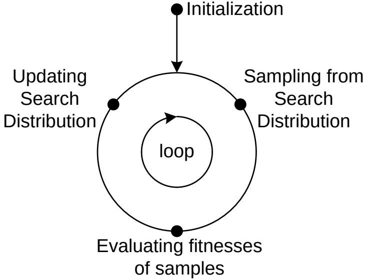

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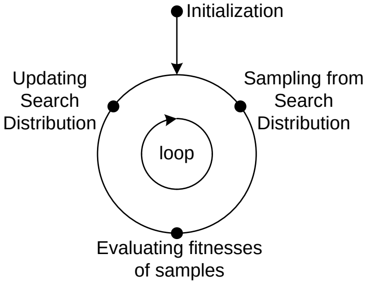

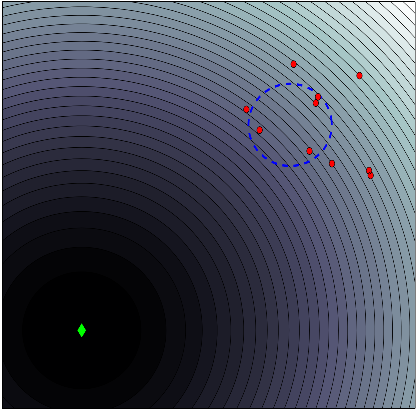

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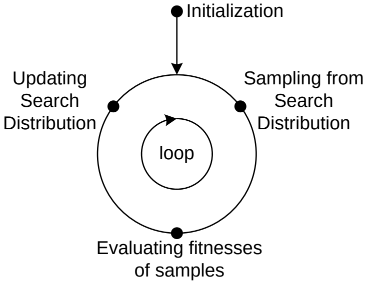

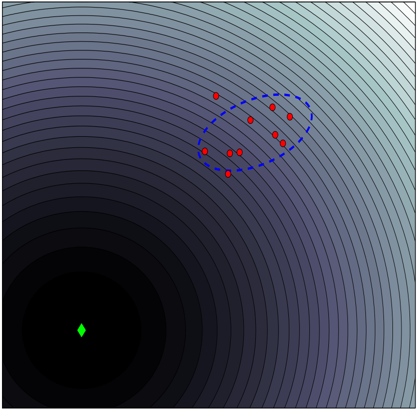

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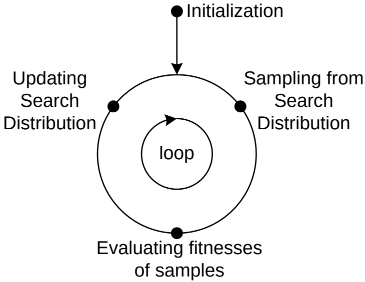

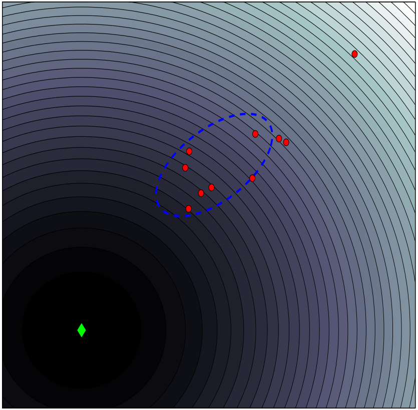

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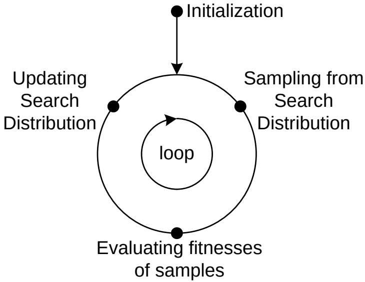

