Separability

Given $f : x = (x_1, \ldots, x_n) \in \mathbb{R}^n \mapsto f(x) \in \mathbb{R}$, let us define the 1-D functions that are cuts of f along the different coordinates:

$$f^i_{(x^i_1,\ldots,x^i_n)}(y) = f(x^i_1, \ldots, x^i_{i-1}, y, x^i_{i+1}, \ldots, x^i_n)$$

for $(x^i_1, \ldots, x^i_n) \in \mathbb{R}^{n-1}$, with $(x^i_1, \ldots, x^i_n) = (x^i_1, \ldots, x^i_{i-1}, x^i_{i+1}, \ldots, x^i_n)$

Definition: A function f is **separable** if for all i, for all $(x^i_1, \ldots, x^i_n) \in \mathbb{R}^{n-1}$, for all $(\hat{x}^i_1, \ldots, \hat{x}^i_n) \in \mathbb{R}^{n-1}$

$$\text{argmin}_y f^i_{(x^i_1,\ldots,x^i_n)}(y) = \text{argmin}_y f^i_{(\hat{x}^i_1,\ldots,\hat{x}^i_n)}(y)$$

a weak definition of separability

Separability (cont)

Proposition: Let f be a **separable** then for all x_i^j

$$\operatorname{argmin} f(x_1, \ldots, x_n) = \left(\operatorname{argmin} f^1_{(x_2^1, \ldots, x_n^1)}(x_1), \ldots, \operatorname{argmin} f^n_{(x_1^n, \ldots, x_{n-1}^n)}(x_n) \right)$$

and f can be optimized using n minimization along the coordinates.

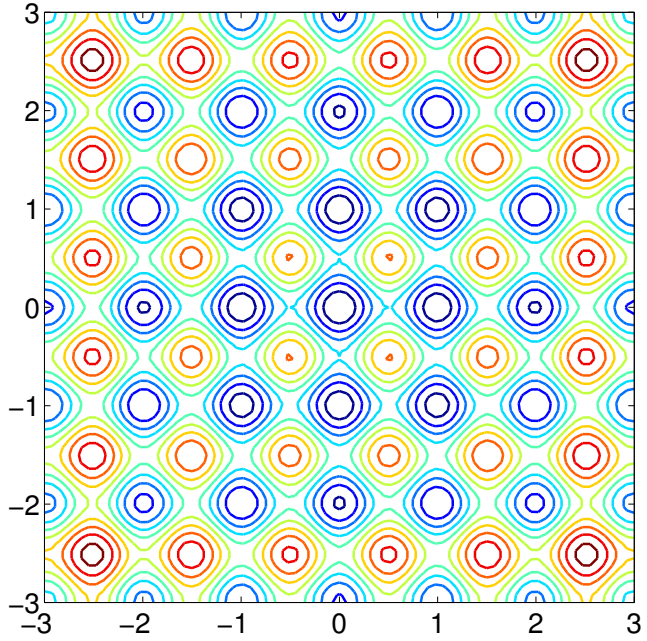
Exercice: prove the previous proposition

Example: Additively Decomposable Functions

Exercice: Let $f(x_1, \ldots, x_n) = \sum_{i=1}^{n} h_i(x_i)$ for h_i having a unique argmin. Prove that f is separable. We say in this case that f is additively decomposable.

Example: Rastrigin function

$$f(x) = 10n + \sum_{i=1}^{n} (x_i^2 - 10\cos(2\pi x_i))$$



Non-separable Problems

Separable problems are typically easy to optimize. Yet **difficult real-word problems are non-separable**.

One needs to be careful when evaluating optimization algorithms that not too many test functions are separable and if so that the *algorithms do not exploit separability*.

