Introduction to Optimization

Derivative-Free Optimization / Blackbox Methods

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Course Overview

Date		Topic
Mon, 21.9.2015		Introduction
Mon, 28.9.2015	D	Basic Flavors of Complexity Theory
Mon, 5.10.2015	D	Greedy algorithms
Mon, 12.10.2015	D	Branch and bound (switched w/ dynamic programming)
Mon, 2.11.2015	D	Dynamic programming *[salle Proto]*
Fri, 6.11.2015	D	Approximation algorithms and heuristics *[S205/S207]*
Mon, 9.11.2015	C	Introduction to Continuous Optimization I *[S118]*
Fri, 13.11.2015	C	Introduction to Continuous Optimization II *[from here onwards always: S205/S207]*
Fri, 20.11.2015	C	Gradient-based Algorithms [+ finishing the intro]
Fri, 27.11.2015	**C**	~~End of Gradient-based Algorithms + Linear Programming~~ ***Stochastic Optimization and Derivative Free Optimization I***
Fri, 4.12.2015	C	Stochastic Optimization and Derivative Free Optimization II
Tue, 15.12.2015		Exam **(most likely in salle Proto)**

Lecture Overview Continuous Optimization

Introduction to Continuous Optimization

- examples (from ML / black-box problems)
- typical difficulties in optimization (e.g. constraints)

Mathematical Tools to Characterize Optima

- reminders about differentiability, gradient, Hessian matrix
- unconstrained optimization
  - first and second order conditions
  - convexity
- constrained optimization

Gradient-based Algorithms

- quasi-Newton method (BFGS)

Derivative-free Optimization/ Stochastic Blackbox Optimization

- CMA-ES (adaptive algorithms / Information Geometry)
- PhD thesis possible on this topic

  strongly related to ML, new promising research area, interesting open questions

Small exercise: finding optima of a constrained problem

Geometrical Interpretation Using an Example

Exercise:

Consider the problem

$$\inf\ \{ f(x,y) \mid (x,y) \in \mathbb{R}^2, g(x,y) = 0\}$$

$f(x,y) = y - x^2 \qquad g(x,y) = x^2 + y^2 - 1$

1) Plot the level sets of f, plot $g = 0$
2) Compute ∇f and ∇g
3) Find the solutions with $\nabla f + \lambda \nabla g = 0$

   equation solving with 3 unknowns (x, y, λ)
4) Plot the solutions of 3) on top of the level set graph of 1)

Descent Methods

Descent Methods

General principle

1. choose an initial point $\boldsymbol{x}_0$, set $t = 1$
2. while not happy
   - choose a descent direction $\boldsymbol{d}_t \neq 0$
   - line search:
     - choose a step size $\sigma_t > 0$
     - set $\boldsymbol{x}_{t+1} = \boldsymbol{x}_t + \sigma_t \boldsymbol{d}_t$
   - set $t = t + 1$

Remaining questions

- how to choose $\boldsymbol{d}_t$?
- how to choose σ_t?

Gradient Descent

Rationale: $\boldsymbol{d}_t = -\nabla f(\boldsymbol{x}_t)$ is a descent direction

indeed for f differentiable

$$f\big(x - \sigma\nabla f(x)\big) = f(x) - \sigma||\nabla f(x)||^2 + o(\sigma||\nabla f(x)||)$$

$$< f(x) \text{ for } \sigma \text{ small enough}$$

Step-size

- optimal step-size: $\sigma_t = \underset{\sigma}{\operatorname{argmin}} f(\boldsymbol{x}_t - \sigma\nabla f(\boldsymbol{x}_t))$
- **Line Search:** total or partial optimization w.r.t. σ
  Total is however often too "expensive" (needs to be performed at each iteration step)
  Partial optimization: execute a limited number of trial steps until a loose approximation of the optimum is found. Typical rule for partial optimization: Armijo rule

see next slide and exercise

Stopping criteria:

norm of gradient smaller than ϵ

The Armijo-Goldstein Rule

Choosing the step size:

- Only to decrease f-value not enough to converge (quickly)
- Want to have a reasonably large decrease in f

Armijo-Goldstein rule:

- also known as backtracking line search
- starts with a (too) large estimate of σ and reduces it until f is reduced enough
- what is enough?
  - assuming a linear f e.g. $m_k(x) = f(x_k) + \nabla f(x_k)^T(x - x_k)$
  - expected decrease if step of σ_k is done in direction $\boldsymbol{d}$: $\sigma_k \nabla f(x_k)^T \boldsymbol{d}$
  - actual decrease: $f(x_k) - f(x_k + \sigma_k \boldsymbol{d})$
  - stop if actual decrease is at least constant times expected decrease (constant typically chosen in [0, 1])

The Armijo-Goldstein Rule

The Actual Algorithm:

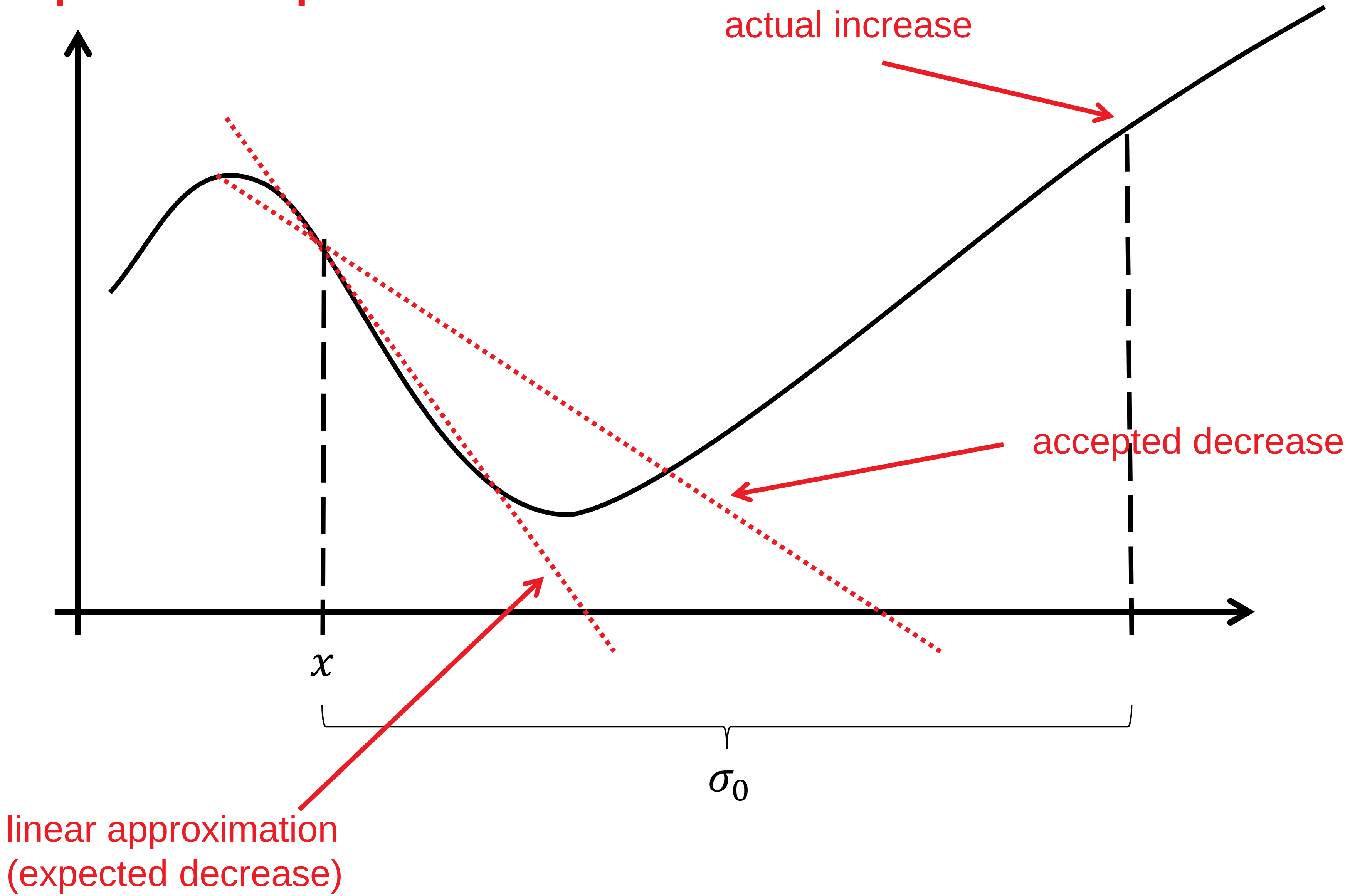
Input: descent direction $\mathbf{d}$, point $\mathbf{x}$, objective function $f(\mathbf{x})$ and its gradient $\nabla f(\mathbf{x})$, parameters $\sigma_0 = 10$, $\theta \in [0,1]$ and $\beta \in (0,1)$
Output: step-size σ

Initialize σ: $\sigma \leftarrow \sigma_0$
while $f(\mathbf{x} + \sigma\mathbf{d}) > f(\mathbf{x}) + \theta\sigma\nabla f(\mathbf{x})^T\mathbf{d}$ **do**
    $\sigma \leftarrow \beta\sigma$
end while

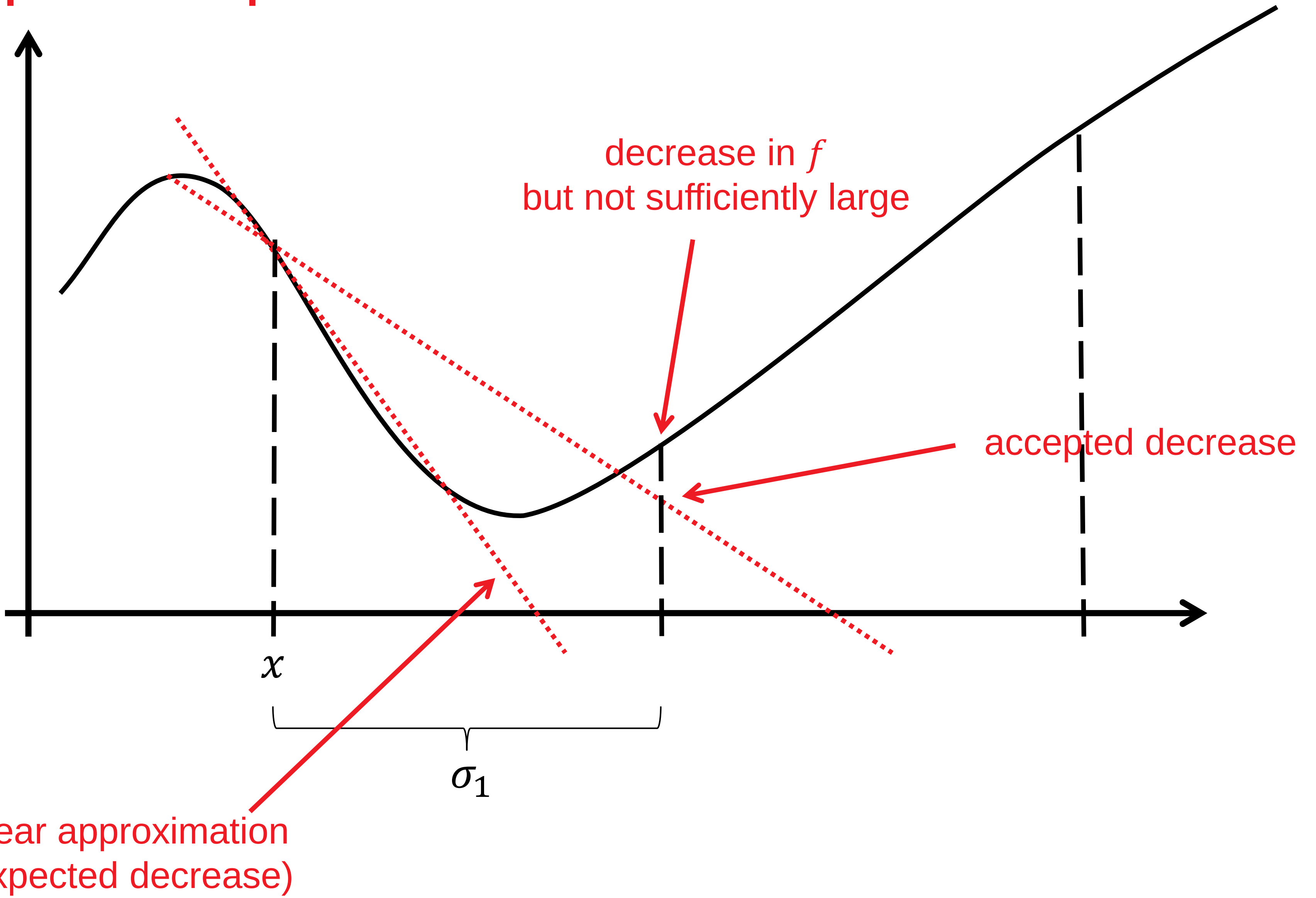
Armijo, in his original publication chose $\beta = \theta = 0.5$.

Choosing $\theta = 0$ means the algorithm accepts any decrease.