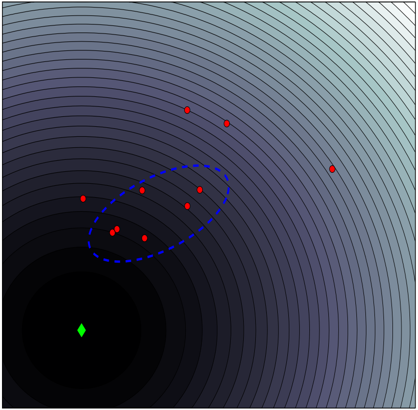

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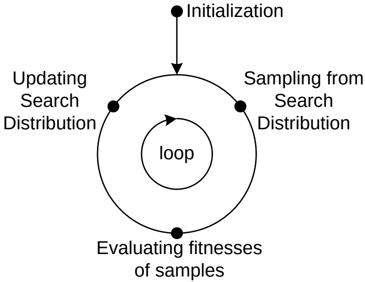

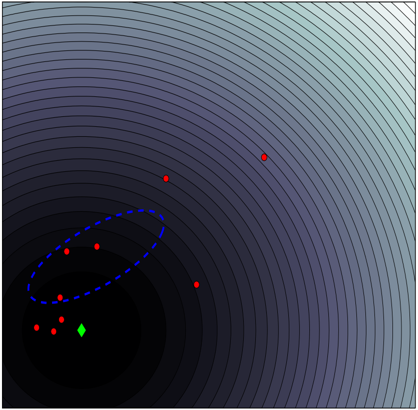

Stochastic Gradient Ascent

Let $p\left(\cdot|\theta\right)$ be the search distribution. We want to update θ towards better expected fitness:

$$J\left(\theta\right) = \mathbb{E}\left[f|\theta\right] = \int f\left(\mathbf{z}\right) p\left(\mathbf{z}|\theta\right) d\mathbf{z}.$$

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- We can compute the 'vanilla' gradient as

$$\begin{aligned}\nabla_\theta J(\theta) &= \int f(\mathbf{z})\, \nabla_\theta p(\mathbf{z}|\theta)\, d\mathbf{z} \\ &= \int f(\mathbf{z})\, \frac{p(\mathbf{z}|\theta)}{p(\mathbf{z}|\theta)} \nabla_\theta p(\mathbf{z}|\theta)\, d\mathbf{z} \quad \text{(log-likelihood trick)} \\ &= \mathbb{E}\left[f(\mathbf{z})\, \nabla_\theta \log p(\mathbf{z}|\theta)\, |\theta\right].\end{aligned}$$

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- Using the Monte-Carlo estimation

$$\begin{aligned}\nabla_\theta J(\theta) &= \mathbb{E}\left[f(\mathbf{z})\,\nabla_\theta \log p(\mathbf{z}|\theta)\,|\theta\right] \\ &\simeq \frac{1}{n}\sum_{i=1}^{n} f(\mathbf{z}_i)\,\nabla_\theta \log p(\mathbf{z}_i|\theta) = \frac{1}{n}\mathbf{G}\mathbf{f},\end{aligned}$$

with

$$\mathbf{G} = \left[\nabla_\theta \log p(\mathbf{z}_1|\theta) \ldots \nabla_\theta \log p(\mathbf{z}_n|\theta)\right],$$

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Now the problem is to compute $\nabla_\theta \log p(\mathbf{z}|\theta)$. A closed form derivation can be obtained if $p(\mathbf{z}|\theta)$ is a Gaussian distribution.

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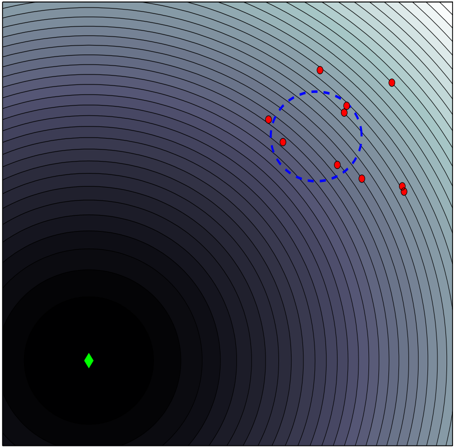

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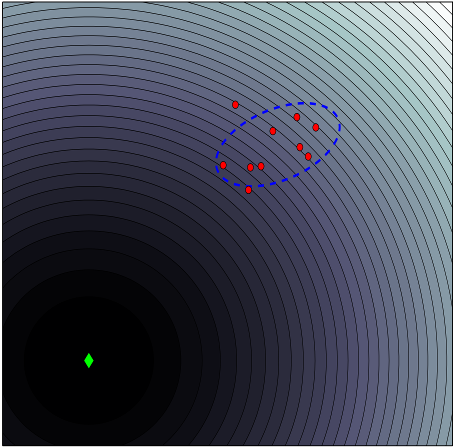