Otherwise: *good performance on test problems will not reflect good performance of the algorithm to solve difficult problems*

Algorithms known to exploit separability:

Many Genetic Algorithms (GA), Most Particle Swarm Optimization (PSO)

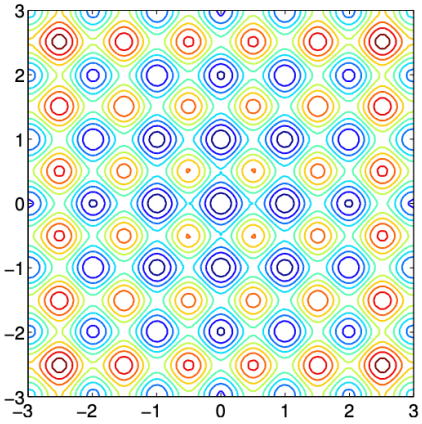
Non-separable Problems

Building a non-separable problem from a separable one

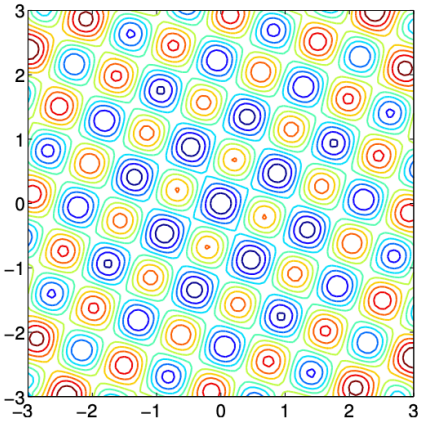
Rotating the coordinate system

- $f : \boldsymbol{x} \mapsto f(\boldsymbol{x})$ separable
- $f : \boldsymbol{x} \mapsto f(\mathbf{R}\boldsymbol{x})$ non-separable

$\mathbf{R}$ rotation matrix



$\mathbf{R}$ $\longrightarrow$



[1] Hansen, Ostermeier, Gawelczyk (1995). On the adaptation of arbitrary normal mutation distributions in evolution strategies: The generating set adaptation. Sixth ICGA, pp. 57-64, Morgan Kaufmann

[2] 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

Ill-conditioned Problems - Case of Convex-quadratic functions

Exercice: Consider a convex-quadratic function $f(x) = \frac{1}{2}(x - x^\star)H(x - x^\star)$ with H a symmetric, positive, definite (SPD) matrix.

1. why is it called a convex-quadratic function? What is the Hessian matrix of f ?

The condition number of the matrix H (with respect to the Euclidean norm) is defined as

$$\text{cond}(H) = \frac{\lambda_{\max}(H)}{\lambda_{\min}(H)}$$

with $\lambda_{\max}()$ and $\lambda_{\min}()$ being respectively the largest and smallest eigenvalues.

Ill-conditioned Problems

Ill-conditioned means a high condition number of the Hessian matrix H.

Consider now the specific case of the function $f(x) = \frac{1}{2}(x_1^2 + 9x_2^2)$

1. Compute its Hessian matrix, its condition number

2. Plots the level sets of f, relate the condition number to the axis ratio of the level sets of f

3. Generalize to a general convex-quadratic function

Real-world problems are often ill-conditioned.

4. Why to you think it is the case?

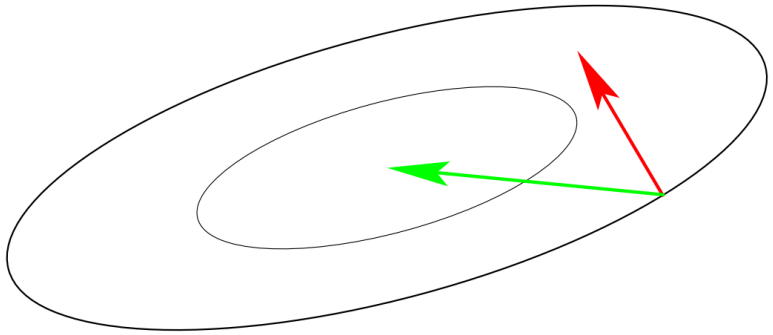
5. why are ill-conditioned problems difficult?

(see also **Exercice 2.5**)

Ill-conditioned Problems

consider the curvature of the level sets of a function

ill-conditioned means "squeezed" lines of equal function value (high curvatures)



gradient direction $-f'(\boldsymbol{x})^{\mathrm{T}}$

Newton direction
$-\boldsymbol{H}^{-1} f'(\boldsymbol{x})^{\mathrm{T}}$

Condition number equals nine here. Condition numbers up to 10^{10} are not unusual in real world problems.