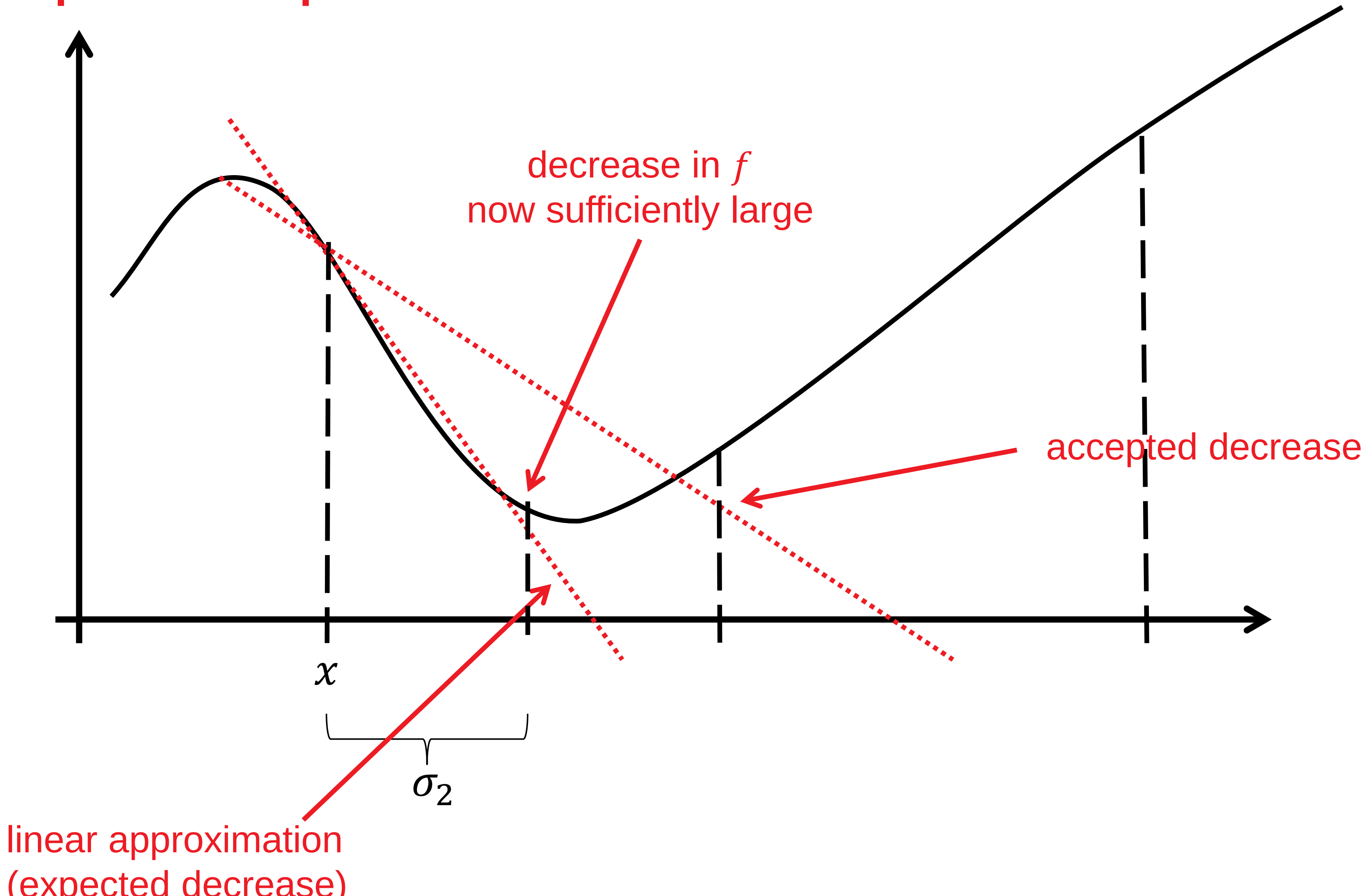
Graphical Interpretation



Graphical Interpretation



Graphical Interpretation



Gradient Descent: Simple Theoretical Analysis

Assume f is twice continuously differentiable, convex and that $\mu I_d \preccurlyeq \nabla^2 f(x) \preccurlyeq L I_d$ with $\mu > 0$ holds, assume a fixed step-size $\sigma_t = \frac{1}{L}$

Note: $A \preccurlyeq B$ means $x^T A x \leq x^T B x$ for all x

$$x_{t+1} - x^* = x_t - x^* - \sigma_t \nabla^2 f(y_t)(x_t - x^*) \text{ for some } y_t \in [x_t, x^*]$$

$$x_{t+1} - x^* = \left(I_d - \frac{1}{L}\nabla^2 f(y_t)\right)(x_t - x^*)$$

Hence $||x_{t+1} - x^*||^2 \leq |||I_d - \frac{1}{L}\nabla^2 f(y_t)|||^2 \; ||x_t - x^*||^2$

$$\leq \left(1 - \frac{\mu}{L}\right)^2 ||x_t - x^*||^2$$

Linear convergence: $||x_{t+1} - x^*|| \leq \left(1 - \frac{\mu}{L}\right) ||x_t - x^*||$

algorithm slower and slower with increasing condition number

Non-convex setting: convergence towards stationary point

Newton Method

- descent direction: $-[\nabla^2 f(x_k)]^{-1}\nabla f(x_k)$ [so-called Newton direction]
- The Newton direction:
  - minimizes the best (locally) quadratic approximation of f: $\tilde{f}(x+\Delta x) = f(x) + \nabla f(x)^T \Delta x + \frac{1}{2}(\Delta x)^T \nabla^2 f(x) \Delta \mathrm{x}$
  - points towards the optimum on $f(x) = (x - x^*)^T A (x - x^*)$
- however, Hessian matrix is expensive to compute in general and its inversion is also not easy

quadratic convergence

(i.e. $\lim_{k\to\infty} \frac{|x_{k+1}-x^*|}{|x_k - x^*|^2} = \mu > 0$)

Remark: Affine Invariance

Affine Invariance: same behavior on $f(x)$ and $f(Ax+b)$ for $A \in \mathrm{GLn}(\mathbb{R})$

- Newton method is affine invariant

  see **http://users.ece.utexas.edu/~cmcaram/EE381V_2012F/Lecture_6_Scribe_Notes.final.pdf**

- same convergence rate on all convex-quadratic functions
- Gradient method not affine invariant

Quasi-Newton Method: BFGS

$x_{t+1} = x_t - \sigma_t H_t \nabla f(x_t)$ where H_t is an approximation of the inverse Hessian

Key Idea of Quasi Newton:

successive iterates x_t, x_{t+1} and gradients $\nabla f(x_t)$, $\nabla f(x_{t+1})$ yield second order information

$$q_t \approx \nabla^2 f(x_{t+1}) p_t$$

where $p_t = x_{t+1} - x_t$ and $q_t = \nabla f(x_{t+1}) - \nabla f(x_t)$

Most popular implementation of this idea: Broyden-Fletcher-Goldfarb-Shanno (BFGS)

- default in MATLAB's **`fminunc`** and python's **`scipy.optimize.minimize`**

Conclusions

I hope it became clear so far...

...what are gradient and Hessian

...what are sufficient and necessary conditions for optimality

...what is the difference between gradient and Newton direction

...and that adapting the step size in descent algorithms is crucial.

Derivative-Free Optimization

Derivative-Free Optimization (DFO)

DFO = blackbox optimization

Why blackbox scenario?

- gradients are not always available (binary code, no analytical model, ...)
- or not useful (noise, non-smooth, ...)

- problem domain specific knowledge is used only within the black box, e.g. within an appropriate encoding
- some algorithms are furthermore function-value-free, i.e. *invariant* wrt. monotonous transformations of f.

Derivative-Free Optimization Algorithms

- (gradient-based algorithms which approximate the gradient by finite differences)

- coordinate descent
- pattern search methods, e.g. Nelder-Mead
- surrogate-assisted algorithms, e.g. NEWUOA or other trust-region methods
- function-value-free algorithms
  - typically stochastic
  - evolution strategies (ESs) and Covariance Matrix Adaptation Evolution Strategy (CMA-ES)
  - differential evolution
  - particle swarm optimization
  - simulated annealing
  - ...

Stochastic Search Template

A stochastic blackbox search template to minimize $f: \mathbb{R}^n \to \mathbb{R}$

Initialize distribution parameters θ, set population size $\lambda \in \mathbb{N}$

While happy do:

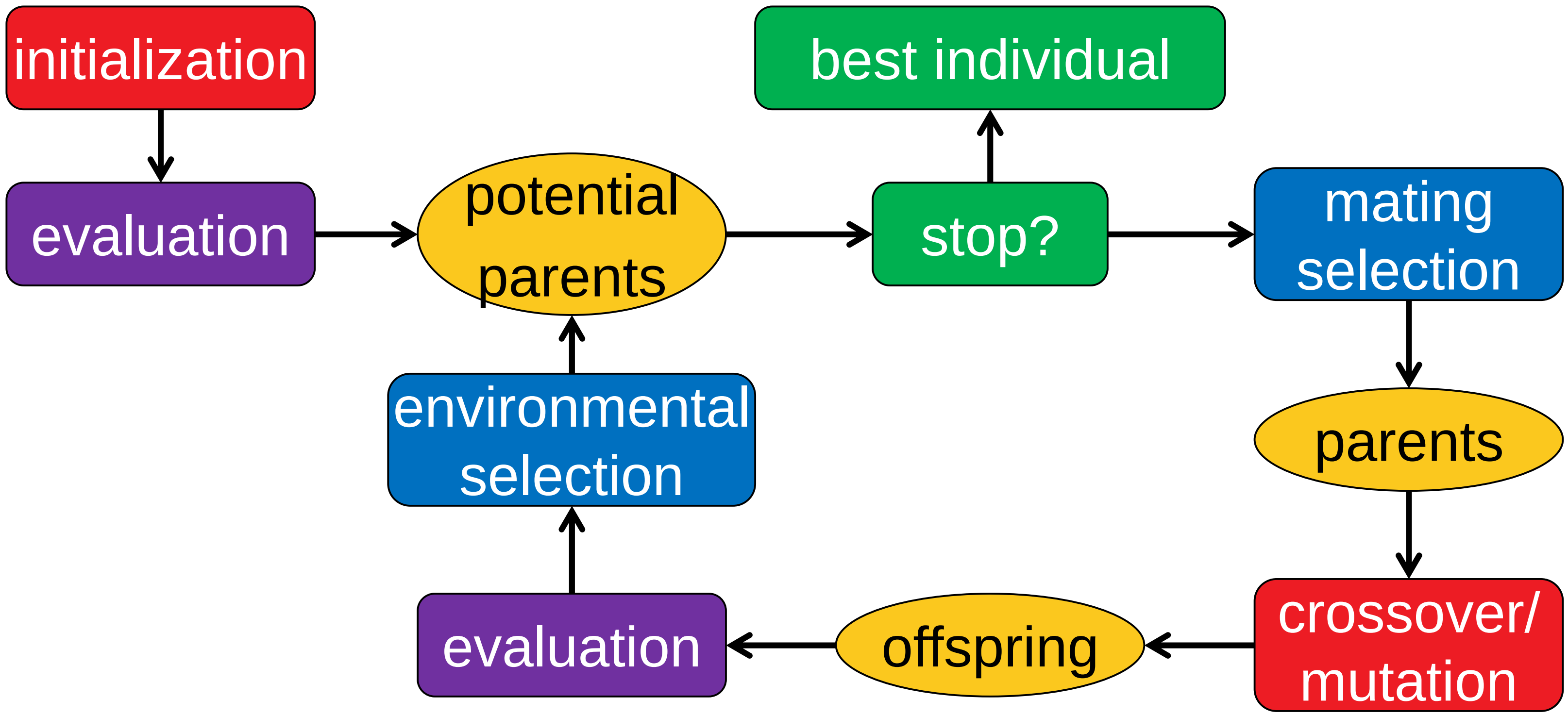
- Sample distribution $P(\boldsymbol{x}|\theta) \to \boldsymbol{x}_1, \dots, \boldsymbol{x}_\lambda \in \mathbb{R}^n$
- Evaluate $\boldsymbol{x}_1, \dots, \boldsymbol{x}_\lambda$ on f
- Update parameters $\theta \leftarrow F_\theta(\theta, \boldsymbol{x}_1, \dots, \boldsymbol{x}_\lambda, f(\boldsymbol{x}_1), \dots, f(\boldsymbol{x}_\lambda))$

- All depends on the choice of P and F_θ

deterministic algorithms are covered as well

- In Evolutionary Algorithms, P and F_θ are often defined implicitly via their operators.