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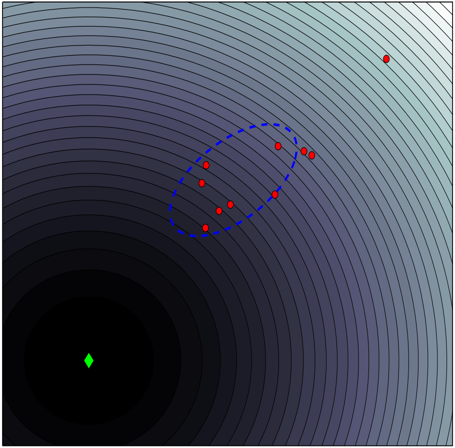

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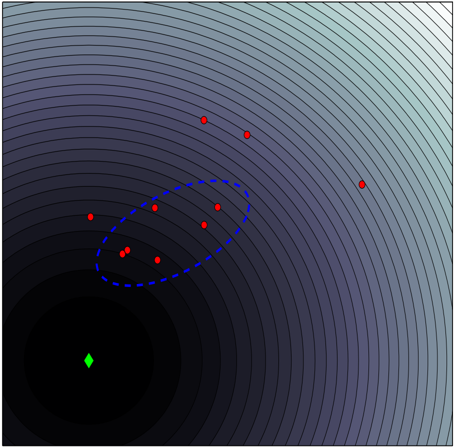

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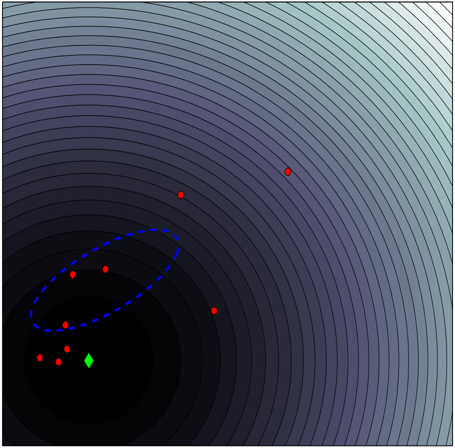

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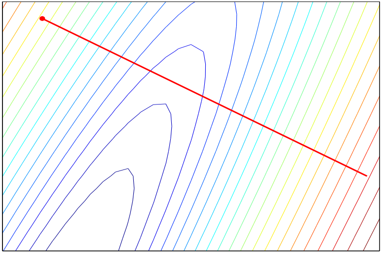

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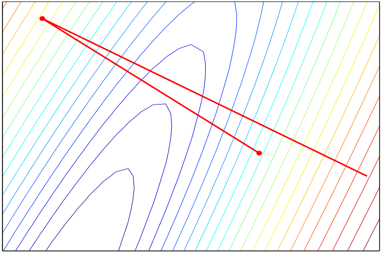

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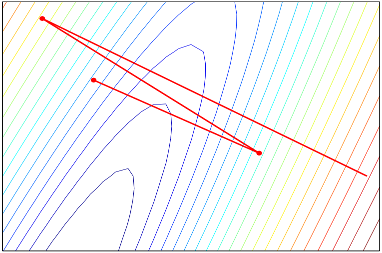

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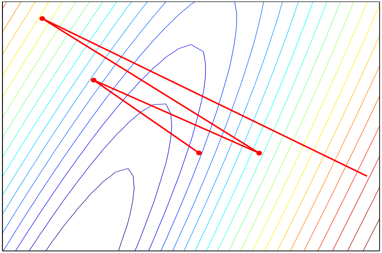

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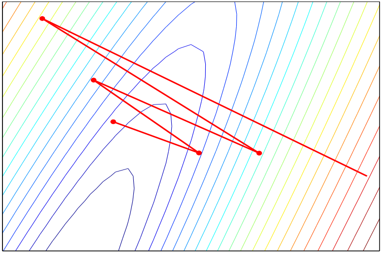

