Numerical optimization : Gradient descents

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Outline of the day

- Numerical optimization :
  White-box scenario : gradient descents
  Black-box scenario : evolutionary algorithms

Single-objective optimization

Definition

An optimization problem is a couple $(\mathcal{X}, f)$ with :

- Search space : set of candidate solutions

$$\mathcal{X}$$

- Objective fonction : quality criteria (or non-quality)

$$f : \mathcal{X} \to \mathbb{R}$$

Solve an optimization problem (minimization)

$$\mathcal{X}^\star = \text{argmin}_{\mathcal{X}} \ f$$

or find an approximation of $\mathcal{X}^\star$.

White-box optimization scenario

Objective function f for $x \in \mathbb{R}^d$,

$$f(x) = \frac{x_2^3 e^{-0.4x_1}}{\sum_k e^{x_k}}$$

White-box optimization definition

Analytic expression of the objective function f is known

In this case, usually the objective fonction is :

- continuous, and differentiable (if we are lucky)

Black-box optimization scenario

$x \longrightarrow$  $\longrightarrow f(x)$

No information on the objective function definition f

Objective fonction :

- can be irregular, non continuous, non differentiable ...
- given by a computation or a simulation

Typology of optimization problems

Classification according to decision variables

- **Combinatorial optimisation** :
  search space is discrete (sometime finite) : NP-hard
- **Numerical optimization** :
  search space is subset of $\mathbb{R}^d$
- **Others** :
  discrete and numerical, program, morphology, topology, etc.

Classification according to information

- **White-box optimisation** :
  Some useful properties are known
- **Black-box optimization** :
  A minimum of *a priori* information is used
  Computation time can be expensive (simulator, in vivo, etc.)
- **Grey-box optimization** : in between

Numerical optimization

Definition : numerical optimization problem

An numerical optimization problem is a couple $(\mathcal{X}, f)$ with :

- Search space : set of candidate solutions

$$\mathcal{X} \text{ connected subset of } \mathbb{R}^d$$

- Objective fonction : quality criteria, minimization

$$f : \mathbb{R}^d \to \mathbb{R}$$

Minimization algorithms in white-box scenario

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Cours master 1, optimisation numérique :
http://www.math.univ-montp2.fr/~di-pietro/Teaching.html

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http://sebastianruder.com/optimizing-gradient-descent/index.html

Descent direction

Definition : descent direction

Let be $\mathcal{X} \subset \mathbb{R}^n$, $f : \mathcal{X} \to \mathbb{R}$, and $x \in \mathcal{X}$.

$w \in \mathcal{X} \setminus \{0\}$ is a descent direction in x when :
it exists a real number $\sigma_0 > 0$ such that :

$$\forall \sigma \in [0, \sigma_0], \quad f(x + \sigma\ w) \leqslant f(x)$$

Descent direction

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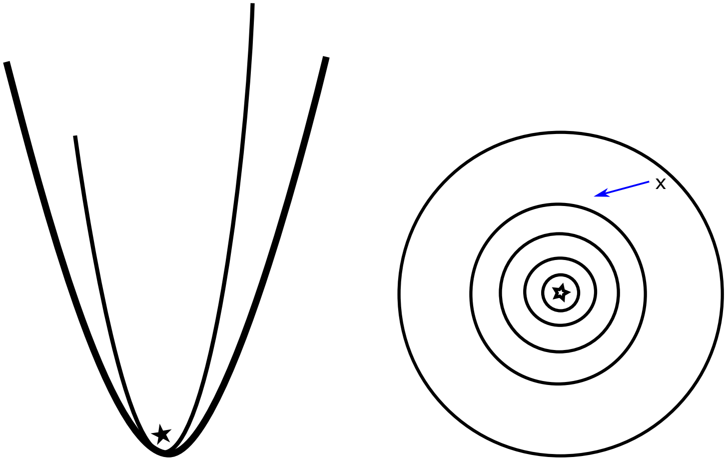
Definition : strict descent direction

Let be $\mathcal{X} \subset \mathbb{R}^n$, $f : \mathcal{X} \to \mathbb{R}$, and $x \in \mathcal{X}$.