Generic Framework of an EA



stochastic operators

“Darwinism”

stopping criteria

Nothing else: just interpretation change

The CMA-ES

Input: $m \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, λ
Initialize: $\mathbf{C} = \mathbf{I}$, and $p_c = \mathbf{0}$, $p_\sigma = \mathbf{0}$,
Set: $c_c \approx 4/n$, $c_\sigma \approx 4/n$, $c_1 \approx 2/n^2$, $c_\mu \approx \mu_w/n^2$, $c_1 + c_\mu \leq 1$, $d_\sigma \approx 1 + \sqrt{\frac{\mu_w}{n}}$,
and $w_{i=1\ldots\lambda}$ such that $\mu_w = \frac{1}{\sum_{i=1}^{\mu} {w_i}^2} \approx 0.3\,\lambda$

While not terminate

$$x_i = m + \sigma y_i, \quad y_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C}), \quad \text{for } i = 1, \ldots, \lambda \qquad \text{sampling}$$

$$m \leftarrow \sum_{i=1}^{\mu} w_i x_{i:\lambda} = m + \sigma y_w \quad \text{where } y_w = \sum_{i=1}^{\mu} w_i y_{i:\lambda} \qquad \text{update mean}$$

$$p_c \leftarrow (1 - c_c)\, p_c + \mathbb{1}_{\{\|p_\sigma\| < 1.5\sqrt{n}\}} \sqrt{1 - (1 - c_c)^2} \sqrt{\mu_w}\, y_w \qquad \text{cumulation for } \mathbf{C}$$

$$p_\sigma \leftarrow (1 - c_\sigma)\, p_\sigma + \sqrt{1 - (1 - c_\sigma)^2} \sqrt{\mu_w}\, \mathbf{C}^{-\frac{1}{2}} y_w \qquad \text{cumulation for } \sigma$$

$$\mathbf{C} \leftarrow (1 - c_1 - c_\mu)\, \mathbf{C} + c_1\, p_c {p_c}^{\mathrm{T}} + c_\mu \sum_{i=1}^{\mu} w_i\, y_{i:\lambda} y_{i:\lambda}^{\mathrm{T}} \qquad \text{update } \mathbf{C}$$

$$\sigma \leftarrow \sigma \times \exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\|p_\sigma\|}{\mathrm{E}\|\mathcal{N}(\mathbf{0},\mathbf{I})\|} - 1\right)\right) \qquad \text{update of } \sigma$$

Not covered on this slide: termination, restarts, useful output, boundaries and encoding

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While not terminate

$\boldsymbol{x}_i = \boldsymbol{m} + \sigma \boldsymbol{y}_i, \quad \boldsymbol{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C}), \quad$ for $i = 1, \ldots, \lambda$ — sampling

$\boldsymbol{m} \leftarrow \sum_{i=1}^{\mu} w_i \boldsymbol{x}_{i:\lambda} = \boldsymbol{m} + \sigma \boldsymbol{y}_w$ where $\boldsymbol{y}_w = \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}$ — update mean

$\boldsymbol{p}_c \leftarrow (1 - c_c)\boldsymbol{p}_c + \mathbb{1}_{\{\|\boldsymbol{p}_\sigma\| < 1.5\sqrt{n}\}} \sqrt{1 - (1 - c_c)^2}\sqrt{\mu_w}\,\boldsymbol{y}_w$ — cumulation for $\mathbf{C}$

$\boldsymbol{p}_\sigma \leftarrow (1 - c_\sigma)\boldsymbol{p}_\sigma + \sqrt{1 - (1 - c_\sigma)^2}\sqrt{\mu_w}\,\mathbf{C}^{-\frac{1}{2}}\boldsymbol{y}_w$ — cumulation for σ

$\mathbf{C} \leftarrow (1 - c_1 - c_\mu)\,\mathbf{C} + c_1 \boldsymbol{p}_c {\boldsymbol{p}_c}^{\mathrm{T}} + \ldots$ — update C

$\sigma \leftarrow \sigma \times \exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\|\boldsymbol{p}_\sigma\|}{\mathsf{E}\|\mathcal{N}(\mathbf{0},\mathbf{I})\|} - 1\right)\right.$

Not covered on this slide: terminati
encoding

Goal:
Understand the main principles of this state-of-the-art algorithm.

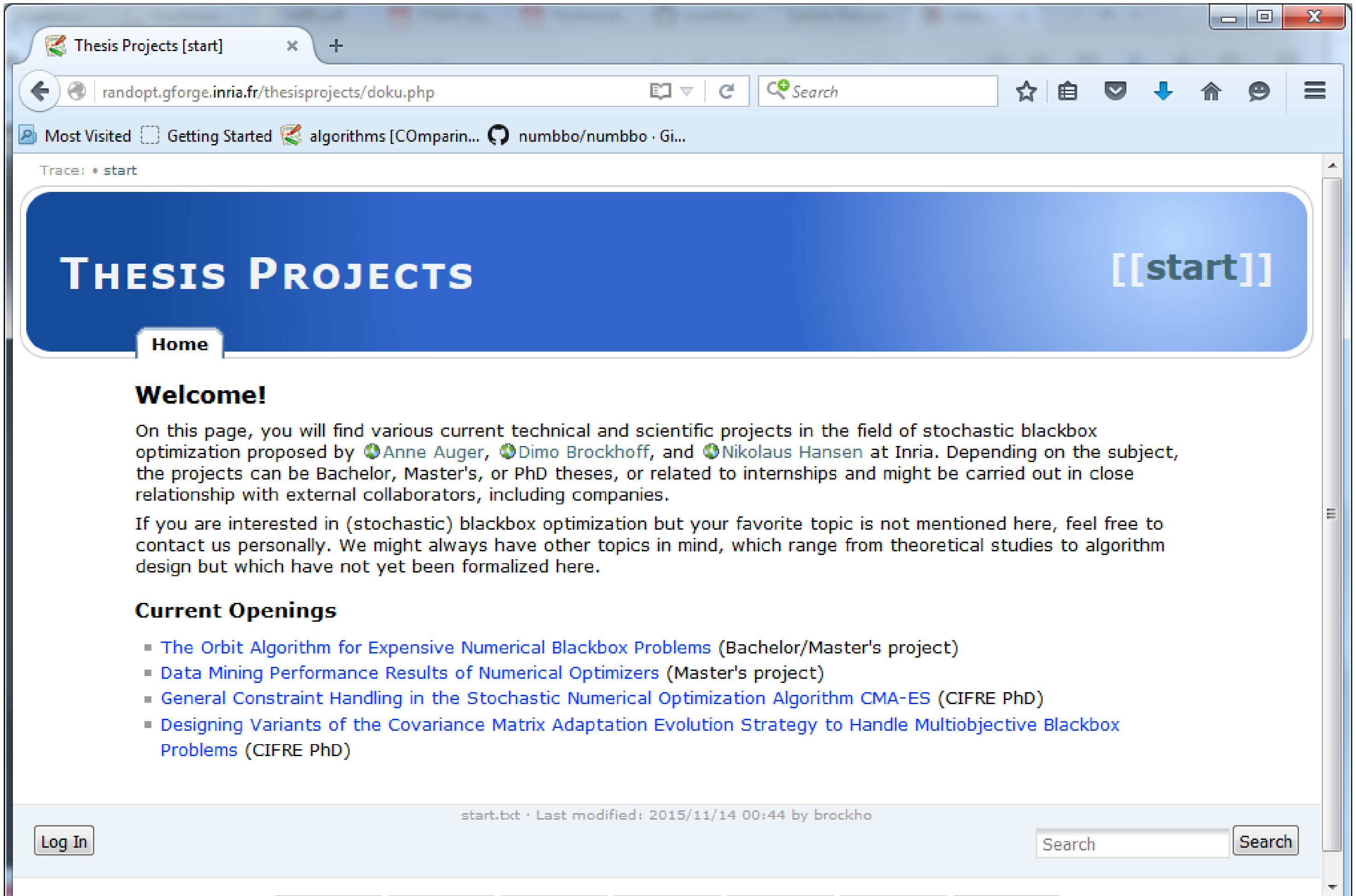
Copyright Notice

- Last slide was taken from
`https://www.lri.fr/~hansen/copenhagen-cma-es.pdf`
(copyright by Nikolaus Hansen, one of the main inventors of the CMA-ES algorithms)
- In the following, I will borrow more slides from there and from
`http://researchers.lille.inria.fr/~brockhof/optimizationSaclay/slides/20151106-continuousoptIV.pdf`
(by Anne Auger)

- In the following and the online material in particular, I refer to these pdfs as [Hansen, p. X] and [Auger, p. Y] respectively.

Announcement: Thesis Projects

- Anne Auger, Nikolaus Hansen, and me propose a couple of research projects for Bachelor's, Master's, and/or PhD theses
- **`randopt.gforge.inria.fr/thesisprojects/`**



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- projects related to CMA-ES and other (stochastic) blackbox optimization algorithms
- ranging from
  - pure theory (e.g. convergence analysis, Markov chain Monte Carlo, Information Geometry, ...) over
  - algorithm design (CMA-ES variants for new problem types such as large-scale, multiobjective, ...) to
  - applications (CIFRE PhD thesis for example)

Note:
Not all possible projects are described, hence contact us.

Back to CMA-ES

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$$\mathbf{C} \leftarrow (1 - c_1 - c_\mu)\, \mathbf{C} + c_1\, p_c {p_c}^{\mathrm{T}} + \ldots$$ update C

$$\sigma \leftarrow \sigma \times \exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\|p_\sigma\|}{\mathsf{E}\|\mathcal{N}(\mathbf{0}, \mathbf{I})\|} - 1\right) \ldots\right.$$

Not covered on this slide: terminati[...]
encoding

Goal:
Understand the main principles of this state-of-the-art algorithm.

CMA-ES: Stochastic Search Template

A stochastic blackbox search template to minimize $\boldsymbol{f}: \mathbb{R}^{\boldsymbol{n}} \to \mathbb{R}$

Initialize distribution parameters θ, set population size $\lambda \in \mathbb{N}$

While happy do:

- Sample distribution $P(\boldsymbol{x}|\theta) \to \boldsymbol{x}_1, \ldots, \boldsymbol{x}_\lambda \in \mathbb{R}^n$
- Evaluate $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_\lambda$ on f
- Update parameters $\theta \leftarrow F_\theta(\theta, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_\lambda, f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_\lambda))$

For CMA-ES and evolution strategies in general:

sample distributions = multivariate Gaussian distributions

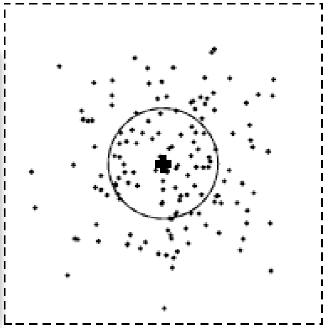
Sampling New Candidate Solutions (Offspring)

Evolution Strategies

New search points are sampled normally distributed

$$\boldsymbol{x}_i \sim \boldsymbol{m} + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \qquad \text{for } i = 1, \ldots, \lambda$$

as perturbations of $\boldsymbol{m}$, where $\boldsymbol{x}_i, \boldsymbol{m} \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, $\mathbf{C} \in \mathbb{R}^{n \times n}$



where

- the mean vector $\boldsymbol{m} \in \mathbb{R}^n$ represents the favorite solution
- the so-called step-size $\sigma \in \mathbb{R}_+$ controls the *step length*
- the covariance matrix $\mathbf{C} \in \mathbb{R}^{n \times n}$ determines the shape of the distribution ellipsoid

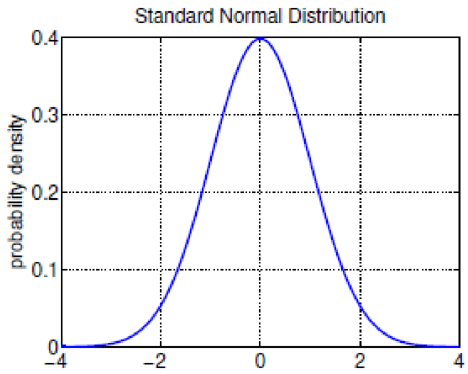
here, all new points are sampled with the same parameters

it remains to show how to adapt the parameters, but for now: normal distributions

from [Auger, p. 10]

Normal Distribution

1-D case



probability density of the 1-D standard normal distribution $\mathcal{N}(0,1)$

(expected (mean) value, variance) = (0,1)

$$p(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$$

General case

- Normal distribution $\mathcal{N}(m, \sigma^2)$

  (expected value, variance) = (m, σ^2)

  density: $p_{m,\sigma}(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-m)^2}{2\sigma^2}\right)$

- A normal distribution is entirely determined by its mean value and variance
- The family of normal distributions is closed under linear transformations: if X is normally distributed then a linear transformation $aX + b$ is also normally distributed
- **Exercice:** Show that $m + \sigma\mathcal{N}(0,1) = \mathcal{N}(m, \sigma^2)$

from [Auger, p. 11]

Normal Distribution

General case

A random variable following a 1-D normal distribution is determined by its mean value m and variance σ^2.

In the n-dimensional case it is determined by its mean vector and covariance matrix

Covariance Matrix

If the entries in a vector $\boldsymbol{X} = (X_1, \ldots, X_n)^T$ are random variables, each with finite variance, then the covariance matrix Σ is the matrix whose (i, j) entries are the covariance of (X_i, X_j)

$$\Sigma_{ij} = \mathrm{cov}(X_i, X_j) = \mathrm{E}\left[(X_i - \mu_i)(X_j - \mu_j)\right]$$

where $\mu_i = \mathrm{E}(X_i)$. Considering the expectation of a matrix as the expectation of each entry, we have

$$\Sigma = \mathrm{E}[(X - \mu)(X - \mu)^T]$$

Σ is symmetric, positive definite

from [Auger, p. 12]

The Multi-Variate (n-Dimensional) Normal Distribution

Any multi-variate normal distribution $\mathcal{N}(\boldsymbol{m}, \mathbf{C})$ is uniquely determined by its mean value $\boldsymbol{m} \in \mathbb{R}^n$ and its symmetric positive definite $n \times n$ covariance matrix $\mathbf{C}$.

density: $p_{\mathcal{N}(\boldsymbol{m},\mathbf{C})}(\boldsymbol{x}) = \frac{1}{(2\pi)^{n/2}|\mathbf{C}|^{1/2}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{m})^{\mathrm{T}}\mathbf{C}^{-1}(\boldsymbol{x}-\boldsymbol{m})\right),$

from [Auger, p. 13]

The Multi-Variate (n-Dimensional) Normal Distribution

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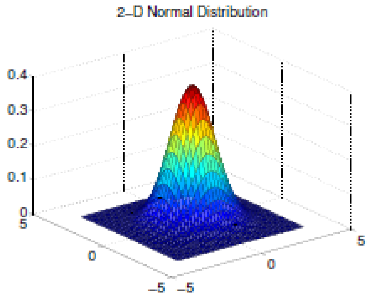
The mean value $\boldsymbol{m}$

- determines the displacement (translation)
- value with the largest density (modal value)
- the distribution is symmetric about the distribution mean



$$\mathcal{N}(\boldsymbol{m}, \mathbf{C}) = \boldsymbol{m} + \mathcal{N}(0, \mathbf{C})$$

from [Auger, p. 13]