Part II: Algorithms

Landscape of Derivative Free Optimization Algorithms

Deterministic Algorithms

Quasi-Newton with estimation of gradient (BFGS) [Broyden et al. 1970]

Simplex downhill [Nelder and Mead 1965]

Pattern search, Direct Search [Hooke and Jeeves 1961]

Trust-region/Model Based methods (NEWUOA, BOBYQA) [Powell, 06,09]

Stochastic (randomized) search methods

Evolutionary Algorithms (continuous domain)

- Differential Evolution [Storn, Price 1997]
- Particle Swarm Optimization [Kennedy and Eberhart 1995]
- **Evolution Strategies, CMA-ES** [Rechenberg 1965, Hansen, Ostermeier 2001]
- Estimation of Distribution Algorithms (EDAs) [Larrañaga, Lozano, 2002]
- Cross Entropy Method (same as EDAs) [Rubinstein, Kroese, 2004]
- Genetic Algorithms [Holland 1975, Goldberg 1989]

Simulated Annealing [Kirkpatrick et al. 1983]

A Generic Template for Stochastic Search

Define $\{P_\theta : \theta \in \Theta\}$, a family of probability distributions on $\mathbb{R}^n$

Generic template to optimize $f : \mathbb{R}^n \to \mathbb{R}$

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

While not terminate

1. Sample $x_1, \ldots, x_\lambda$ according to P_θ
2. Evaluate $x_1, \ldots, x_\lambda$ on f
3. Update parameters $\theta \leftarrow F(\theta, x_1, \ldots, x_\lambda, f(x_1), \ldots, f(x_\lambda))$

the update of θ should drive P_θ to concentrate on the optima of f

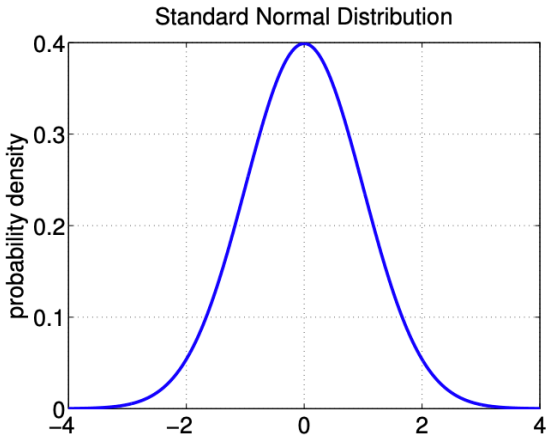
To obtain an optimization algorithm we need:

❶ to define $\{P_\theta, \theta \in \Theta\}$

❷ to define F the update function of θ

Which probability distribution to sample candidate solutions?

Normal distribution - 1D 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 $\mathcal{N}(\boldsymbol{m}, \sigma^2)$

(expected value, variance) $= (\boldsymbol{m}, \sigma^2)$

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

- 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 $\boldsymbol{m} + \sigma\mathcal{N}(0,1) = \mathcal{N}(\boldsymbol{m}, \sigma^2)$

Generalization to n Variables: Independent Case

Assume X1 ~ $\mathcal{N}(\mu_1, \sigma_1^2)$ denote its density $p(x_1) = \frac{1}{Z_1} \exp\left(-\frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2 \right)$

Assume X2~ $\mathcal{N}(\mu_2, \sigma_2^2)$ denote its density $p(x_2) = \frac{1}{Z_1} \exp\left(-\frac{1}{2\sigma_2^2}(x_2 - \mu_2)^2 \right)$

Assume X1 and X2 are **independent**, then (X1,X2) is a Gaussian vector with

$$p(x_1, x_2) =$$

Generalization to n Variables: Independent Case

Assume X1 ~ $\mathcal{N}(\mu_1, \sigma_1^2)$ denote its density $p(x_1) = \frac{1}{Z_1} \exp\left(-\frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2 \right)$