$w \in \mathcal{X} \setminus \{0\}$ is strict descent direction in x when :
it exists a real number $\sigma_0 > 0$ such that :

$$\forall \sigma \in [0, \sigma_0], \quad f(x + \sigma \; w) < f(x)$$

Descent direction



Descent algorithm

Descent Algorithm

Choose an initial solution $x \in \mathcal{X}$
repeat
  Find a strict descent direction in x : $w \in \mathcal{X} \setminus \{0\}$
  Choose a real number $\sigma > 0$
  $x \leftarrow x + \sigma \ w$
until stopping criterium is false

Descent algorithm

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  Find a strict descent direction in x : $w \in \mathcal{X} \setminus \{0\}$
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  $x \leftarrow x + \sigma\ w$
until stopping criterium is false

Open questions :

- How to choose the descent direction w as a function of x ?
- How to choose the step size σ ?
- How to define the stopping criterium ?

Gradient direction

Intuitions

from physic,

the **gradient** shows the speed vector of the trajectory (surface),

i.e. the direction, the way, and the amplitude of the speed vector of the surface.

Formal definition

If f is differentiable in $x \in \mathbb{R}^d$,

the gradient of f in x is equal to :

$$\nabla f(x) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \dots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

Gradient : first example

$$f(x) = 2 + 4x_1 + x_2 + 2x_1^2 + 2x_1x_2 + x_1^2x_2$$

Gradient : first example

$f(x) = 2 + 4x_1 + x_2 + 2x_1^2 + 2x_1x_2 + x_1^2x_2$

$$\nabla f(x) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{pmatrix}$$

with :

$\frac{\partial f}{\partial x_1} = 4 + 4x_1 + 2x_2 + 2x_1x_2$

$\frac{\partial f}{\partial x_2} = 1 + 2x_1 + x_1^2$

Gradient : Mean Square Error example

Multiple linear regression on data $\{(x_i, y_i) \mid i \in \{1, \ldots, n\}\}$
with linear model $m_\beta(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$

Mean Square Error function :

$$f(\beta) = \frac{1}{2n} \sum_{i=1}^{n} (m_\beta(x_i) - y_i)^2$$

$$f(\beta) = \frac{1}{2n} \sum_{i=1}^{n} (\beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} - y_i)^2$$

Gradient : Mean Square Error example

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$$\nabla f(\beta) = \begin{pmatrix} \frac{\partial f}{\partial \beta_0} \\ \frac{\partial f}{\partial \beta_1} \\ \frac{\partial f}{\partial \beta_2} \end{pmatrix}$$

Gradient : Mean Square Error example

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Mean Square Error function :

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$$f(\beta) = \frac{1}{2n} \sum_{i=1}^{n} (\beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} - y_i)^2$$

with :

$\frac{\partial f}{\partial \beta_0} = \frac{1}{n} \sum_{i=1}^{n} (\beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} - y_i)$

$\frac{\partial f}{\partial \beta_1} = \frac{1}{n} \sum_{i=1}^{n} x_{i,1} (\beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} - y_i)$

$\frac{\partial f}{\partial \beta_2} = \frac{1}{n} \sum_{i=1}^{n} x_{i,2} (\beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} - y_i)$

Gradient, and descent directions

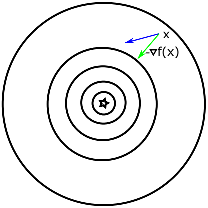
Result

Let be f a continuously differentiable function on open set with $x \in \mathbb{R}$. The notation . is the scalar production on $\mathbb{R}^d$.

If $w \in \mathcal{X} \setminus \{0\}$ is a descent direction,
then $\nabla f(x).w \leqslant 0$

gradient vector is at the opposite direction of descent direction.