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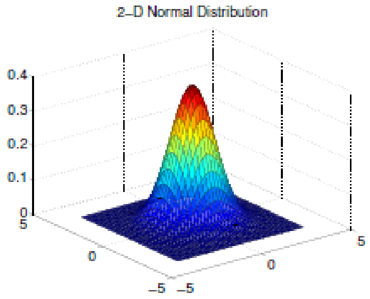


The covariance matrix $\mathbf{C}$

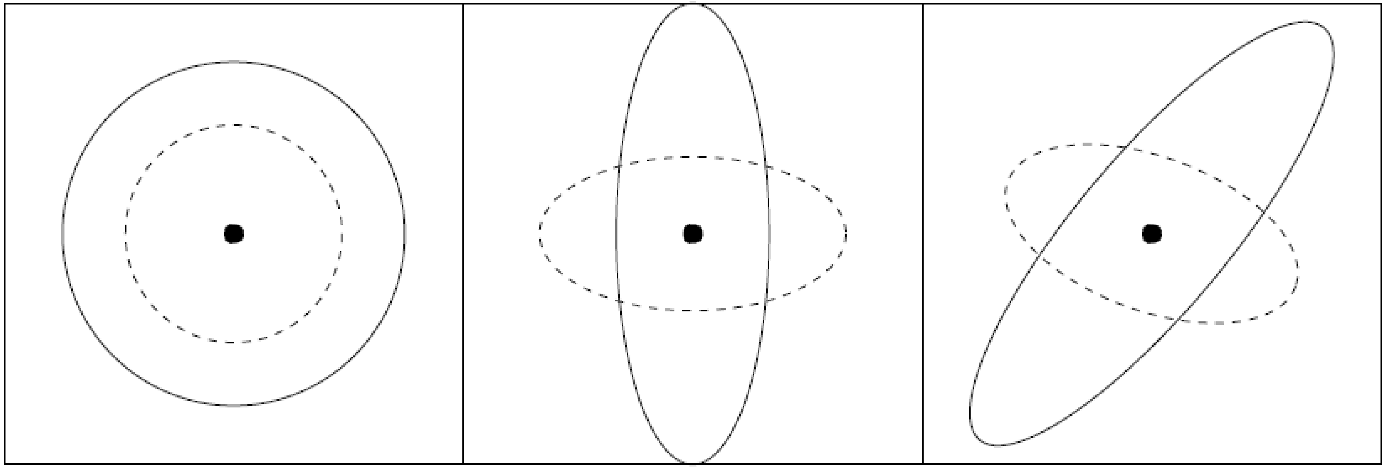
- determines the shape
- geometrical interpretation: any covariance matrix can be uniquely identified with the iso-density ellipsoid $\{\boldsymbol{x} \in \mathbb{R}^n \,|\, (\boldsymbol{x}-\boldsymbol{m})^{\mathrm{T}}\mathbf{C}^{-1}(\boldsymbol{x}-\boldsymbol{m}) = 1\}$

from [Auger, p. 13]

Covariance Matrix: Lines of Equal Density

. . . any covariance matrix can be uniquely identified with the iso-density ellipsoid $\{\mathbf{x} \in \mathbb{R}^n \mid (\mathbf{x} - \mathbf{m})^{\mathrm{T}}\mathbf{C}^{-1}(\mathbf{x} - \mathbf{m}) = 1\}$

Lines of Equal Density



$\mathcal{N}(\mathbf{m}, \sigma^2\mathbf{I}) \sim \mathbf{m} + \sigma\mathcal{N}(\mathbf{0}, \mathbf{I})$
one degree of freedom σ
components are independent standard normally distributed

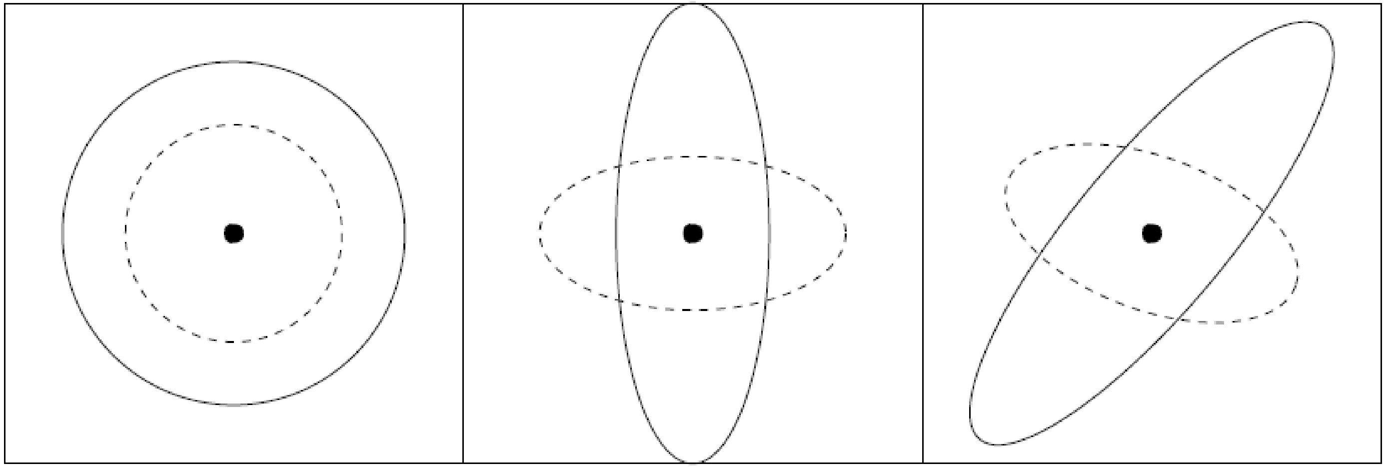
where $\mathbf{I}$ is the identity matrix (isotropic case) and $\mathbf{D}$ is a diagonal matrix (reasonable for separable problems) and $\mathbf{A} \times \mathcal{N}(\mathbf{0}, \mathbf{I}) \sim \mathcal{N}(\mathbf{0}, \mathbf{A}\mathbf{A}^{\mathrm{T}})$ holds for all $\mathbf{A}$.

from [Auger, p. 14]

Covariance Matrix: Lines of Equal Density

...any covariance matrix can be uniquely identified with the iso-density ellipsoid $\{x \in \mathbb{R}^n \mid (x - m)^{\mathrm{T}} \mathbf{C}^{-1}(x - m) = 1\}$

Lines of Equal Density



$\mathcal{N}(m, \sigma^2 \mathbf{I}) \sim m + \sigma \mathcal{N}(\mathbf{0}, \mathbf{I})$
one degree of freedom σ
components are independent standard normally distributed

$\mathcal{N}(m, \mathbf{D}^2) \sim m + \mathbf{D}\mathcal{N}(\mathbf{0}, \mathbf{I})$
n degrees of freedom
components are independent, scaled

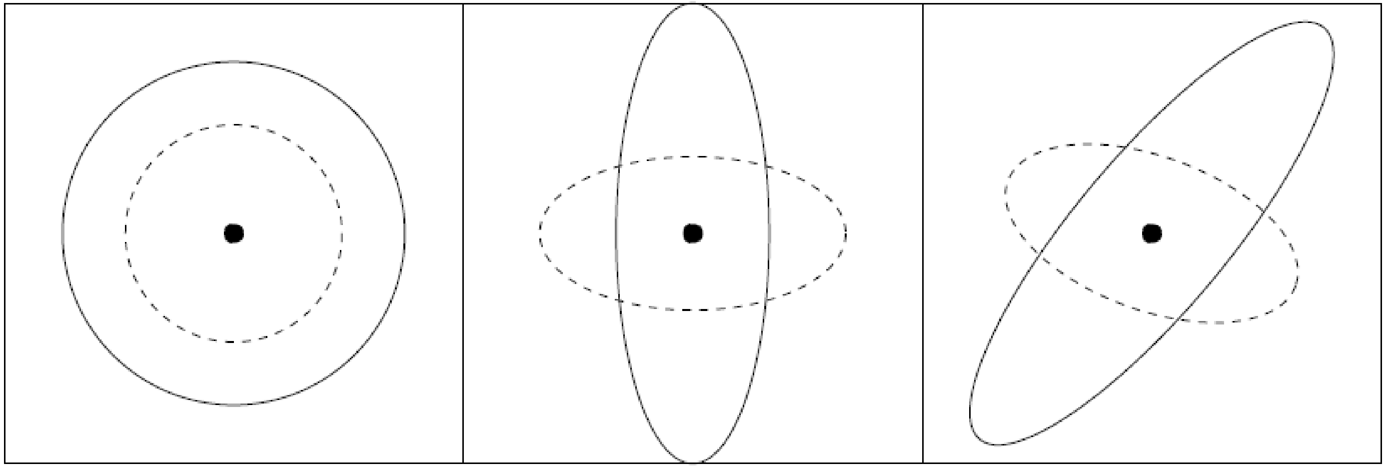
where $\mathbf{I}$ is the identity matrix (isotropic case) and $\mathbf{D}$ is a diagonal matrix (reasonable for separable problems) and $\mathbf{A} \times \mathcal{N}(\mathbf{0}, \mathbf{I}) \sim \mathcal{N}(\mathbf{0}, \mathbf{A}\mathbf{A}^{\mathrm{T}})$ holds for all $\mathbf{A}$.

from [Auger, p. 14]

Covariance Matrix: Lines of Equal Density

...any covariance matrix can be uniquely identified with the iso-density ellipsoid $\{x \in \mathbb{R}^n \mid (x - m)^{\mathrm{T}} \mathbf{C}^{-1}(x - m) = 1\}$

Lines of Equal Density



$\mathcal{N}(m, \sigma^2 \mathbf{I}) \sim m + \sigma \mathcal{N}(\mathbf{0}, \mathbf{I})$	$\mathcal{N}(m, \mathbf{D}^2) \sim m + \mathbf{D}\mathcal{N}(\mathbf{0}, \mathbf{I})$	$\mathcal{N}(m, \mathbf{C}) \sim m + \mathbf{C}^{\frac{1}{2}}\mathcal{N}(\mathbf{0}, \mathbf{I})$
one degree of freedom σ	n degrees of freedom	$(n^2 + n)/2$ degrees of freedom
components are independent standard normally distributed	components are independent, scaled	components are correlated

where $\mathbf{I}$ is the identity matrix (isotropic case) and $\mathbf{D}$ is a diagonal matrix (reasonable for separable problems) and $\mathbf{A} \times \mathcal{N}(\mathbf{0}, \mathbf{I}) \sim \mathcal{N}(\mathbf{0}, \mathbf{A}\mathbf{A}^{\mathrm{T}})$ holds for all $\mathbf{A}$.

from [Auger, p. 14]

Adaptation of Sample Distribution Parameters

Adaptation: What do we want to achieve?

New search points are sampled normally distributed

$$\boldsymbol{x}_i \sim \boldsymbol{m} + \sigma \mathcal{N}_i(\boldsymbol{0}, \mathbf{C}) \qquad \text{for } i = 1, \ldots, \lambda$$

where $\boldsymbol{x}_i, \boldsymbol{m} \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, $\mathbf{C} \in \mathbb{R}^{n \times n}$

- the mean vector should represent the favorite solution
- the step-size controls the step-length and thus convergence rate

  should allow to reach fastest convergence rate possible
- the covariance matrix $\mathbf{C} \in \mathbb{R}^{n \times n}$ determines the shape of the distribution ellipsoid

  adaptation should allow to learn the "topography" of the problem
  particulary important for ill-conditionned problems
  $\mathbf{C} \propto \boldsymbol{H}^{-1}$ on convex quadratic functions

from [Auger, p. 16]

Adaptation of the Mean

Evolution Strategies

Terminology

μ: # of parents, λ: # of offspring

Plus (elitist) and comma (non-elitist) selection

$(\mu + \lambda)$-ES: selection in $\{\text{parents}\} \cup \{\text{offspring}\}$
(μ, λ)-ES: selection in $\{\text{offspring}\}$

$(1 + 1)$-ES

Sample one offspring from parent $\boldsymbol{m}$

$$\boldsymbol{x} = \boldsymbol{m} + \sigma \mathcal{N}(\mathbf{0}, \mathbf{C})$$

If $\boldsymbol{x}$ better than $\boldsymbol{m}$ select

$$\boldsymbol{m} \leftarrow \boldsymbol{x}$$

why?

from [Hansen, p. 35]

The $(\mu/\mu, \lambda)$-ES

Non-elitist selection and intermediate (weighted) recombination

Given the i-th solution point $\boldsymbol{x}_i = \boldsymbol{m} + \sigma \underbrace{\mathcal{N}_i(\mathbf{0}, \mathbf{C})}_{=: \boldsymbol{y}_i} = \boldsymbol{m} + \sigma \boldsymbol{y}_i$

