An introduction to optimization for machine learning

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Foreword

This course was given during a summer school on AI in Godomey, Benin, July-Aug. 2025. The school was organized by the Benin Excellence NGO and the Vallet Foundation (cf.

https://www.fondationvallet.org/eeia).

- The course provides basic concepts for numerical optimization
- for an audience interested in machine learning
- with a background corresponding to 1 year after high school
- through examples coded in python from scratch.
- Limitation: the algorithms are not exactly those used in state-of-the-art deep learning, but the main concepts, related to gradient descent, will be presented.

The code, the slides and the project statement are available at https://github.com/ML-for-B-E/Optimisation

Course outline

An introduction to optimization for machine learning

- Introduction
 - Objectives, acknowledgements
 - Optimization problem formulation
 - Examples of optimization usages
 - Basic mathematical concepts for optimization

- 2 Steepest descent algorithm
 - Fixed step steepest descent algorithm
- Line search Improved gradient based searches
 - Search directions for acceleration
 - A word about constraints
 - Making it more global: restarts
- 4 Application to neural network
- Bibliography

Optimization = a quantitative formulation of decision

Optimization is a¹ way of mathematically modeling decision.

$$\min_{x \in \mathcal{S}} f(x)$$



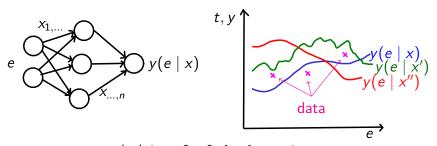
- x vector of decision parameters (variables):
 dimensions, investment, tuning of a
 machine / program, . . .
- f(x): decision cost x
- S: set of possible values for x, search space

¹non unique, incomplete when considering human beings_or life → ◆ ≥ → ∞ 0

Example of optimization : Learning as optimization

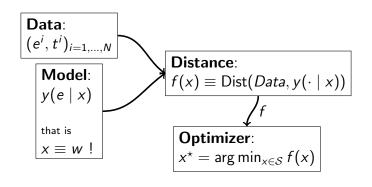
Neural net as a parameterized function

Find x, the weights and biases of the Neural Network (NN) so that the function $y(\cdot \mid x)$ approaches the observed data



where $y(e \mid x) = X^L \Phi^L (\dots \Phi^2 (X^2 \Phi^1 (X^1 e)) \dots)$, X^1, \dots, X^L the weights/biases arranged as matrices for each of the L layers, Φ^i is a vector of activation functions (reLU, linear, sigmoid, leaky reLU) for the i-th layer.

Learning as optimization: the big picture

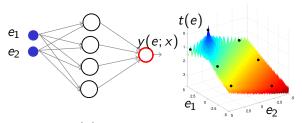


 \Rightarrow Learned model : $y(\cdot; x^*)$

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Optimization example: neural net regression

learn a function from a discrete limited set of observations



- ullet e entries or inputs, $t(e) \in \mathbb{R}$ target function to learn
- Observed data set, ":" : $(e^i, t^i \equiv t(e^i))$, i = 1, ..., N
- Model y(e; x): a NN with inputs e and weights & biases x, supposed to mimick t(e)
- Distance data-model as sum-of-squares error:

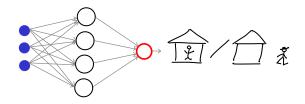
$$f(x) = \frac{1}{2N} \sum_{i=1}^{N} (t^{i} - y(e^{i}; x))^{2}$$



Optimization example: NN classification (1/3)

Ex: Predict if a person stays at home or goes out based on longitude, latitude and temperature = a 2 classes (out/in) classification problem.

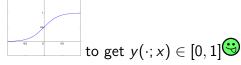
TP: Predict gender based on a person's measurements.



- e entries (ex: e_1 longitude, e_2 latitude, e_3 temperature)
- $t(e) \in \{0,1\}$ target function to learn (t=1) if person stays, t=0 otherwise)
- Observed data set: (e^i, t^i) , i = 1, ..., N

Optimization example: NN classification (2/3)

- y(e;x): output of the NN $\in \mathbb{R} \neq \{0,1\}$: the space of the function to learn is discrete, that of the NN is continuous
- Trick: predict the probability that t(e) = 1. This probability is in [0,1] which is continuous ... yet bounded
- Logistic regression trick: pass the NN output through a sigmoid



• Benefit: the model has a probabilistic interpretation. y(e; x) is the probability that t(e) = 1, t(e) Bernouilli variable.