If $\nabla f(x) \neq 0$,
then $w = -\nabla f(x)$ is strict descent direction in x.



Method of gradient descent

Algorithm of gradient descent

Choose initial solution $x \in \mathcal{X}$

repeat

$w \leftarrow -\nabla f(x)$

Choose a real number $\sigma > 0$

$x \leftarrow x + \sigma \; w$

until stopping criterium is false

Method of gradient descent

Algorithm of gradient descent

Choose initial solution $x \in \mathcal{X}$
repeat
$w \leftarrow -\nabla f(x)$
Choose a real number $\sigma > 0$
$x \leftarrow x + \sigma \ w$
until stopping criterium is false

Open questions :

- How to choose the step size σ ?
- How to define the stopping criterium ?

Gradient descent with fix step size

Algorithm of gradient descent with fix step size

Choose a step size $\sigma \in \mathbb{R}^+$
Choose initial solution $x \in \mathcal{X}$
repeat
  $w \leftarrow -\nabla f(x)$
  $x \leftarrow x + \sigma \; w$
until stopping criterium is false

- Define the gradient function of the two examples
- Code the gradient descent algorithm
- Test the gradient descent on the two examples

Gradient descent with fix step size

Algorithm of gradient descent with fix step size

Choose a step size $\sigma \in \mathbb{R}^+$
Choose initial solution $x \in \mathcal{X}$
repeat
  $w \leftarrow -\nabla f(x)$
  $x \leftarrow x + \sigma \ w$
until stopping criterium is false

Open questions :

- How to choose the step size σ ?
- How to define the stopping criterium ?

Step size : basic, and simple case

When the expression of f is simple,
compute directly by "hand" with algebra/analysis,

$$\sigma = \text{argmin}_{\sigma > 0} f(x - \sigma \nabla f(x))$$

Step size : in practice, most of the time

Try and test

From large value of σ,
decrease by a factor τ until the value of σ is relevant.

Choose a $\tau \in]0, 1[$
Choose initial σ
while $f(x - \sigma \nabla f(x)) > f(x)$ **do**
  $\sigma = \tau\sigma$
end while

- Code the step size adaptation

Newton Method (1669)

Newton algorithm (dimension 1)

Choose initial solution $x \in \mathcal{X}$
repeat
$w \leftarrow \frac{-1}{f''(x)} f'(x)$
$x \leftarrow x + w$
until stopping criterium is false

Newton algorithm (dimension n)

Choose initial solution $x \in \mathcal{X}$
repeat
$w \leftarrow -[H(f)(x)]^{-1} \nabla f(x)$
$x \leftarrow x + w$
until stopping criterium is false

H is the Hersian matrix (matrix of second order partial derivatives)

- Code a Newton descent on two examples

Variants and improvements of gradient descent

- (Batch) gradient descent :
  $\nabla f(\theta) = \mathbb{E}_{j \in 1 \ldots p}[\frac{\partial f}{\partial \theta}(\theta; x^{(j)}, y^{(j)})]\,; \quad \theta \leftarrow \theta + \sigma\ \nabla f(\theta)$
- Stochastic gradient descent :
  $\nabla f(\theta; j) = \frac{\partial f}{\partial \theta}(\theta; x^{(j)}, y^{(j)})\,;$
  $\forall j$ rnd order, $\theta \leftarrow \theta + \sigma\ \nabla f(\theta; j)$
- Momentum gradient descent :
  $v_t = \gamma v_{t-1} + \sigma \nabla f(\theta)\,; \quad \theta \leftarrow \theta - v_t$
- Nesterov accelerated gradient descent (NAG) :
  $v_t = \gamma v_{t-1} + \sigma \nabla f(\theta - \gamma v_{t-1})\,; \quad \theta \leftarrow \theta - v_t$
- Adagrad gradient descent :
  $g_{t,i} = \nabla_i f(\theta)\,;\ \ G_{t,ii} = \sum_{t' \leqslant t} g_{t',i}^2\,;\ \ \forall i,\ \theta_i \leftarrow \theta_i - \frac{\sigma}{\sqrt{G_{t,ii} + \epsilon}} g_{t,i}$
- AdaDelta gradient descent :
  $E[g^2]_t = \gamma E[g^2]_{t-1} + (1-\gamma) g_t^2\,;$
  $E[\Delta\theta^2]_t = \gamma E[\Delta\theta^2]_{t-1} + (1-\gamma)\Delta\theta_t^2\,;$
  $\Delta\theta_t = -\frac{\sqrt{E[\Delta\theta^2]_{t-1} + \epsilon}}{\sqrt{E[g^2]_t + \epsilon}} g_t\,;\ \ \theta_t \leftarrow \theta_{t-1} + \Delta\theta_t$