Let $\boldsymbol{x}_{i:\lambda}$ the i-th ranked solution point, such that $f(\boldsymbol{x}_{1:\lambda}) \leq \cdots \leq f(\boldsymbol{x}_{\lambda:\lambda})$.
The new mean reads

$$\boldsymbol{m} \leftarrow \sum_{i=1}^{\mu} w_i \boldsymbol{x}_{i:\lambda} = \boldsymbol{m} + \sigma \underbrace{\sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}}_{=: \boldsymbol{y}_w}$$

where

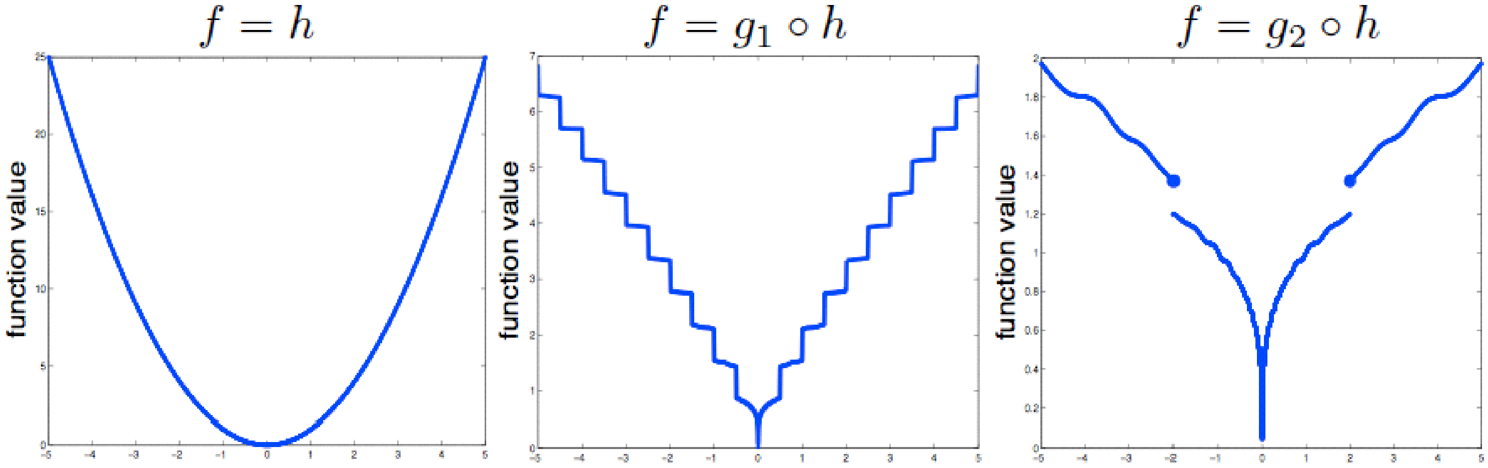
$$w_1 \geq \cdots \geq w_\mu > 0, \quad \sum_{i=1}^{\mu} w_i = 1, \quad \frac{1}{\sum_{i=1}^{\mu} {w_i}^2} =: \mu_w \approx \frac{\lambda}{4}$$

The best μ points are selected from the new solutions (non-elitistic) and weighted intermediate recombination is applied.

from [Hansen, p. 34]

Invariance Against Order-Preserving f-Transformations

Invariance: Function-Value Free Property



Three functions belonging to the same equivalence class

A *function-value free search algorithm* is invariant under the transformation with any order preserving (strictly increasing) g.

Invariances make

- observations meaningful
- algorithms predictable and/or "robust"

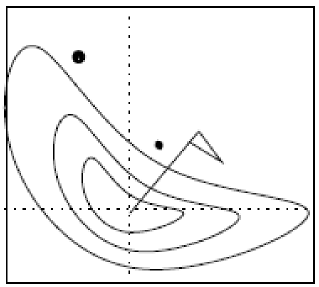
as a rigorous notion of generalization

from [Hansen, p. 37]

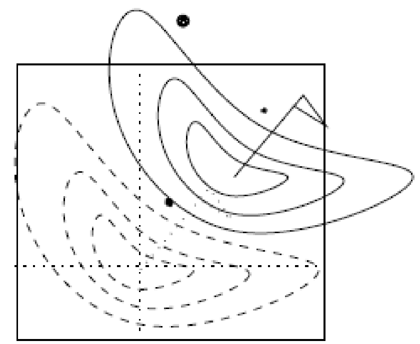
Basic Invariance in Search Space

- translation invariance

is true for most optimization algorithms



$$f(\boldsymbol{x}) \leftrightarrow f(\boldsymbol{x}-\boldsymbol{a})$$



Identical behavior on f and f_a

$$\begin{aligned} f: &\quad \boldsymbol{x} \mapsto f(\boldsymbol{x}), & \boldsymbol{x}^{(t=0)} &= \boldsymbol{x}_0 \\ f_a: &\quad \boldsymbol{x} \mapsto f(\boldsymbol{x}-\boldsymbol{a}), & \boldsymbol{x}^{(t=0)} &= \boldsymbol{x}_0 + \boldsymbol{a} \end{aligned}$$

No difference can be observed w.r.t. the argument of f

from [Hansen, p. 38]

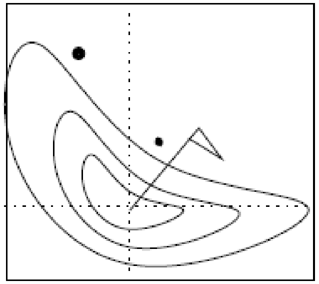
Invariance Against Search Space Rotations

Rotational Invariance in Search Space

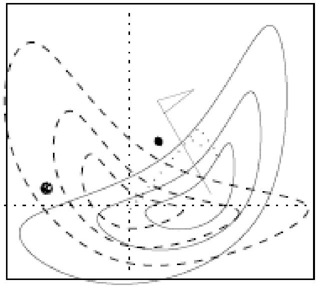
- invariance to orthogonal (rigid) transformations $\mathbf{R}$, where $\mathbf{R}\mathbf{R}^{\mathrm{T}} = \mathbf{I}$

e.g. true for simple evolution strategies

recombination operators might jeopardize rotational invariance



$$f(\boldsymbol{x}) \leftrightarrow f(\mathbf{R}\boldsymbol{x})$$



Identical behavior on f and $f_{\mathbf{R}}$

$$f: \quad \boldsymbol{x} \mapsto f(\boldsymbol{x}), \qquad \boldsymbol{x}^{(t=0)} = \boldsymbol{x}_0$$
$$f_{\mathbf{R}}: \quad \boldsymbol{x} \mapsto f(\mathbf{R}\boldsymbol{x}), \quad \boldsymbol{x}^{(t=0)} = \mathbf{R}^{-1}(\boldsymbol{x}_0)$$

45

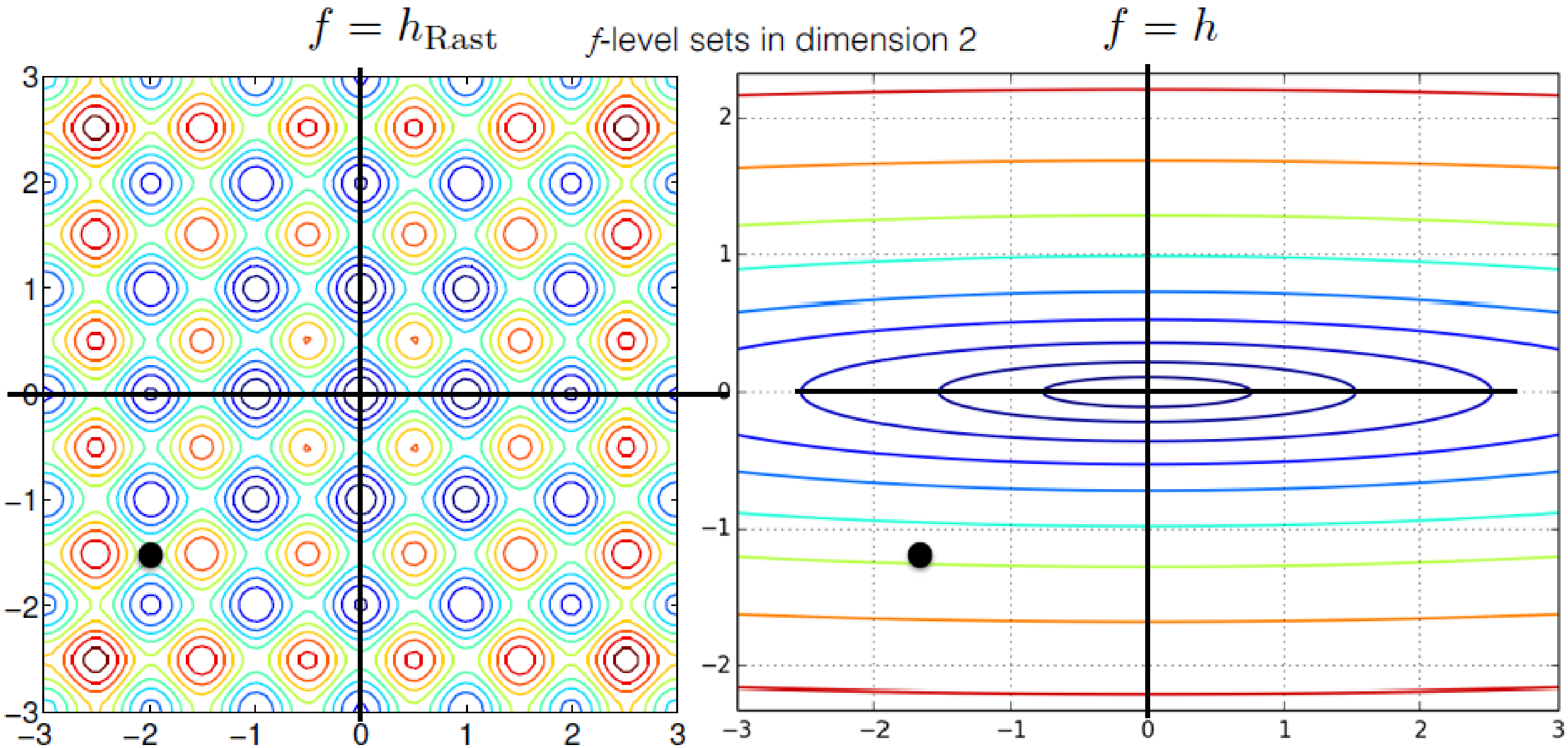
No difference can be observed w.r.t. the argument of f

[4] Salomon 1996. "Reevaluating Genetic Algorithm Performance under Coordinate Rotation of Benchmark Functions; A survey of some theoretical and practical aspects of genetic algorithms." BioSystems, 39(3):263-278

[5] Hansen 2000. Invariance, Self-Adaptation and Correlated Mutations in Evolution Strategies. *Parallel Problem Solving from Nature PPSN VI*

from [Hansen, p. 39]

Invariance Under Rigid Search Space Transformations

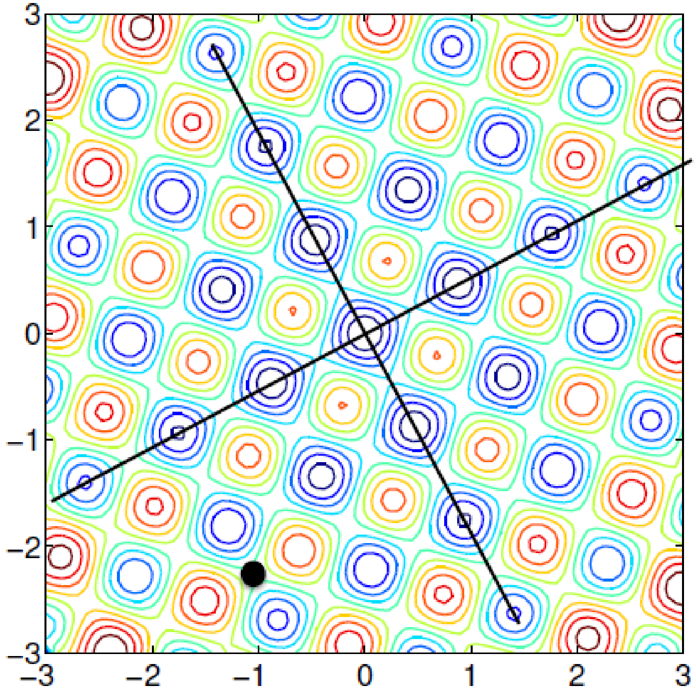


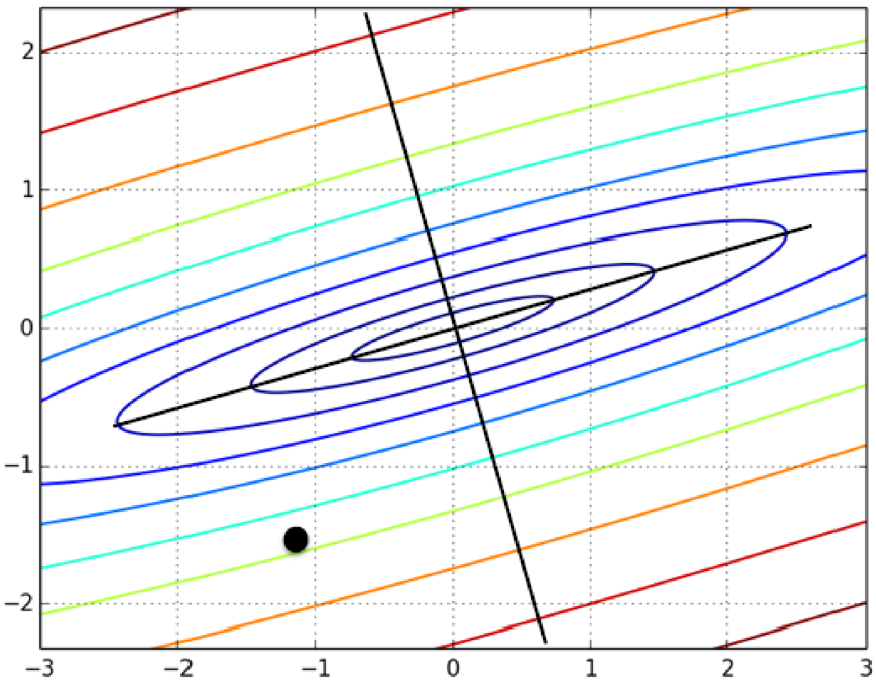
for example, invariance under search space rotation
(separable $\Leftrightarrow$ non-separable)

from [Hansen, p. 40]