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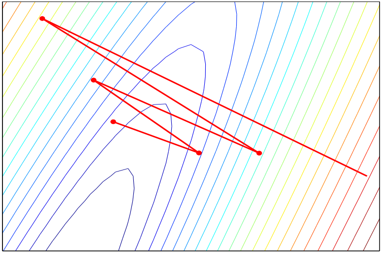

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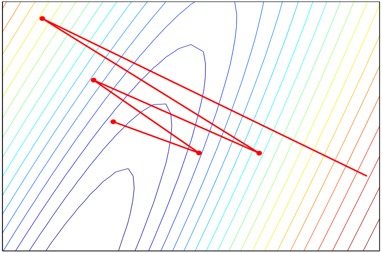

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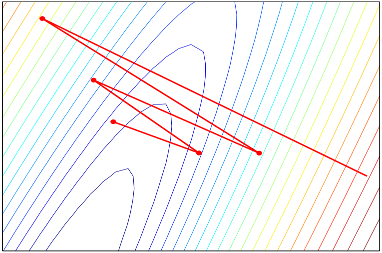

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  - Re-weight gradient elements according to their uncertainties, resp.

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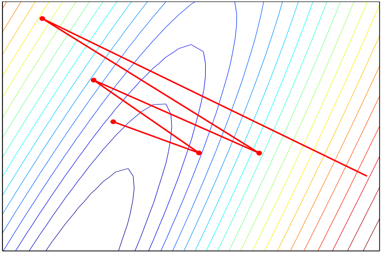

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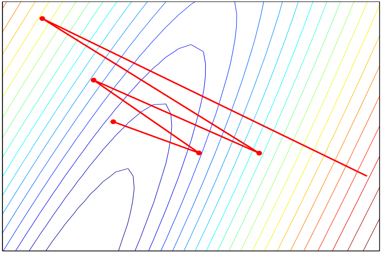

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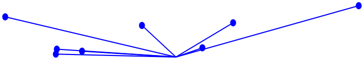

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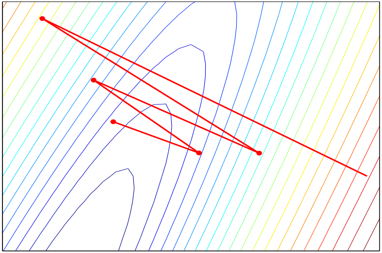

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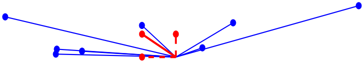

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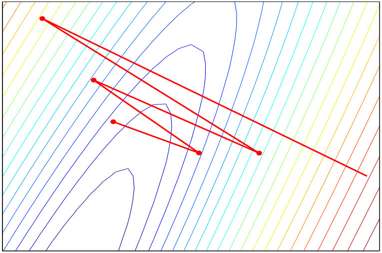

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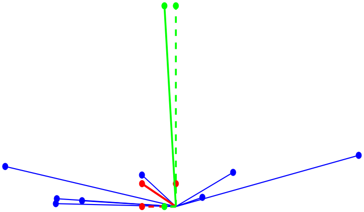

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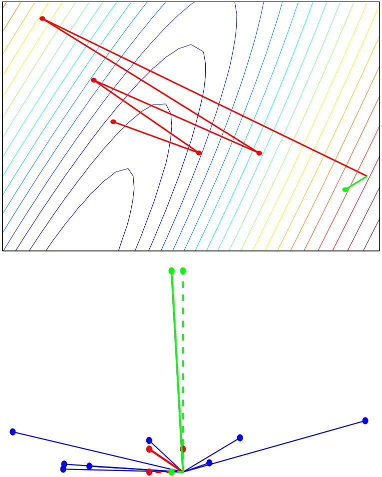

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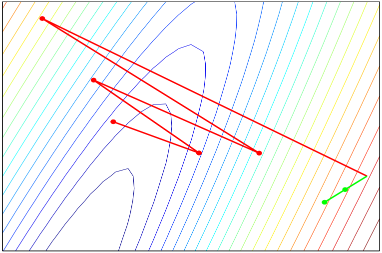