Optimization example: NN classification (3/3)

Cross-entropy error as model-data distance:

$$f(x) = -\sum_{i=1}^{N} \{t^{i} \log(y(e^{i}; x)) + (1 - t^{i}) \log(1 - y(e^{i}; x))\}$$

Proof:

- y(e;x) is the probability that t(e)=1, 1-y(e;x) is the probathat t(e)=0, $0 \le y(e;x) \le 1$.
- The probability of t knowing e can be written $y(e;x)^t \times (1-y(e;x))^{1-t}$
- The likelihood of the N i.i.d observations is $\prod_{i=1}^{N} \left[y(e^i; x)^{t^i} \times (1 y(e^i; x))^{1-t^i} \right], \text{ to be maximized}$
- The likelihood is turned into an error, to be minimized, by taking
 log(likelihood)

Other examples of optimization use

Optimization example: design

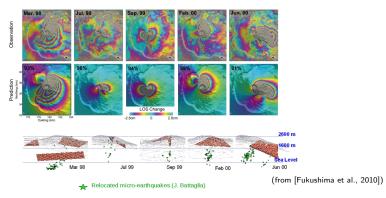


(from [Sgueglia et al., 2018])

x= aircraft parameters (here distributed electrical propulsion) $f()=-1\times$ performance metric (aggregation of $-1\times$ range, cost, take-off length, ...)

At the minimum, the design is "optimal".

Optimization example: model identification



x = dike position, geometry, internal pressure

f()= distance between measures (from RADARSAT-1 satellite) and model (boundary elements, non trivial computation)

At the minimum, the model best matches measurements and should correspond to the underground phenomenon.

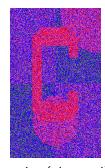
Optimization example: image denoising

$$\min_{x} f(x) \quad , \quad f(x) = \frac{1}{2} \sum_{i=1}^{N_{\text{pixels}}} (y_i - x_i)^2 + \lambda \sum_{i=1}^{N_{\text{pixels}}} \sum_{j \text{ near } i} |x_i - x_j|$$

 $\lambda \geq 0$ regularization constant



target image



noisy (observed) $= y_i$'s



denoised (optimized)

 $=x^{\star}$

(from [Ravikumar and Singh, 2017])

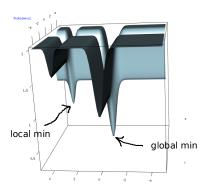
Basic mathematical concepts for optimization

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Local versus global optimum

$$\min_{x \in \mathcal{S} \subset \mathbb{R}^n} f(x)$$



Python code to generate such a 3D plot given in the Code folder, 3D_plots.py

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Gradient of a function

Gradient of a function = direction of steepest ascent = vector of partial derivatives

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

Hessian of a function

It is the matrix of second derivatives,

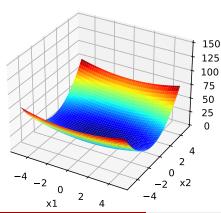
$$\nabla^{2}f(x) = \begin{bmatrix} \frac{\partial^{2}f(x)}{\partial x_{1}^{2}} & \frac{\partial^{2}f(x)}{\partial x_{1}\partial x_{2}} & \cdots & \frac{\partial^{2}f(x)}{\partial x_{1}\partial x_{n}} \\ \frac{\partial^{2}f(x)}{\partial x_{1}\partial x_{2}} & \frac{\partial^{2}f(x)}{\partial x_{2}^{2}} & \cdots & \frac{\partial^{2}f(x)}{\partial x_{2}\partial x_{n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^{2}f(x)}{\partial x_{1}\partial x_{n}} & \frac{\partial^{2}f(x)}{\partial x_{2}\partial x_{n}} & \cdots & \frac{\partial^{2}f(x)}{\partial x_{n}^{2}} \end{bmatrix}$$

= the matrix of curvatures = the gradient of the gradient.