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Assume X1 and X2 are **independent**, then (X1,X2) is a Gaussian vector with

$$p(x_1, x_2) = p(x_1)p(x_2) = \frac{1}{Z_1 Z_2} \exp\left(-\frac{1}{2}(x - \mu)^T \Sigma^{-1} (x - \mu) \right)$$

with $x = (x_1, x_2)^T$ $\mu = (\mu_1, \mu_2)^T$ $\Sigma = \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix}$

Generalization to n Variables: Independent Case

Assume X1 ~ $\mathcal{N}(\mu_1, \sigma_1^2)$ denote its density $\quad p(x_1) = \frac{1}{Z_1} \exp\left(-\frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2 \right)$

Assume X2~ $\mathcal{N}(\mu_2, \sigma_2^2)$ denote its density $\quad p(x_2) = \frac{1}{Z_1} \exp\left(-\frac{1}{2\sigma_2^2}(x_2 - \mu_2)^2 \right)$

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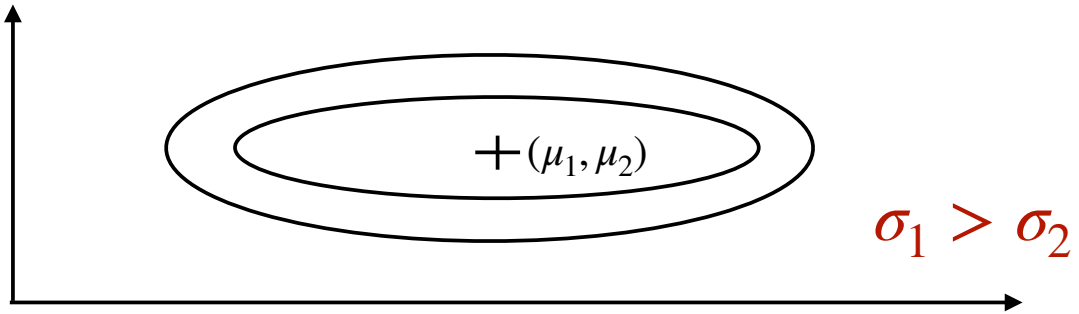
with $\quad x = (x_1, x_2)^T \qquad \mu = (\mu_1, \mu_2)^T \qquad \Sigma = \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix}$



Generalization to n Variables: General Case

Gaussian Vector - Multivariate Normal Distribution

A random vector $X = (X_1, \ldots, X_n) \in \mathbb{R}^n$ is a Gaussian vector (or multivariate normal) if and only if for all real numbers $a_1, \ldots, a_n$, the random variable $a_1X_1 + \ldots + a_nX_n$ has a normal distribution.

Gaussian Vector - Multivariate Normal Distribution

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)

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

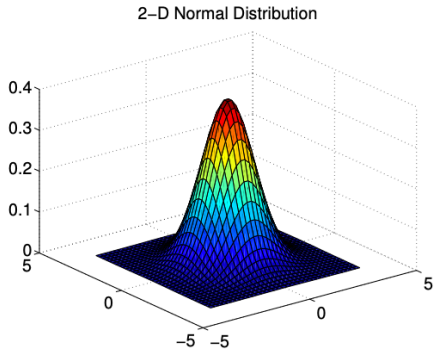
where $\mu_i = \mathrm{E}(X_i)$. Considering the expectation of a matrix as the expectation of each entry, we have

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

Σ is symmetric, positive definite

Density of a n-dimensional Gaussian vector $\mathcal{N}(m, C)$:

$$p_{\mathcal{N}(m.C)}(x) = \frac{1}{(2\pi)^{n/2}\,|\,C\,|^{1/2}} \exp\left(-\frac{1}{2}(x-m)^{\top} C^{-1}(x-m)\right)$$



The mean vector m:

determines the displacement

is the value with the largest density

the distribution is symmetric around the mean

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

The covariance matrix:

determines the geometrical shape (see next slides)

Geometry of a Gaussian Vector

Consider a Gaussian vector $\mathcal{N}(m, C)$, remind that lines of equal densities are given by:

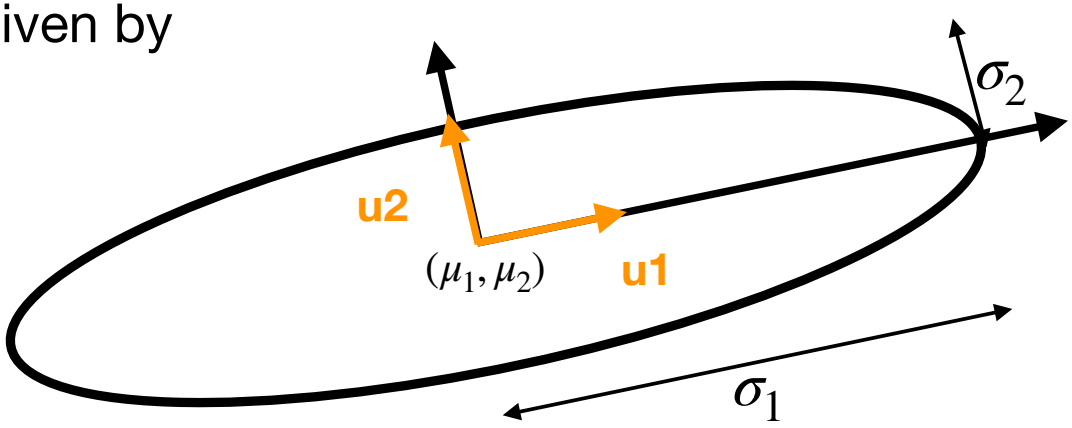
$$\{x \,|\, \Delta^2 = (x-m)^T C^{-1}(x-m) = \text{cst}\}$$

Decompose $C = U\Lambda U^\top$ with *U* orthogonal, i.e.

$$C = \begin{pmatrix} u_1 & u_2 \\ | & | \end{pmatrix} \begin{pmatrix} \sigma_1^2 & 0 \\ 0 | & \sigma_2^2 \end{pmatrix} \begin{pmatrix} u_1 & - \\ u_2 & - \end{pmatrix}$$

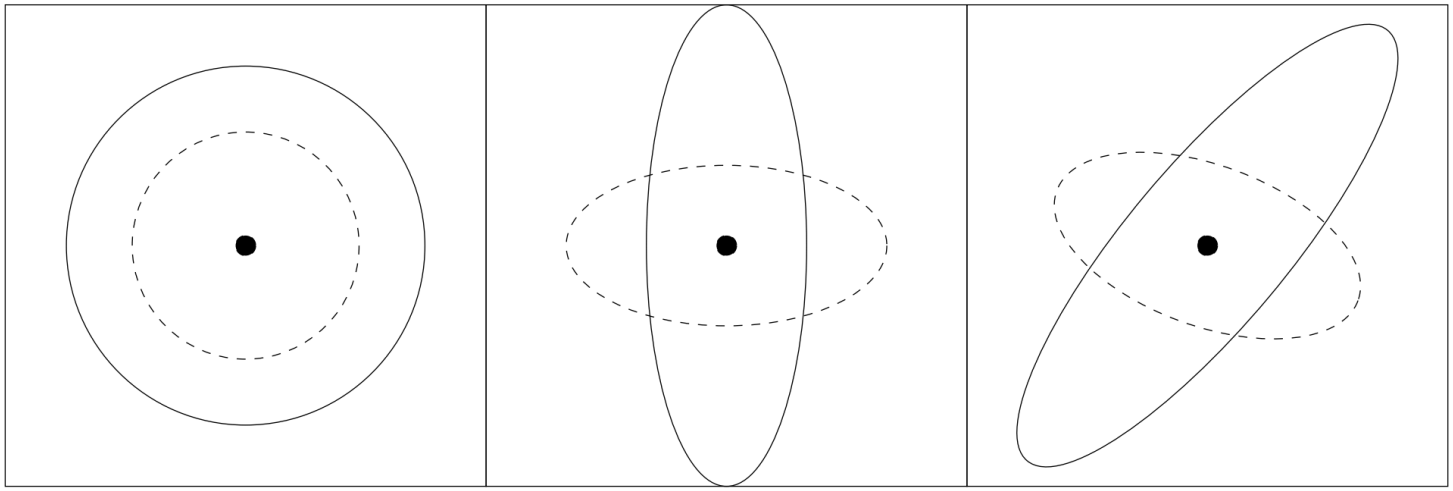
Let $Y = U^\top(x-m)$, then in the coordinate system, (u1,u2), the lines of equal densities are given by

$$\{x \,|\, \Delta^2 = \frac{Y_1^2}{\sigma_1^2} + \frac{Y_2^2}{\sigma_2^2} = \text{cst}\}$$