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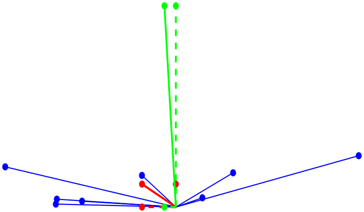

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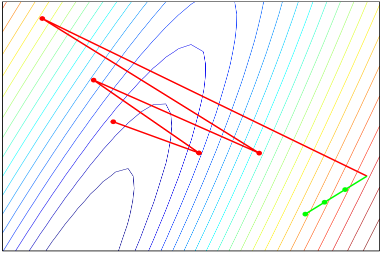

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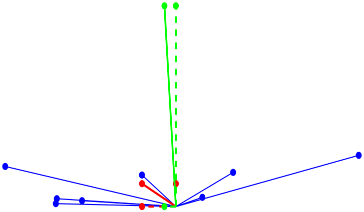

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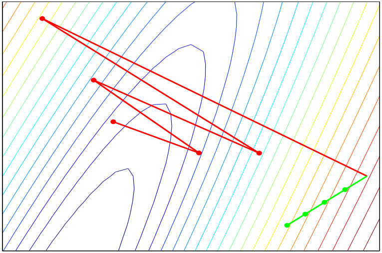

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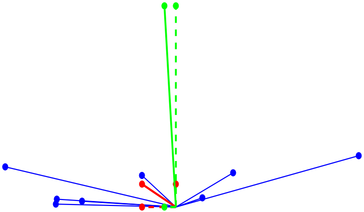

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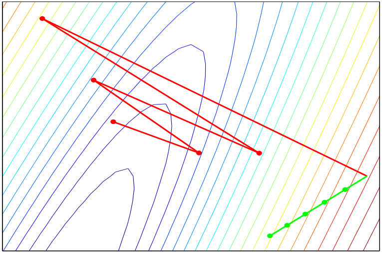

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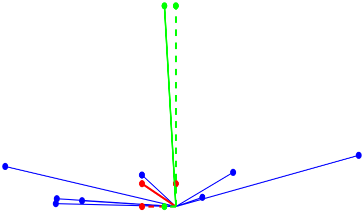

Formulation of Natural Gradient

Assume the distance between two adjacent distributions $p(\cdot|\theta)$ and $p(\cdot|\theta + \delta\theta)$ is defined by their KL divergence. The natural gradient $\tilde{\nabla}_\theta J(\theta)$ is given by the necessary condition

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- If $\mathbf{F}$ is invertable, we can compute the (estimated) natural gradient as

$$\tilde{\nabla}_\theta J\left(\theta\right) = \mathbf{F}^{-}\nabla_\theta J\left(\theta\right),\ \tilde{\nabla}^s_\theta J\left(\theta\right) = \mathbf{F}^{-}\nabla^s_\theta J\left(\theta\right).$$

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  - The FIM suggest a natural grouping of elements in θ. Groups are orthogonal with each other.

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    - This special form permits a iterative algorithm to compute $\mathbf{F}_k^{-}$ from $\mathbf{F}_{k+1}^{-}$ with complexity $O\left(k^2\right)$.

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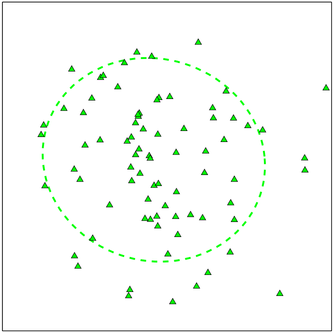

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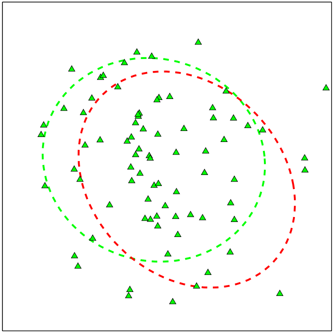