Quadratic function and Hessian I

$$f(x) = \frac{1}{2}x^{\mathsf{T}}Hx$$
 , $\nabla^2 f(x) = H$

a good approximation to what happens on any function when converging quadratic



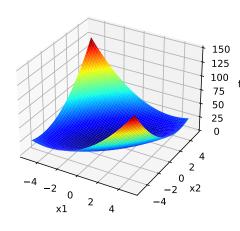
$$H = \begin{bmatrix} 1 & 0 \\ 0 & 5 \end{bmatrix}$$

(guess the eigenvalues and eigenvectors)



Quadratic function and Hessian II

quadratic

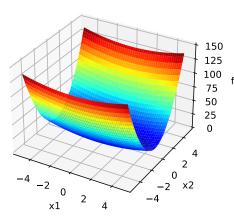


the same rotated by $45^{\circ}\,$

$$\begin{aligned} H &= \begin{bmatrix} 3 & -2 \\ -2 & 3 \end{bmatrix} \\ \text{eig.vect} &= \begin{bmatrix} \sqrt{2}/2 & -\sqrt{2}/2 \\ \sqrt{2}/2 & \sqrt{2}/2 \end{bmatrix} \\ \text{eig.val} &= [1, 5] \end{aligned}$$

Quadratic function and Hessian III

quadratic

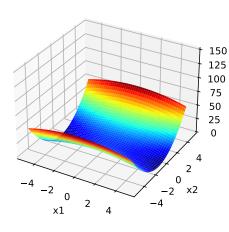


increased curvature f (condition number)

$$H = \begin{bmatrix} 1 & 0 \\ 0 & 10 \end{bmatrix}$$

Quadratic function and Hessian IV

quadratic



Non positive definite Hessian

$$H = \begin{bmatrix} -1 & 0 \\ 0 & 5 \end{bmatrix}$$

what is the problem ?

Numerical approximation of the gradient

By forward finite differences

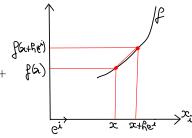
$$\frac{\partial f(x)}{\partial x_i} \approx \frac{f(x + he^i) - f(x)}{h}$$

Proof: by Taylor,

$$f(x + he^{i}) = f(x) + he^{i}^{\top} \cdot \nabla f(x) + h^{2}/2e^{i}^{\top} \nabla^{2} f(x + \rho he^{i})e^{i}, \ \rho \in]0,1[$$

$$\frac{\partial f(x)}{\partial x_{i}} = \frac{f(x + he^{i}) - f(x)}{h} - h/2e^{i}^{\top} \nabla^{2} f(x + \rho he^{i})e^{i}$$

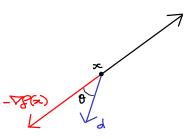
and make h very small \square



Other (better but more difficult to implement) schemes: central differences, automatic differentiation (e.g., in TensorFlow or PyTorch), (semi-)analytic differentiation (e.g., backpropagation in NN).

Descent direction

A search direction d which makes an acute angle with $-\nabla f(x)$ is a descent direction, i.e., for a small enough step, f is guaranteed to decrease!

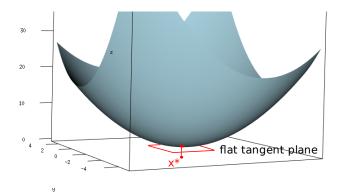


Proof: by Taylor,
$$\forall \alpha$$
, $\exists \epsilon \in [0,1]$ such that $f(x + \alpha d) = f(x) + \alpha d^{\top} \cdot \nabla f(x) + \frac{\alpha^2}{2} d^{\top} \nabla^2 f(x + \alpha \epsilon d) d$ $\lim_{\alpha \to 0^+} \frac{f(x + \alpha d) - f(x)}{\alpha} = d^{\top} \cdot \nabla f(x) = -1 \times \|\nabla f(x)\| \cos(d, -\nabla f(x))$ is negative if the cosine is positive \Box

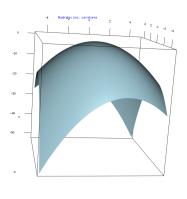
Necessary optimality condition (1)