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

Lines of Equal Density



$\mathcal{N}(\boldsymbol{m}, \sigma^2 \mathbf{I}) \sim \boldsymbol{m} + \sigma \mathcal{N}(\mathbf{0}, \mathbf{I})$

one degree of freedom σ

components are independent standard normally distributed

$\mathcal{N}(\boldsymbol{m}, \mathbf{D}^2) \sim \boldsymbol{m} + \mathbf{D}\,\mathcal{N}(\mathbf{0}, \mathbf{I})$

n degrees of freedom

components are independent, scaled

$\mathcal{N}(\boldsymbol{m}, \mathbf{C}) \sim \boldsymbol{m} + \mathbf{C}^{\frac{1}{2}} \mathcal{N}(\mathbf{0}, \mathbf{I})$

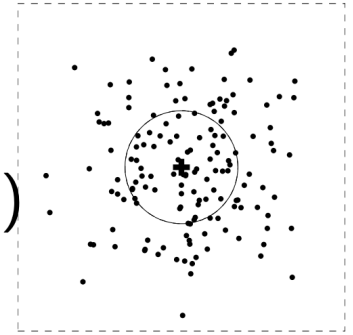
$(n^2 + n)/2$ degrees of freedom

components are correlated

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

Evolution Strategies

New search points are sampled normally distributed



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

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

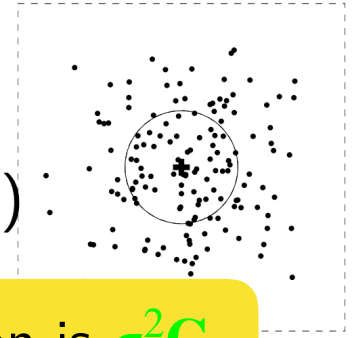
- the mean vector $\boldsymbol{m} \in \mathbb{R}^n$ represents the favorite solution
- the so-called step-size $\sigma \in \mathbb{R}_+$ controls the *step length*
- the covariance matrix $\mathbf{C} \in \mathbb{R}^{n \times n}$ determines the shape of the distribution ellipsoid

here, all new points are sampled with the same parameters

Evolution Strategies

New search points are sampled normally distributed

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



In fact, the covariance matrix of the sampling distribution is $\sigma^2\mathbf{C}$ but it is convenient to refer to $\mathbf{C}$ as the covariance matrix (it is a covariance matrix but not of the sampling distribution)

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

How to update the different parameters $m, \sigma, \mathbf{C}$?

Update the Mean: a Simple Algorithm the (1+1)-ES

Notation and Terminology:

one solution kept from one iteration to the next

(1+1)-ES

one new solution sampled at each iteration

The + means that we keep the best between current solution and new solution, we talk about *elitist* selection

(1+1)-ES algorithm (update of the mean)

sample one candidate solution from the mean $\mathbf{m}$

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

if $\mathbf{x}$ is better than $\mathbf{m}$ (i.e. if $f(\mathbf{x}) \leq f(\mathbf{m})$), select $\mathbf{m}$

$$\mathbf{m} \leftarrow \mathbf{x}$$

The (1+1)-ES algorithm is a simple algorithm, yet:

- the elitist selection is not robust to outliers

we cannot loose solutions accepted by "chance", for instance that look good because the noise gave it a low function value

- there is no population (just a single solution is sampled) which makes it less robust

In practice, one should rather use a:

$$(\mu/\mu, \lambda)\text{-ES}$$

The μ best solutions are selected and recombined (to form the new mean)

λ solutions are sampled at each iteration

The $(\mu/\mu, \lambda)$-ES - Update of the Mean Vector

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

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

Notation: we denote $\boldsymbol{y}_{i:\lambda}$ the vector such that $\boldsymbol{x}_{i:\lambda} = \boldsymbol{m} + \sigma \boldsymbol{y}_{i:\lambda}$

Exercice: realize that $\boldsymbol{y}_{i:\lambda}$ is generally not distributed as $\mathcal{N}(\mathbf{0}, \mathbf{C})$

The new mean reads

$$\boldsymbol{m} \leftarrow \sum_{i=1}^{\mu} w_i \, \boldsymbol{x}_{i:\lambda}$$

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.