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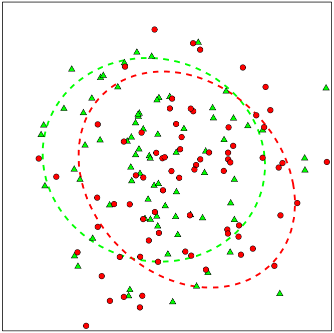

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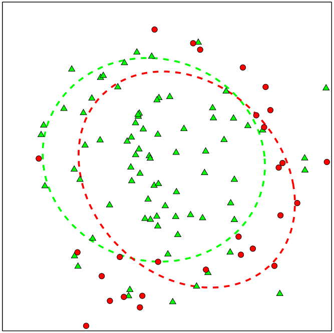

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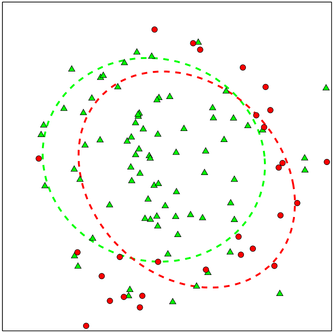

Reusing samples: fewer fitness evaluations.

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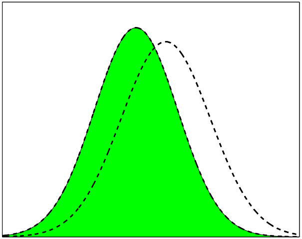

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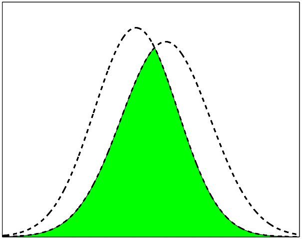

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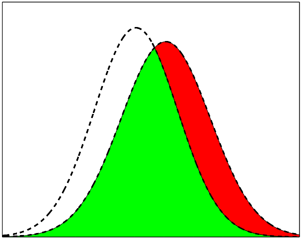

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A typical problem with the Monte-Carlo gradient estimation is that the variance is too big. The *fitness baseline* is introduced to reduce the variance.

$$\begin{aligned}\nabla_\theta J &= \nabla_\theta \int f(\mathbf{z})\, p(\mathbf{z}|\theta)\, d\mathbf{z} - \underbrace{\nabla_\theta \int b p(\mathbf{z}|\theta)\, d\mathbf{z}}_{=0} \\ &= \nabla_\theta \int [f(\mathbf{z}) - b]\, p(\mathbf{z}|\theta)\, d\mathbf{z},\end{aligned}$$

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- But it affects the *variance* of the estimation: For natural gradient

$$\mathbb{V}\left[\tilde{\nabla}_\theta J(\theta)\right] \propto b^2 \mathbb{E}\left[\mathbf{u}^\top \mathbf{u}\right] - 2b\mathbb{E}\left[\mathbf{u}^\top \mathbf{v}\right] + const$$

with

$$\mathbf{u} = \mathbf{F}^- \nabla_\theta \log p(\mathbf{z}|\theta)\,,\ \mathbf{v} = f(\mathbf{z})\, \mathbf{u}.$$

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- $\mathbb{V}\left[\tilde{\nabla}_\theta J\left(\theta\right)\right]$ is of quadratic form, we can minimize it. The *optimal fitness baseline* is given by

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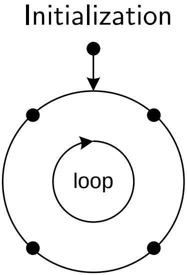
    - The block diagonal structure of **F** suggests using a *block fitness baseline*, where different baseline values are computed for orthogonal groups of parameters in θ.

Putting Things Together



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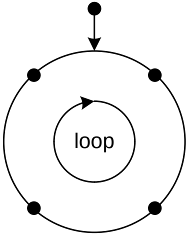
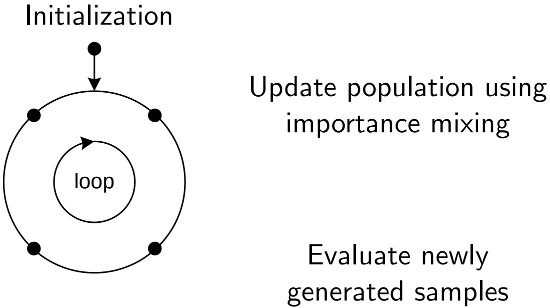
Initialization