A necessary condition for a differentiable function to have a minimum at x^* is that it is flat at this point, i.e., its gradient is null

$$x^{\star} \in \arg\min_{x \in \mathcal{S}} f(x) \Rightarrow \nabla f(x^{\star}) = 0$$

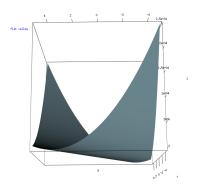


Necessary optimality condition (2)



necessary is not sufficient (works with a max)

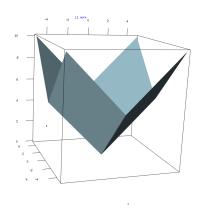
Necessary optimality condition (3)



 $\nabla f(x^*) = 0$ does not make x^* unique (flat valley)



Necessary optimality condition (4)



 $\nabla f()$ not defined everywhere, example with L1 norm = $\sum_{i=1}^{n} |x_i|$

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Optimizers as iterative algorithms

We look for
$$x^* \in \arg\min_{x \in \mathcal{S}} f(x)$$
 , $\mathcal{S} = \mathbb{R}^n$

- Except for special cases (e.g., convex quadratic problems), the solution is not obtained analytically through the optimality conditions ($\nabla f(x^*) = 0$ + higher order conditions).
- We typically use iterative algorithms: x^{i+1} depends on previous iterates, x^1, \ldots, x^i and their f's.
- Often calculating $f(x^i)$ takes more computation than the optimization algorithm itself.
- Qualities of an optimizer: robustness, speed of convergence.
 Have to strike a compromise between them.



Fixed step steepest descent algorithm (1)

Repeat steps along the steepest descent direction, $-\nabla f(x^t)$ [Cauchy, 1847, Curry, 1944]. The size of the steps is proportional to the gradient norm.

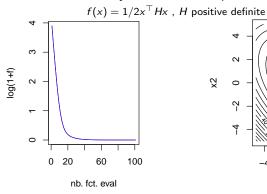
```
Require: f(), \bar{\alpha} \in ]0,1], x^1, \epsilon^{\text{step}}, \epsilon^{\text{grad}}, i^{\text{max}}
    i \leftarrow 0. f^{\text{bestSoFar}} \leftarrow \text{max\_double}
    repeat
        i \leftarrow i + 1
        calculate f(x^i) and \nabla f(x^i)
        if f(x^i) < f^{\text{bestSoFar}} then
            update x^{\text{bestSoFar}} and f^{\text{bestSoFar}} with current iterate
        end if
        direction: d^i = -\nabla f(x^i) / \|\nabla f(x^i)\|
        step: x^{i+1} = x^i + \bar{\alpha} \|\nabla f(x^i)\| d^i
    until i > i^{\text{max}} or ||x^i - x^{i-1}|| < \epsilon^{\text{step}} or ||\nabla f(x^i)|| / \sqrt{n} < \epsilon^{\text{grad}}
    return x<sup>bestSoFar</sup> and f<sup>bestSoFar</sup>
```

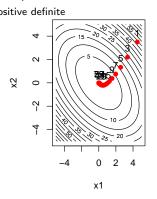
(code organization)

- In src/optimcourse: ressource files for the optimization
 - gradient_descent.py,restarted_gradient_descent.py: gradient-based descent algorithms; the current gradient fixed-step version, and the ones coming up (other direction, with a line search), a version with randomly restarted searches.
 - random_search.py: a random search algorithm.
 - test_functions.py: a collection of test functions.
 - 3D_plots.py: plots a 2 dimensional function in 3D + contour plot.
 - optim_utilities.py: additional routines.
- In src/optimcourse: ressource files for the NN coded from scratch
 - activation_functions.py: the collection of activation functions.
 - forward_propagation.py: a collection of routines for the forward propagation in a NN.
- In notebooks: notebooks and main script for starting the descent algorithms and learning the NNs.

Fixed step steepest descent algorithm (2)

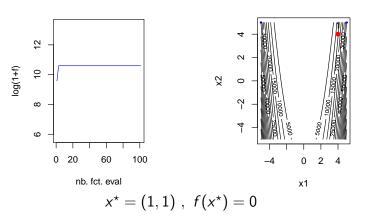
- The choice of the step size factor $\bar{\alpha}$ is critical : the steeper the function, the smaller $\bar{\alpha}$. Default value = 0.1
- The true code (cf. gradient_descent.R) is a bit longer because it is necessary to record the points visited.