Variants and improvements of gradient descent

- Adam gradient descent :
  $m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t$; $v_t = \beta_2 v_{t-1} + (1-\beta_2) g_t^2$;
  $\hat{m}_t = m_t/(1-\beta_1^t)$; $\hat{v}_t = v_t/(1-\beta_2^t)$; $\theta_{t+1} = \theta_t - \frac{\sigma}{\sqrt{v_t}+\epsilon}\hat{m}_t$
- AdaMax gradient descent :
  $m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t$; $v_t = \max(\beta_2 v_{t-1}, |g_t|)$;
  $\hat{m}_t = m_t/(1-\beta_1^t)$; $\theta_{t+1} = \theta_t - \frac{\sigma}{v_t}\hat{m}_t$
- Nadam gradient descent :
  $m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t$; $v_t = \beta_2 v_{t-1} + (1-\beta_2) g_t^2$;
  $\hat{m}_t = m_t/(1-\beta_1^t)$; $\hat{v}_t = v_t/(1-\beta_2^t)$;
  $\theta_{t+1} = \theta_t - \frac{\sigma}{\sqrt{v_t}+\epsilon}(\beta_1 \hat{m}_t + \frac{(1-\beta_1)g_t}{1-\beta_1^t})$

Black-box optimization scenario

$x \longrightarrow$  $\longrightarrow f(x)$

No information on the objective function definition f

Objective fonction :

- can be irregular, non continuous, non differentiable ...
- given by a computation or a simulation

Optimization methods

- Bayesian optimization :
  Jonas Mockus, 1970 - 1980, well-known Kriging method
  0. Function is represented as random function
  1. Assume a prior of the behavior of function
  2. Sample some x
  3. Update the post-perior the distribution
- Evolutionary algorithm :
  Bio-inspired algorithms
  (genetic algorithm, evo. strategy, genetic prog., etc.)
  ES : Ingo Rechenberg, Hans-Paul Schwefel, early 1960

Introduction to evolution strategy

Bibliography :

Summer school on artificial evolution

Anne Auger, june 2012 :
https://sites.google.com/site/ecoleea2012/programme

Evolutionary algorithm : evolution strategy

Evolutionary algorithm

Choose initial population Parents *i.e. set of solutions*
repeat
  Genitors = select(Parents)
  Children = random variation (Genitors)
  Parents = replacement(Children, Parents)
until stopping criterium is false

Evolution strategy (continuous optimization)

Initialize distribution parameter θ
repeat
  Sample population $(x_1, \ldots, x_\lambda)$ using distribution $P(x|\theta)$
  Evaluate $(x_1, \ldots, x_\lambda)$ on f
  Update parameter $\theta = F_\theta(\theta, x_1, \ldots, x_\lambda, f(x_1), \ldots, f(x_\lambda))$
until stopping criterium is false

$(1+1)$-Evolution Strategy

Basic idea

Parameter $\theta = m$:

current position of the best known candidate solution

Iterate :

1. Sample one solution "around" m
2. If better, update parameter m

$(1+1)$-Evolution Strategy

Basic idea

Parameter $\theta = m$:

current position of the best known candidate solution

Iterate :