Update population using importance mixing

Putting Things Together



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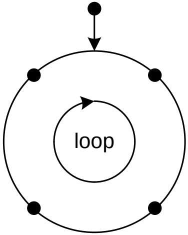

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Evaluate newly generated samples

Compute optimal baseline $\mathbf{b}^*$ and $\tilde{\nabla}_\theta^s J(\theta)$

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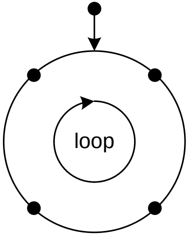


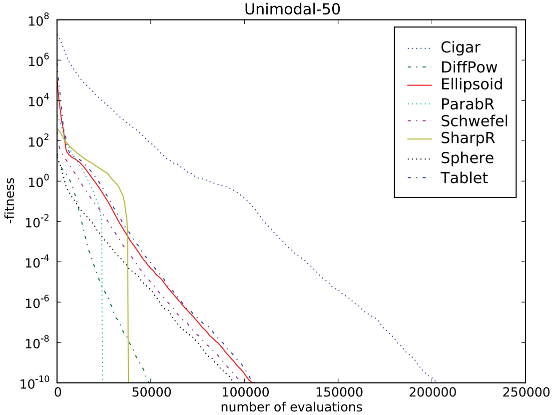
Update:
$\theta \leftarrow \theta + \alpha \tilde{\nabla}_{\theta}^{s} J(\theta)$

Update population using importance mixing

Compute optimal baseline $\mathbf{b}^*$ and $\tilde{\nabla}_{\theta}^{s} J(\theta)$

Evaluate newly generated samples

Empirical Results - Standard Blackbox Benchmarks



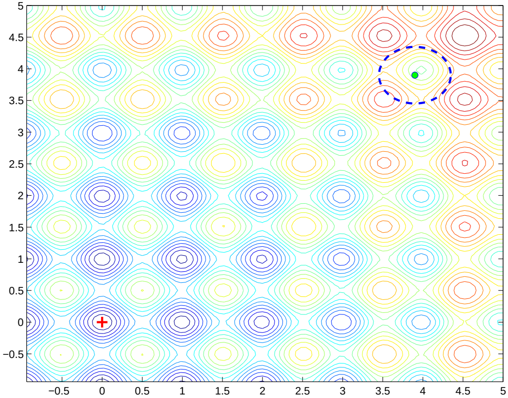
Empirical Results - Importance Mixing and Optimal Baseline

Percentage of runs that prematurely converged, while varying the type of fitness baseline used.

Baseline	premature convergence
None	52%
Uniform	50%
Block	0%

Importance Mixing reduces the number of fitness evaluations by a factor of $3 \sim 4$.

Empirical Results - Multimodal



eNES is able to jump over deceptive local optima.

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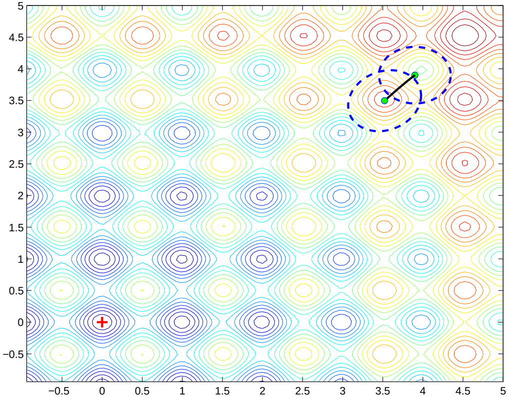

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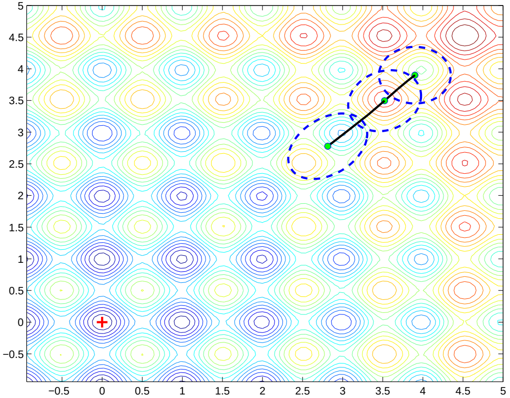