Fixed step steepest descent algorithm (3)

 $\bar{\alpha}=0.1$ on f(x)= Rosenbrock (banana shaped) function in d=2 dimensions, example of divergence:



Descent with line search

At each iteration, search for the best step size in the descent² direction d^i (which for now is $-\nabla f(x^i)/\|\nabla f(x^i)\|$ but it is general). Same algorithm as before, just change the **step** instruction:

```
Require: ...
  initializations but no \alpha now ...
  repeat
     increment i, calculate f(x^i) and \nabla f(x^i) ...
     direction: d^i = -\nabla f(x^i)/\|\nabla f(x^i)\| or any other descent
     direction
     step: \alpha^i = \arg\min_{\alpha>0} f(x^i + \alpha d^i)
                x^{i+1} = x^i + \alpha^i d^i
  until stopping criteria
  return best so far
```

²if d^i is not a descent direction, $-d^i$ is. Proof left as exercise.

Approximate line search (1)

Notation: during line search i,

$$x = x^{i} + \alpha d^{i}$$

$$f(\alpha) = f(x^{i} + \alpha d^{i})$$

$$\frac{df(0)}{d\alpha} = \sum_{j=1}^{n} \frac{\partial f(x^{i})}{\partial x_{j}} \frac{\partial x_{j}}{\partial \alpha} = \sum_{j=1}^{n} \frac{\partial f(x^{i})}{\partial x_{j}} d^{i}_{j} = \nabla f(x^{i})^{\top} . d^{i}$$

In practice, perfectly optimizing for α^i is too expensive and not useful \Rightarrow approximate the line search by a sufficient decrease condition:

find
$$\alpha^i$$
 such that $f(x^i + \alpha^i d^i) < f(x^i) + \delta \alpha^i \nabla f(x^i)^\top d^i$

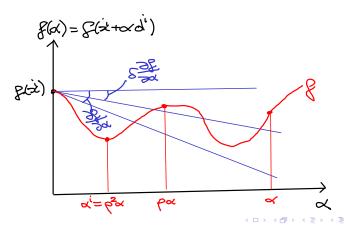
where $\delta \in [0,1]$, i.e., achieve a δ proportion of the progress promised by order 1 Taylor expansion.

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Approximate line search (2)

Sufficient decrease condition rewritten with line search notation:

find
$$\alpha^i$$
 such that $f(\alpha^i) < f(x^i) + \delta \alpha^i \frac{df(0)}{d\alpha}$



Approximate line search (3)

At iteration *i*:

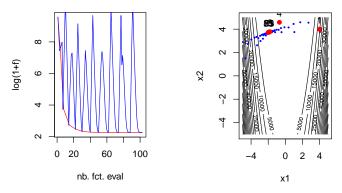
Backtracking line search (Armijo)

```
Require: d^i a descent direction, x^i, \delta \in [0,1], \rho \in ]0,1[, C>0 (defaults: \delta = 0.1, \rho = 0.5, C=1) initialize step size: \alpha = \max(C \times \|\nabla f(x^i)\|, \sqrt{n}/100) while f(x^i + \alpha d^i) \geq f(x^i) + \delta \alpha \nabla f(x^i)^\top d^i do decrease step size: \alpha \leftarrow \rho \times \alpha end while return \alpha^i \leftarrow \alpha
```

From now on, use line search, and the number of calls to f is no longer equal to the iteration number since many function calls can be done during a line search within a single iteration.

Approximate line search (4)

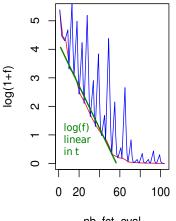
Look at what line search does to f(x) = Rosenbrock where fixed step size diverged



Better, but not perfect: oscillations make progress very slow.