1. Sample one solution "around" m
2. If better, update parameter m

Basic version of $(1+1)$-Evolution Strategy

Choose initial mean $m \in \mathbb{R}^d$
repeat
  $x' \leftarrow Norm_d(m, \sigma^2)$
  if $f(x')$ is better than $f(m)$ **then**
    $m \leftarrow x'$
  end if
until stopping criterium is false

$(1+1)$-Evolution Strategy

Basic version of $(1+1)$-Evolution Strategy

Choose initial mean $m \in \mathbb{R}^d$
repeat
    $x^{'} \leftarrow Norm_d(m, \sigma^2)$
    if $f(x^{'})$ is better than $f(m)$ **then**
        $m \leftarrow x^{'}$
    end if
until stopping criterium is false

From the previous jupyter notebook,

- Code the basic $(1+1)$-ES
- Test the code on the 2 examples with different step sizes

$(1+1)$-Evolution Strategy

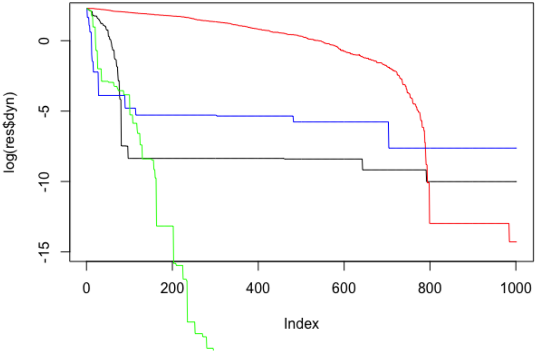
$(1+1)$-ES

Choose randomly initial mean $m \in \mathbb{R}^d$
repeat
  $x^{'} \leftarrow Norm_d(m, \sigma.C)$
  if $f(x^{'})$ is better than $f(m)$ **then**
    $m \leftarrow x^{'}$
  end if
until stopping criterium is false

Parameters of the algorithm :
  $\sigma \in \mathbb{R}$: step size
  Matrice $C \in \mathbb{R}^{d \times d}$: covariance matrix

Open questions :
  How to choose the step size ?
  How to choose the covariance matrix ?

Search dynamic according to step size



- black : $\sigma = 0.1$
- red : $\sigma = 0.01$
- blue : $\sigma = 0.5$
- green : adaptive σ

$(1+1)$-Evolution Strategy with One-fifth success rule

$(1+1)$-Evolution Strategy with $1/5$ success rule

Choose randomly initial solution $m \in \mathbb{R}^n$
repeat
  $x^{'} \leftarrow m + \sigma \, \mathcal{N}_d(0, C)$
  if $x^{'}$ is better than m **then**
    $m \leftarrow x^{'}$
    $\sigma \leftarrow \sigma \times exp(1/3)$
  else
    $\sigma \leftarrow \sigma / exp(1/3)^{1/4}$
  end if
until stopping criterium is false

From the previous jupyter notebook,

- Code the basic $(1+1)$-ES with $1/5$ success rule
- Compare the results with fix step size

Larger populations : $(\mu/\mu, \lambda)$-Evolution Strategy

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

Choose randomly initial mean $m \in \mathbb{R}^n$
repeat
  for $i \in \{1 \dots \lambda\}$ **do**
    $x_i' \leftarrow m + \sigma \, \mathcal{N}_d(0, C)$
    Evaluate x_i' with f
  end for
  Select the μ best solutions from $\{x_1', \dots, x_\lambda'\}$
  Let be $x_{:j}$ those solutions ranking by increasing order of f :
    $f(x_{:1}) \leq \dots \leq f(x_{:\mu})$

  $m \leftarrow \sum_{j=1}^{\mu} w_j x_{:j}'$
until stopping criterium is false

avec $\hat{w}_i = \log(\mu + 0.5) - \log(i)$ et $w_i = \hat{w}_i / \sum_{i=1}^{\mu} \hat{w}_i$

Advanced Evolution Strategy : CMA-ES

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

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

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

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

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

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

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

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