Invariance Under Rigid Search Space Transformations

$f = h_{\text{Rast}} \circ R$ $\quad$ f-level sets in dimension 2 $\quad$ $f = h \circ R$



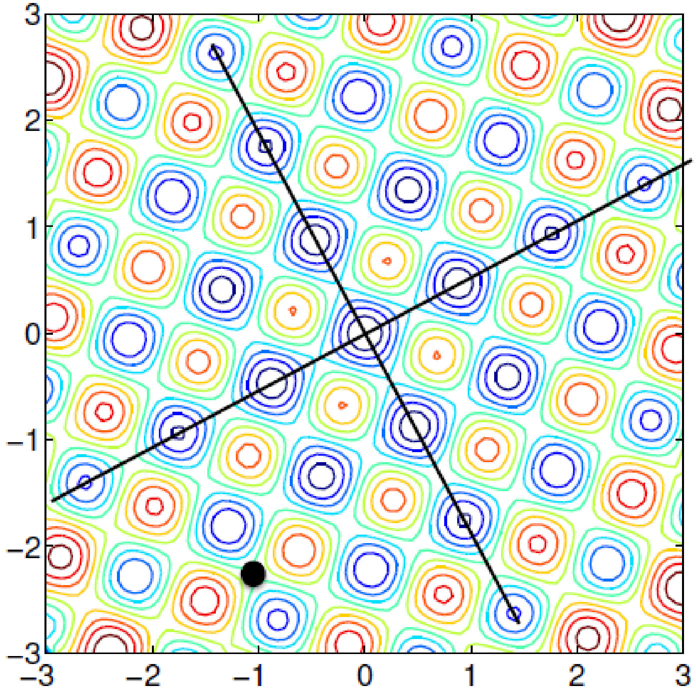


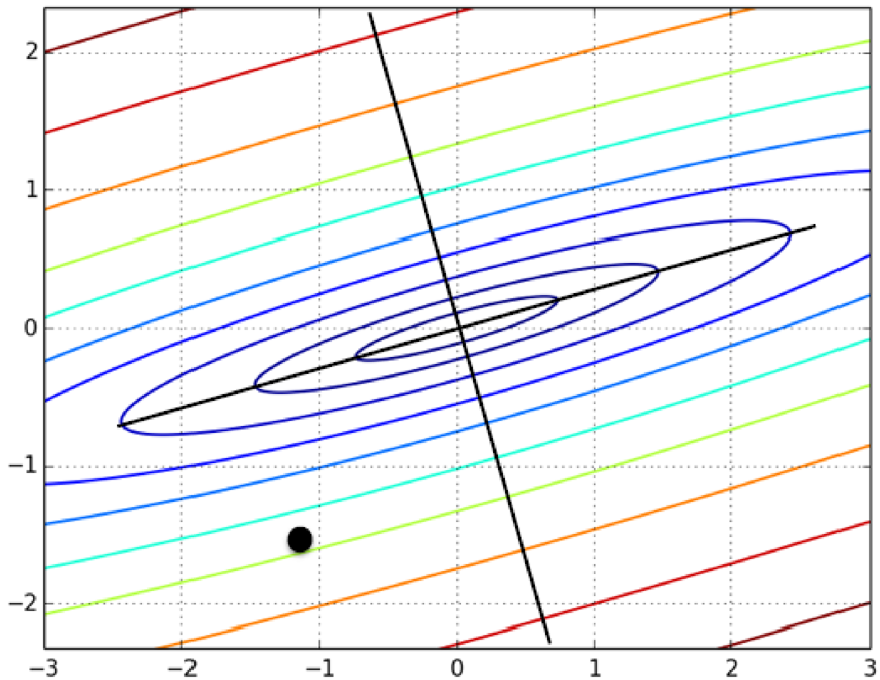
for example, invariance under search space rotation
(separable ⇔ non-separable)

from [Hansen, p. 41]

Invariance Under Rigid Search Space Transformations

$f = h_{\text{Rast}} \circ R$ f-level sets in dimension 2 $f = h \circ R$





for example, invariance un
(separable ⇔ non-separab

mainly Nelder-Mead and CMA-ES have this property

Invariance

The grand aim of all science is to cover the greatest number of empirical facts by logical deduction from the smallest number of hypotheses or axioms.

— Albert Einstein

- Empirical performance results
  - from benchmark functions
  - from solved real world problems

  are only useful if they do generalize to other problems

- Invariance is a strong non-empirical statement about generalization

  generalizing (identical) performance from a single function to a whole class of functions

consequently, invariance is important for the evaluation of search algorithms

from [Hansen, p. 43]

Step-Size Adaptation

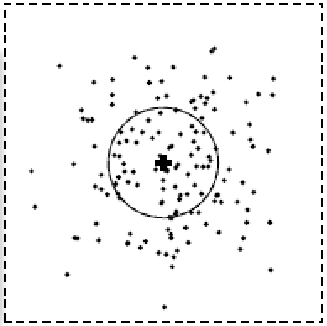
Evolution Strategies

Recalling

New search points are sampled normally distributed

$$x_i \sim m + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \qquad \text{for } i = 1, \ldots, \lambda$$

as perturbations of m, where $x_i, m \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, $\mathbf{C} \in \mathbb{R}^{n \times n}$



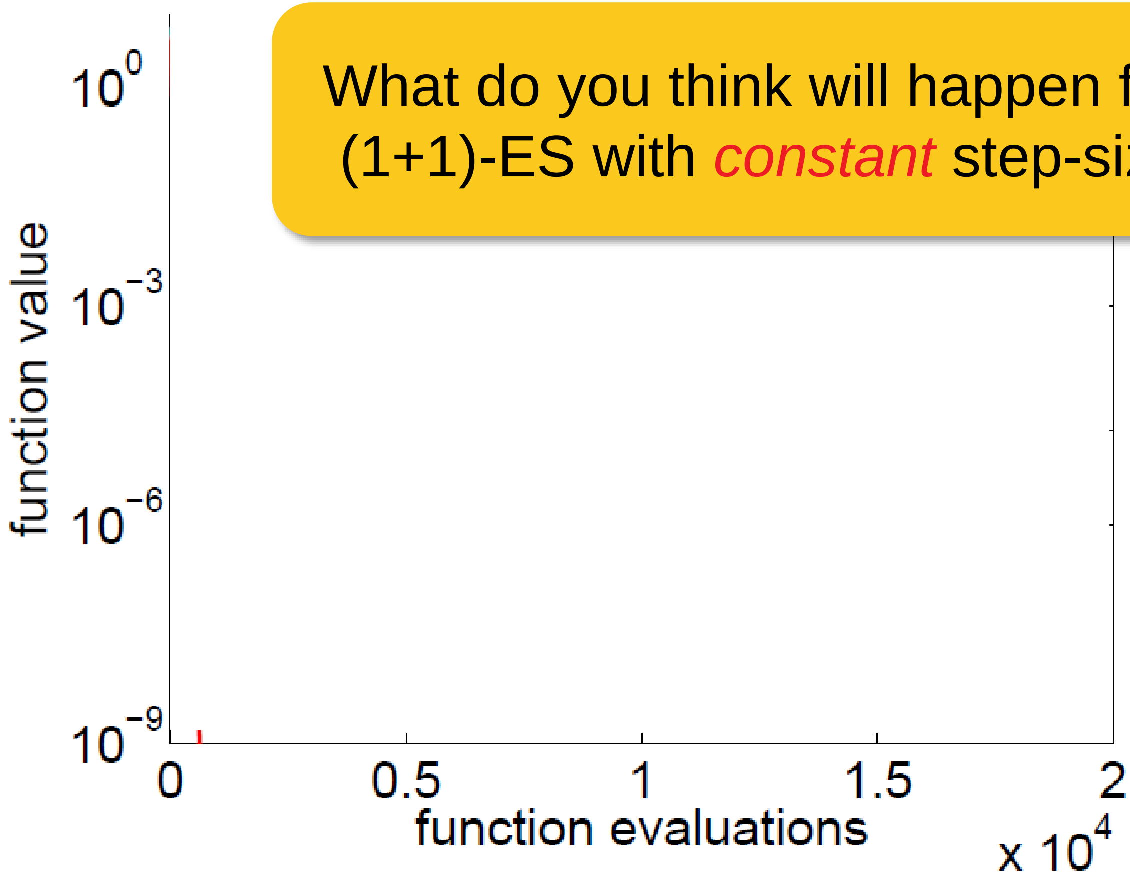
where

- the mean vector $m \in \mathbb{R}^n$ represents the favorite solution and $m \leftarrow \sum_{i=1}^{\mu} w_i x_{i:\lambda}$
- the so-called step-size $\sigma \in \mathbb{R}_+$ controls the *step length*
- the covariance matrix $\mathbf{C} \in \mathbb{R}^{n \times n}$ determines the shape of the distribution ellipsoid

The remaining question is how to update σ and $\mathbf{C}$.

from [Hansen, p. 45]

Why Step-Size Control?



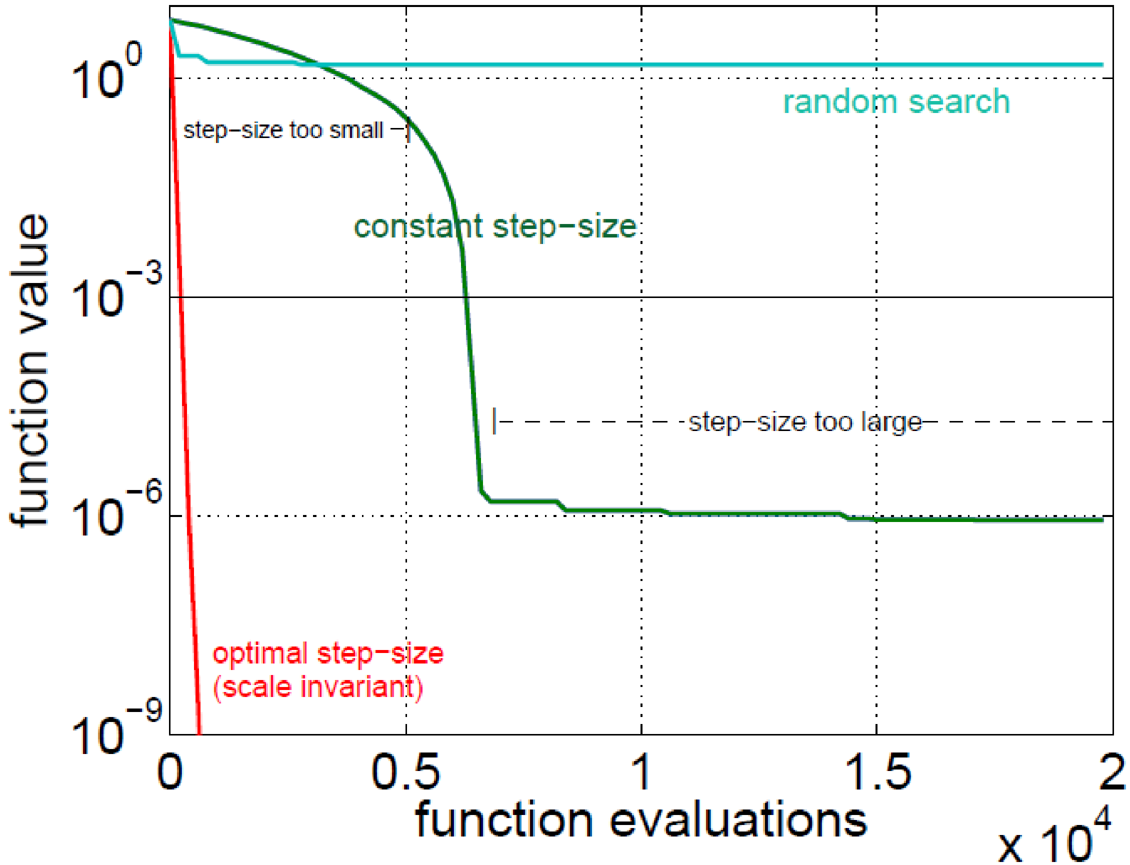
What do you think will happen for a (1+1)-ES with *constant* step-size?

$$f(\mathbf{x}) = \sum_{i=1}^{n} x_i^2$$

in $[-0.2, 0.8]^n$
for $n = 10$

from [Auger, p. 22]

Why Step-Size Control?