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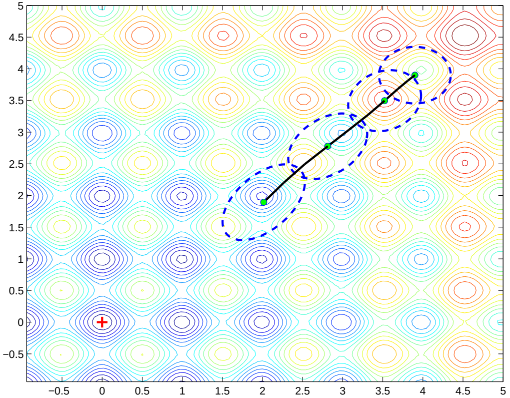

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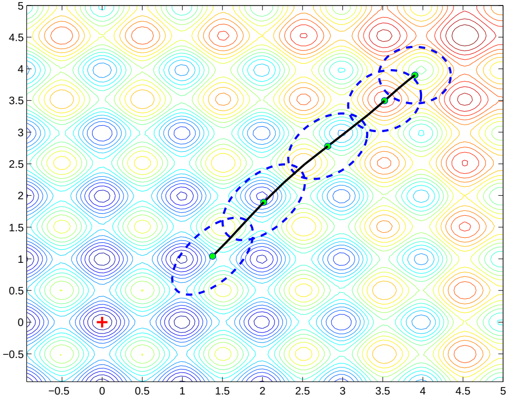

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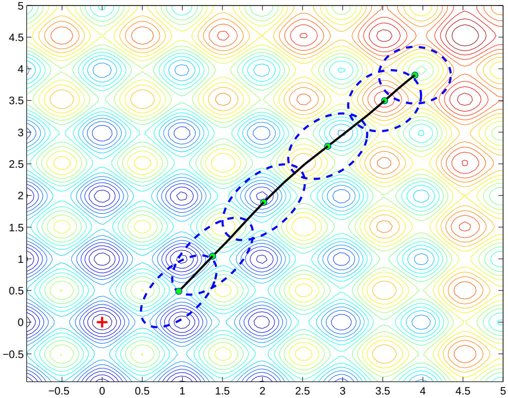

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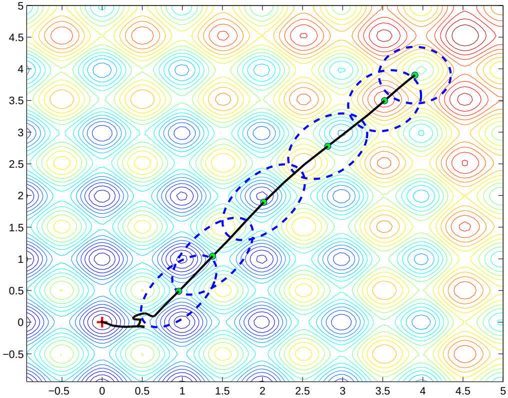

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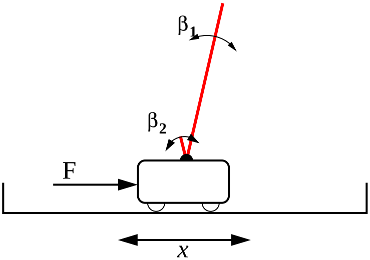
Empirical Results - Double Pole Balancing



Non-Markovian double pole balancing, average numbers of evaluations.

Method	SANE	ESP	NEAT	CMA	CoSyNE	FEM	NES
Eval.	262, 700	7, 374	6, 929	3, 521	1, 249	2, 099	1, 753

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- Derivation of exact Fisher information matrix.
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- Importance mixing reduces the number of fitness evaluations.
- Optimal fitness baselines reduces the variance of gradient estimation.
- Competitive performance on standard benchmarks, including non-Markovian double pole balancing tasks.

Try it Out?

PyBrain

The Python Machine Learning Library

http://www.pybrain.org

Thank you!