Gradient convergence speed

 $f(x) = \frac{1}{2}x^{T}Hx$ in n = 10 dimensions, H > 0, not aligned with the axes, condition number = 10.



nb. fct. eval

Empirically (for proofs and more info cf. [Ravikumar and Singh, 2017]): on convex and differentiable functions, gradient search with line search progresses at a speed such that $f(x^t) \propto \xi \gamma^t$ where $\gamma \in [0,1[$. Equivalently, to achieve $f(x^t) < \varepsilon, \ t > \mathcal{O}(\log(1/\varepsilon))$

 $\log f(x^t) \propto t \log(\gamma) + \log(\xi) \implies \log(\gamma) < 0$ slope of the green curve.

$$\begin{split} \xi \gamma^t &< \varepsilon \Leftrightarrow t > \frac{\log(\varepsilon) - \log(\xi)}{\log(\gamma)} = \frac{-1}{\log(\gamma)} \log(\xi/\varepsilon) \\ \Rightarrow & t > \mathcal{O}(\log(1/\varepsilon)) \; . \end{split}$$

Gradient descent oscillations

Perfect line search solves

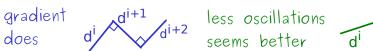
$$\alpha^{i} = \arg\min_{\alpha>0} f(\alpha)$$
 where $f(\alpha) = f(x^{i} + \alpha d^{i})$

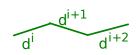
Necessary conditions of optimal step size:

$$\frac{df(\alpha^i)}{d\alpha} = \sum_{j=1}^n \frac{\partial f(x^i + \alpha^i d^i)}{\partial x_j} \frac{\partial x_j}{\partial \alpha} = \nabla f(x^{i+1})^\top . d^i = 0$$

If the direction is the gradient,

$$-d^{i+1}$$
. $d^i=0$ i.e. d^{i+1} and d^i perpendicular





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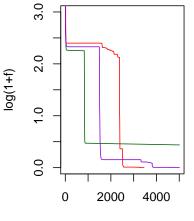
Changing the search direction

Improved gradient searches slightly (but importantly) change the search direction from minus the gradient:

- Momentum : search direction = minus gradient moved a bit towards previous search direction.
- Nesterov [Nesterov, 1983] : search direction = momentum direction with an anticipation about point of the next gradient.
- Adam [Kingma and Ba, 2014]: state-of-the-art in deep learning. Stochastic gradient method with independent adaptation of each variable based on momentum.

Comparison of methods (1)

Rosenbrock, d = 2: ability to handle curved ravines



nb. fct. eval

green=gradient, red=momentum, violet=NAG

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A word about constraints

$$\left\{\begin{array}{ll} \min_{x\in\mathcal{S}}f(x) &, \quad \mathcal{S}=\mathbb{R}^n\\ \text{such that } g_i(x)\leq 0 &, \quad i=1,m \end{array}\right.$$

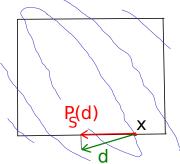
Bound constraints

 \mathcal{S} is an hypercube of \mathbb{R}^n , $\mathcal{S} = [LB, UB] \subset \mathbb{R}^n$.

It could be described by constraints, $g_{2i-1}(x) := LB_i - x_i \le 0$, $g_{2i}(x) := x_i - UB_i \le 0$, i = 1, ..., d but these constraints are so simple that they can be directly handled by projection.

If x^i is at a bound and the search direction d^i takes it outside $\mathcal{S} = [LB, UB]$, project the search direction vector onto the active bound.

Exercise: how to code this?



^aThis can even happen for a convex function in a convex S, as the drawing shows.

Constraints handling by penalizations (1)

$$\begin{cases} \min_{x \in \mathcal{S} \in \mathbb{R}^d} f(x) \\ \text{such that } g(x) \leq 0 \end{cases}$$

(vector notation for the constraints)

We give two techniques to aggregate f and the g_i 's into a new objective function (to minimize).

External penalty function: penalize points that do not satisfy the constraints

$$f_r(x) = f(x) + r \left[\max(0, g(x)) \right]^2$$
, $r > 0$

- Pros: simple, $\nabla f_r()$ continuous accross the constraint boundary (if f and g are)
- Cons: Convergence by the infeasible domain (hence external), need to find r large enough to reduce infeasibility, but not too large because of numerical issue (high curvature accross constraint)

Constraints handling by penalizations (2)

Lagrangian: for problems without duality gap³, e.g., convex problems, there exists Lagrange multipliers λ^* such that

$$x^{\star} \in \arg\min_{x \in \mathcal{S}} L(x; \lambda^{\star})$$
 where $L(x; \lambda^{\star}) \coloneqq f(x) + \lambda^{\star} g(x)$

The Lagrangian $L(; \lambda^*)$ is (when no duality gap) a valid penalty function.