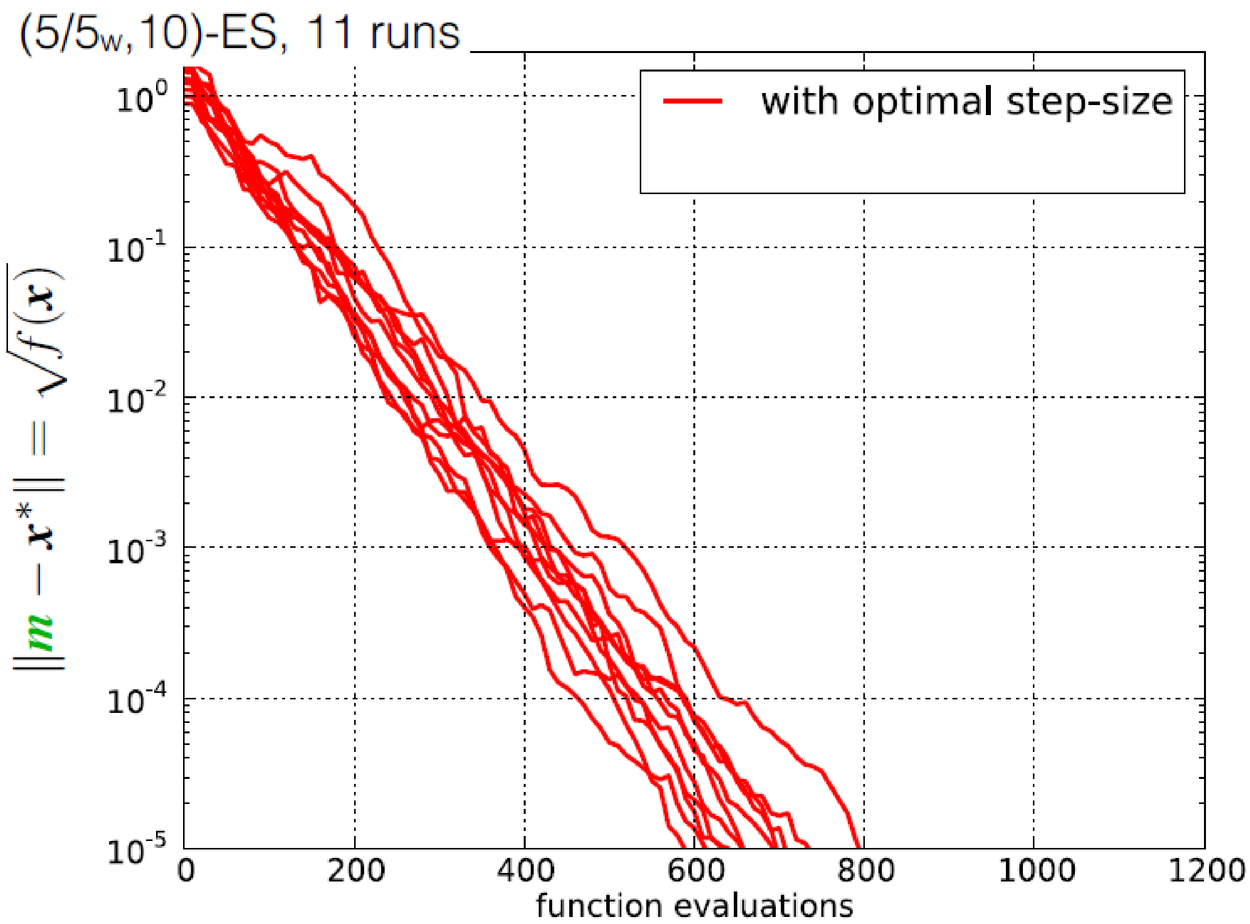


$$f(\mathbf{x}) = \sum_{i=1}^{n} x_i^2$$

in $[-0.2, 0.8]^n$
for $n = 10$

from [Auger, p. 22]

Why Step-Size Control?



$$f(\boldsymbol{x}) = \sum_{i=1}^{n} x_i^2$$

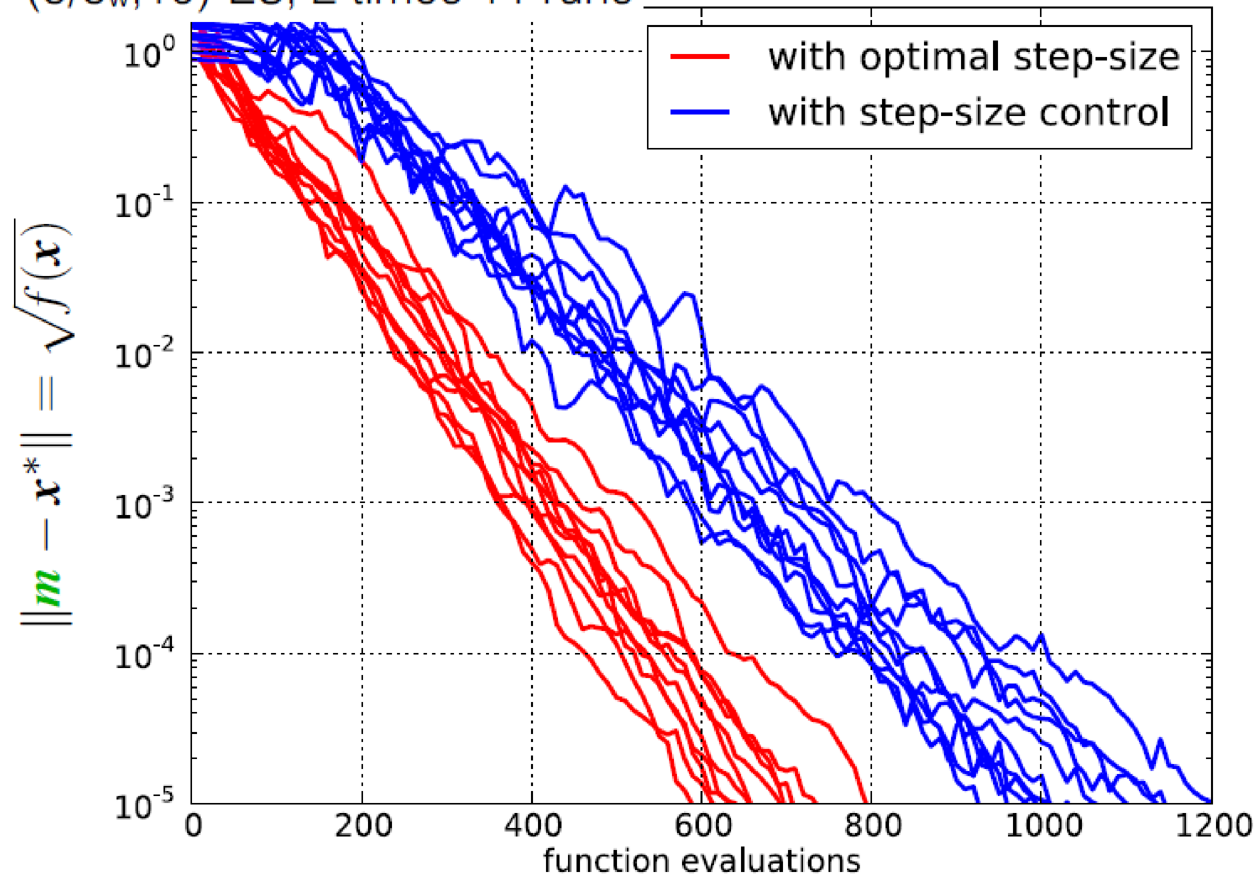
for $n = 10$ and $\boldsymbol{x}^0 \in [-0.2, 0.8]^n$

with optimal step-size σ

from [Hansen, p. 47]

Why Step-Size Control?

(5/5w,10)-ES, 2 times 11 runs



$$f(\boldsymbol{x}) = \sum_{i=1}^{n} x_i^2$$

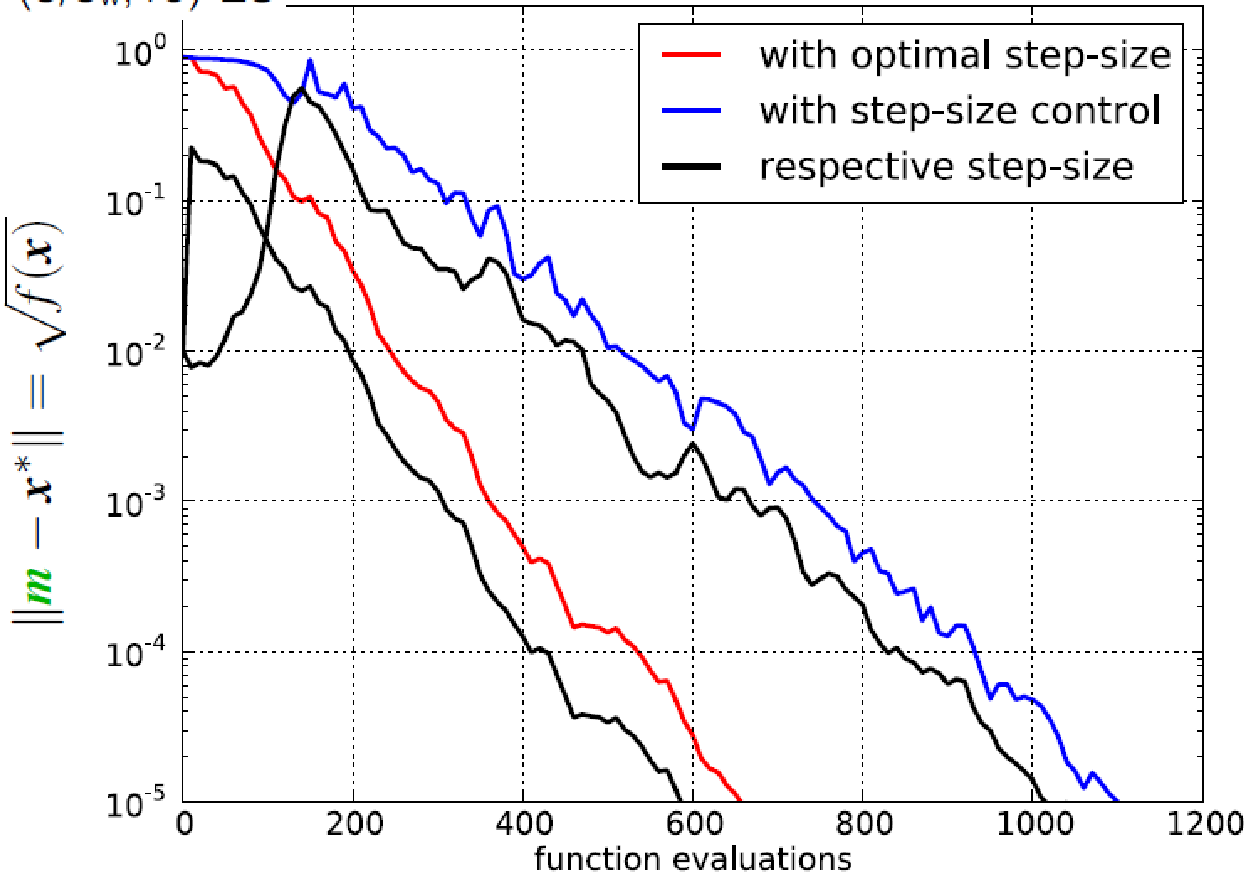
for $n = 10$ and $\boldsymbol{x}^0 \in [-0.2, 0.8]^n$

with optimal versus adaptive step-size σ with too small initial σ

from [Hansen, p. 48]

Why Step-Size Control?

(5/5w,10)-ES



$$f(\boldsymbol{x}) = \sum_{i=1}^{n} x_i^2$$

for $n = 10$ and $\boldsymbol{x}^0 \in [-0.2, 0.8]^n$

comparing number of f-evals to reach $\|\boldsymbol{m}\| = 10^{-5}$: $\frac{1100-100}{650} \approx$ 1.5

from [Hansen, p. 49]

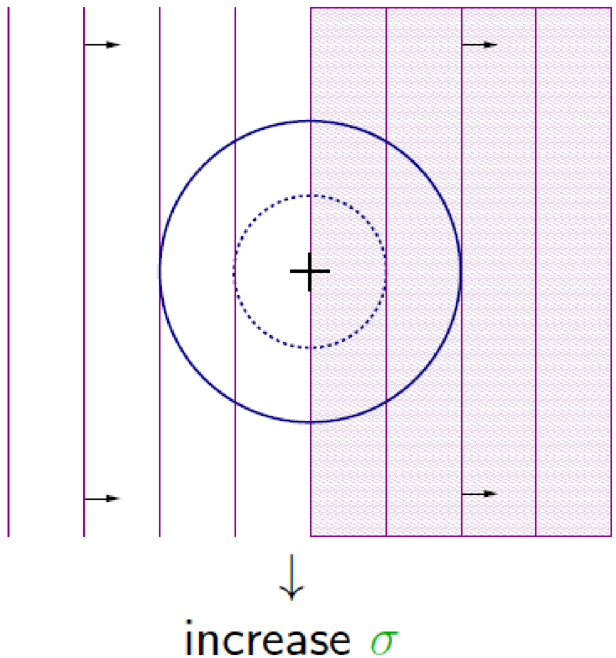
Adapting the Step-Size

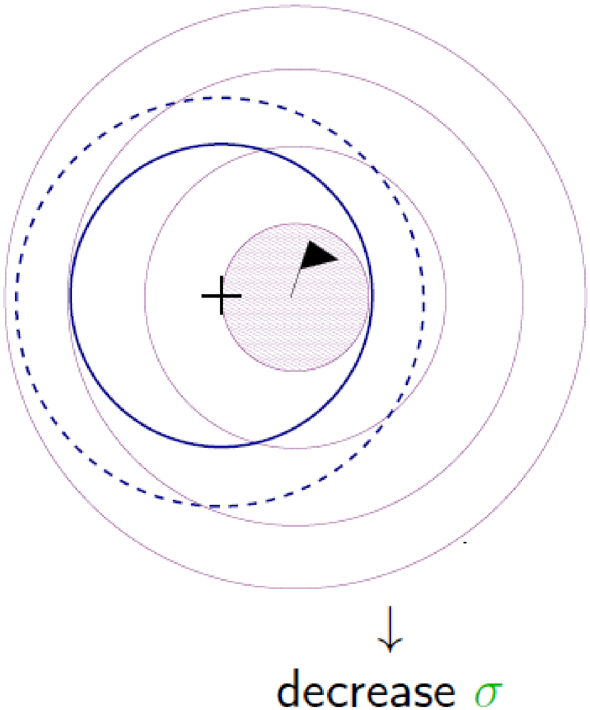
- How to actually adapt the step-size during the optimization?

Most common:

- 1/5 success rule
- Cumulative Step-Size Adaptation (CSA, as in standard CMA-ES)
- others possible (Two-Point Adaptation, self-adaptive step-size, ...)