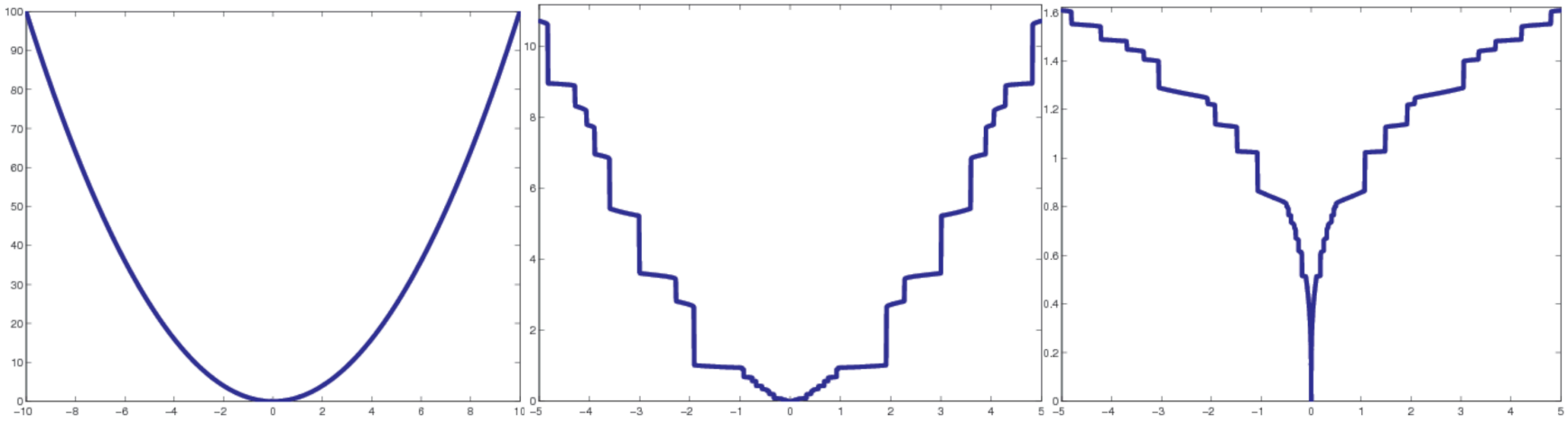
What changes in the previous slide if instead of optimizing f, we optimize $g \circ f$ where $g : \mathrm{Im}(f) \to \mathbb{R}$ is strictly increasing?

Invariance Under Monotonically Increasing Functions

Comparison-based/ranking-based algorithms:

Update of all parameters uses only the ranking:

$$f(x_{1:\lambda}) \leq f(x_{2:\lambda}) \leq \ldots \leq f(x_{\lambda:\lambda})$$



$$g(f(x_{1:\lambda})) \leq g(f(x_{2:\lambda})) \leq \ldots \leq g(f(x_{\lambda:\lambda}))$$

for all $g : \mathrm{Im}(f) \to \mathbb{R}$ strictly increasing

A Template for Comparison-based Stochastic Search

Define $\{P_\theta : \theta \in \Theta\}$, a family of probability distributions on $\mathbb{R}^n$

Generic template to optimize $f : \mathbb{R}^n \to \mathbb{R}$

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

While not terminate

1. Sample $x_1, \ldots, x_\lambda$ according to P_θ
2. Evaluate $x_1, \ldots, x_\lambda$ on f
3. Rank the solutions and find π the permutation such
$$f(x_{\pi(1)}) \leq f(x_{\pi(2)}) \leq \ldots \leq f(x_{\pi(\lambda)})$$
4. Update parameters $\theta \leftarrow F(\theta, x_1, \ldots, x_\lambda, \pi)$