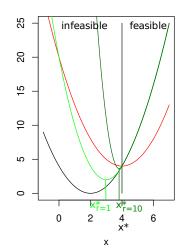
- Pros: duality provides a way to calculate λ^* , yields a feasible solution.
- Cons: estimating λ^* has a numerical cost. For most problems with local optima there is a duality gap \Rightarrow rely on augmented Lagrangians⁴.



³cf. duality, out of scope for this course

Constraints handling by penalizations (3)

Example:
$$f(x) = (x-2)^2$$
, $g(x) = 4 - x \le 0$, $x^* = 4$, convex problem



f and g in black, $L(x; \lambda^* = 4)$ in red, exterior penalty $f_r()$ with r = 1 and 10 in light and dark green, respectively.

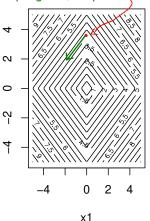
The Lagrangian is a valid penalty here.

As r grows, $x_r^{\star} \to x^{\star}$ but the curvature of $f_r()$ increases.

Comments on gradient based descent algorithms

Use on nondifferentiable functions: theoretically may converge at a point which is not a minimum even on convex functions (e.g., if an iterate is at a kink). This rarely happens in practice. Try function $f(x) = \sum_{i=1}^{n} |x_i|$ ("L1norm") with the code.

forward finite difference estimation to the gradient: no progress, stops at \



Main flaw: gets trapped in local minima.

Restarted local searches

Simple principle: restart descent searches from initial points chosen at random.

Use randomness to make deterministic descent searches more robust.

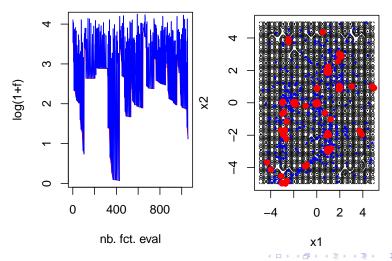
A mix between 2 extremes: local vs global, line search vs volume search, specific (to unimodal differentiable functions) vs without assumption, efficient vs very slow.

Simplistic implementation at a cost \times nb_restarts:

```
Require: budget, nb_restarts
for i in 1 to nb_restarts do
    xinit <- runif(n=d,min=LB,max=UB)
    res<-gradient_descent(xinit,budget=budget/nb_restarts)
    update global search results
end for</pre>
```

Restarted local searches: example

Execution of the restarted_descent file. fun <-rastrigin, d<-2, budget<-1000, nb_restart<-10:



Application to neural network

The practical applications are available through the project notebook on github, cf. https://github.com/ML-for-B-E/Optimisation/notebook/project.ipynb

Conclusions

- Numerical optimization is a fundamental technique for quantitative decision making, statistical modeling, machine learning, . . .
- The enthousiasm for machine learning has led to very many optimization algorithms which we did not discuss in this introductory course: see for example [Sun et al., 2019, Sra et al., 2012].
- Also not covered yet emerging: Bayesian optimization for hyper-parameters tuning (regularization constants, number of NN layers, types of neurons, parameters of the gradient based algorithms) [Snoek et al., 2012].

Bibliographical references for the class

This course is based on

- [Ravikumar and Singh, 2017] : a detailed up-to-date presentation of the main convex optimization algorithms for machine learning (level end of undergraduate, bac +3)
- [Minoux, 2008]: a classic textbook for optimization, written before the ML trend but still useful (level end of undergraduate / bac+3)
- [Bishop, 2006]: a reference book for machine learning with some pages on optimization (level end of undergraduate / bac+3)
- [Schmidt et al., 2007] : L1 regularization techniques (research article)
- [Sun, 2019] : review of optimization methods and good practices for tuning neural nets.

The content of these references has been simplified for this class.

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