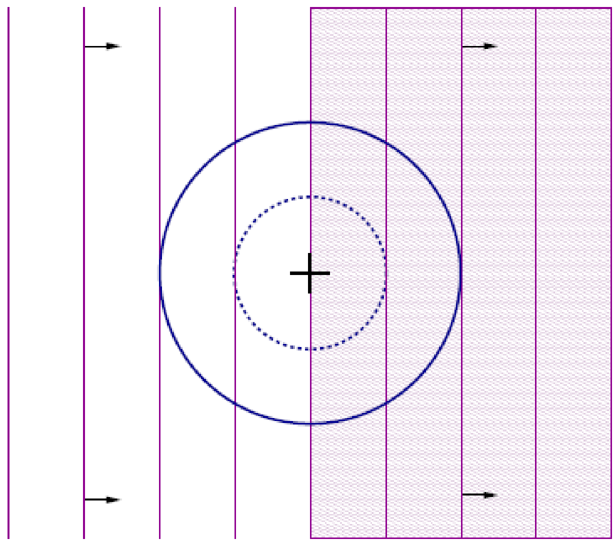
One-fifth success rule

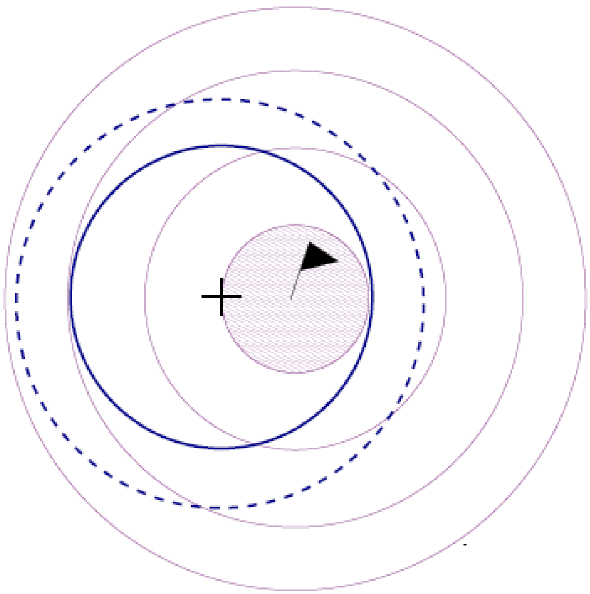




from [Auger, p. 32]

One-fifth success rule





Probability of success (p_s)

Probability of success (p_s)

1/2

1/5

"too small"

from [Auger, p. 33]

One-Fifth Success Rule

One-fifth success rule

p_s: # of successful offspring / # offspring (per generation)

$$\sigma \leftarrow \sigma \times \exp\left(\frac{1}{3} \times \frac{p_s - p_{\text{target}}}{1 - p_{\text{target}}}\right)$$

Increase σ if $p_s > p_{\text{target}}$
Decrease σ if $p_s < p_{\text{target}}$

$(1+1)$-ES

$p_{target} = 1/5$

IF *offspring better parent*

$p_s = 1$, $\sigma \leftarrow \sigma \times \exp(1/3)$

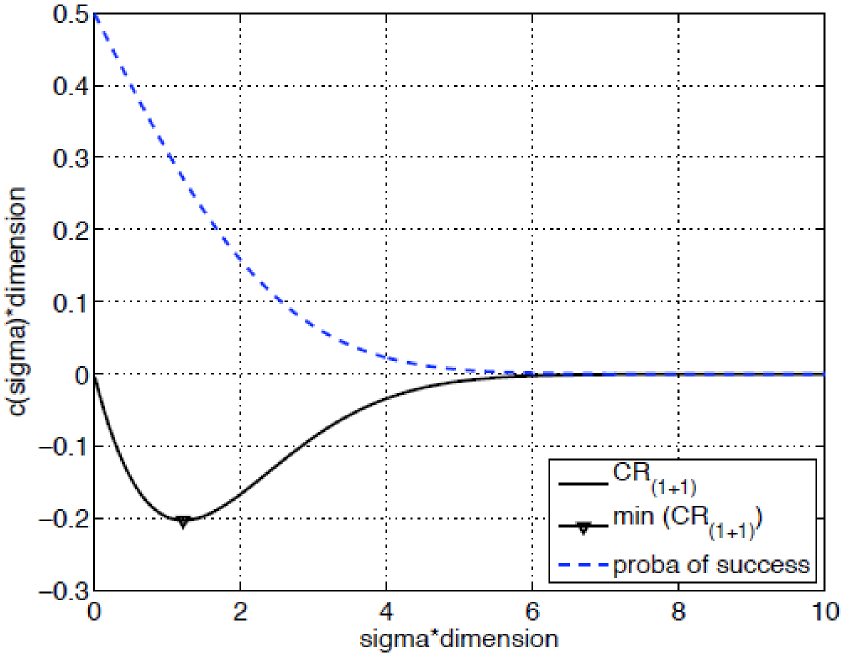
ELSE

$p_s = 0$, $\sigma \leftarrow \sigma / \exp(1/3)^{1/4}$

from [Auger, p. 34]

Why 1/5?

Asymptotic convergence rate and probability of success of scale-invariant step-size (1+1)-ES



sphere - asymptotic results, i.e. $n = \infty$ (see slides before)

1/5 trade-off of optimal probability of success on the sphere and corridor

from [Auger, p. 35]

Cumulative Step-Size Adaptation (CSA)

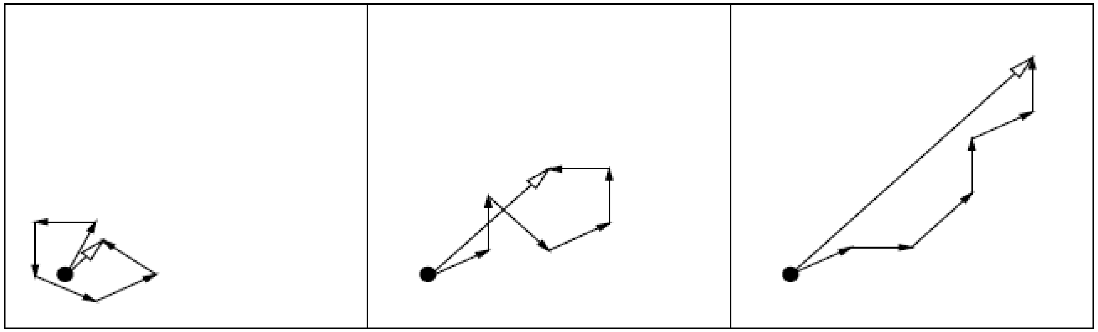
Path Length Control (CSA)

The Concept of Cumulative Step-Size Adaptation

$$\begin{aligned} \mathbf{x}_i &= \mathbf{m} + \sigma\, \mathbf{y}_i \\ \mathbf{m} &\leftarrow \mathbf{m} + \sigma\, \mathbf{y}_w \end{aligned}$$

Measure the length of the *evolution path*

the pathway of the mean vector $\mathbf{m}$ in the generation sequence



$\Downarrow$ decrease σ $\qquad\qquad$ $\Downarrow$ increase σ

from [Auger, p. 36]

Path Length Control (CSA)

The Equations

Initialize $\boldsymbol{m} \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, evolution path $\boldsymbol{p}_\sigma = \boldsymbol{0}$,
set $c_\sigma \approx 4/n$, $d_\sigma \approx 1$.

$$\boldsymbol{m} \leftarrow \boldsymbol{m} + \sigma \boldsymbol{y}_w \quad \text{where } \boldsymbol{y}_w = \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda} \qquad \text{update mean}$$

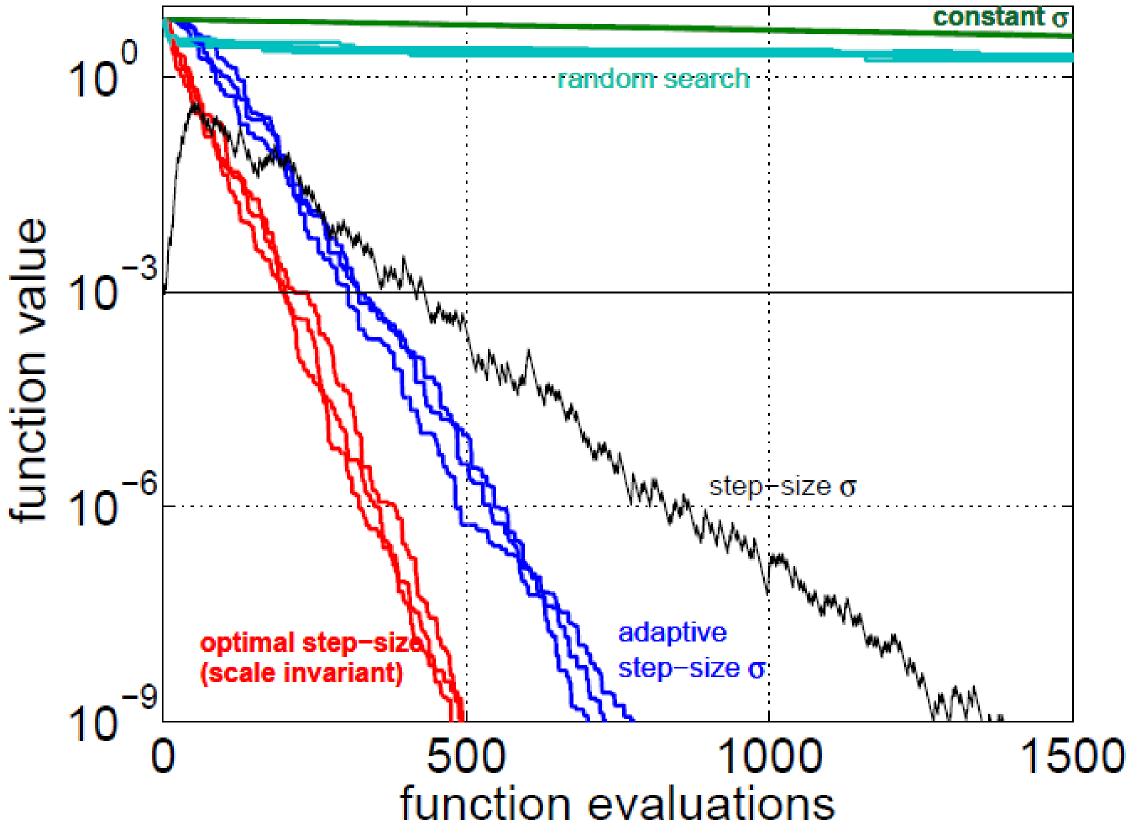
$$\boldsymbol{p}_\sigma \leftarrow (1 - c_\sigma)\, \boldsymbol{p}_\sigma + \underbrace{\sqrt{1 - (1 - c_\sigma)^2}}_{\text{accounts for } 1 - c_\sigma} \; \underbrace{\sqrt{\mu_w}}_{\text{accounts for } w_i} \; \boldsymbol{y}_w$$

$$\sigma \leftarrow \sigma \times \underbrace{\exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\|\boldsymbol{p}_\sigma\|}{\mathsf{E}\|\mathcal{N}(\boldsymbol{0}, \mathbf{I})\|} - 1\right)\right)}_{>1 \iff \|\boldsymbol{p}_\sigma\| \text{ is greater than its expectation}} \qquad \text{update step-size}$$

from [Auger, p. 37]

Step-size adaptation

What is achived



$$f(x) = \sum_{i=1}^{n} x_i^2$$

in $[-0.2, 0.8]^n$
for $n = 10$

Linear convergence

from [Auger, p. 38]

Covariance Matrix Adaptation

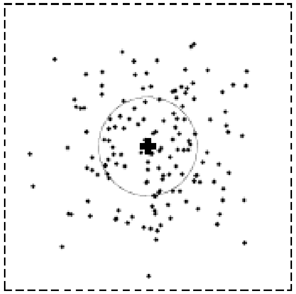
Recap CMA-ES: What We Have So Far

Evolution Strategies

Recalling

New search points are sampled normally distributed

$$x_i \sim m + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \qquad \text{for } i = 1, \ldots, \lambda$$



as perturbations of m, where $x_i, m \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, $\mathbf{C} \in \mathbb{R}^{n \times n}$

where

- the mean vector $m \in \mathbb{R}^n$ represents the favorite solution
- the so-called step-size $\sigma \in \mathbb{R}_+$ controls the *step length*
- the covariance matrix $\mathbf{C} \in \mathbb{R}^{n \times n}$ determines the shape of the distribution ellipsoid

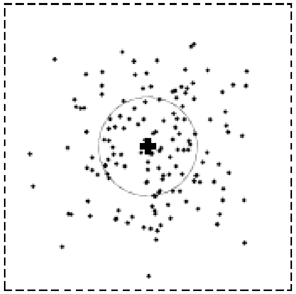
The remaining question is how to update $\mathbf{C}$.

from [Auger, p. 40]

Evolution Strategies

Recalling

New search points are sampled normally distributed



$$\boldsymbol{x}_i \sim \boldsymbol{m} + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \qquad \text{for } i = 1, \ldots, \lambda$$

as perturbations of $\boldsymbol{m}$, where $\boldsymbol{x}_i, \boldsymbol{m} \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, $\mathbf{C} \in \mathbb{R}^{n \times n}$

where

- the mean vector $\boldsymbol{m} \in \mathbb{R}^n$ represents the favorite solution
- the so-called step-size
- the covariance matrix
  of the distribution elli

...which is what we will see in the last lecture next Friday

The remaining question is how to update $\mathbf{C}$.

from [Auger, p. 40]