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. 2024. 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

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 will be simplified for this class.

Optimization = a quantitative formulation of decision

Optimization is a[1] 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
- $\mathcal{S}$: set of possible values for x, search space

[1] non unique, incomplete when considering human beings or life

Optimization in ML: the big picture

Data: $(e^i, t^i)_{i=1,\ldots,N}$

Model: $y(e \mid x)$

Distance: $f(x) \equiv \text{Dist}(Data, y(\cdot \mid x))$

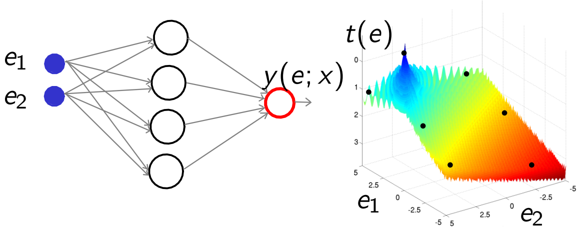
$\Big\downarrow f$

Optimizer: $x^\star = \arg\min_{x \in \mathcal{S}} f(x)$

$\Rightarrow$ $\boxed{\textbf{Learned model} : y(\cdot; x^\star)}$

Optimization example: neural net regression

learn a function from a discrete limited set of observations

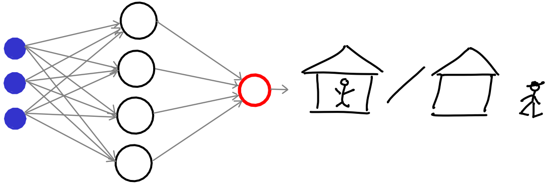


x = neural network (NN) weights and biases
$f()$ = an error of the NN predictions (sum-of-squares error):

- e entries, $t(e)$ target function to learn
- observed data set, "•" : (e^i, t^i), $i = 1, \ldots, N$
- $y(e;x)$: output of the NN, the expected value of $t(e)$
- $f(x) = 1/2 \sum_{i=1}^{N} (t^i - y(e^i;x))^2$

Optimization example: neural net classification

Predict if a person stays at home or goes out based on longitude, latitude and temperature = a 2 classes classification problem.



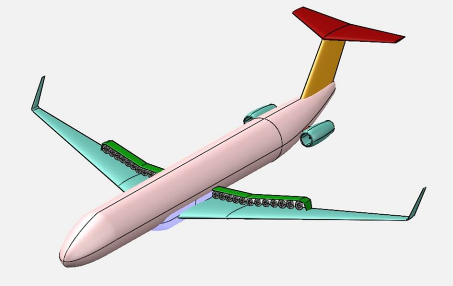
x = neural network (NN) weights and biases
$f()$ = an error of the NN predictions (a cross-entropy error):

- e entries: e_1 longitude, e_2 latitude, e_3 temperature
- $t = 1$ if person stays, $t = 0$ otherwise
- Observed data set: (e^i, t^i), $i = 1, \ldots, N$
- $y(e; x)$: output of the NN, the probability that $t(e) = 1$
- $f(x) = -\sum_{i=1}^{N} \{ t^i \log(y(e^i; x)) + (1 - t^i) \log(1 - y(e^i; x)) \}$

- View the relationship between the entry e and the class t as probabilistic (generalizes deterministic functions): $t(e)$ is a Bernoulli variable with a given probability that $t(e) = 1$
- The NN models this probability: $y(e; x)$ is the probability that $t(e) = 1$, $1 - y(e; x)$ is the proba that $t(e) = 0$, $0 \leq y(e; x) \leq 1$.
- 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 $\prod_{i=1}^{N} \left[y(e^i; x)^{t^i} \times (1 - y(e^i; x))^{1-t^i} \right]$, to be maximized
- The likelihood is turned into an error, to be minimized, by taking $-\log(\text{likelihood})$,

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

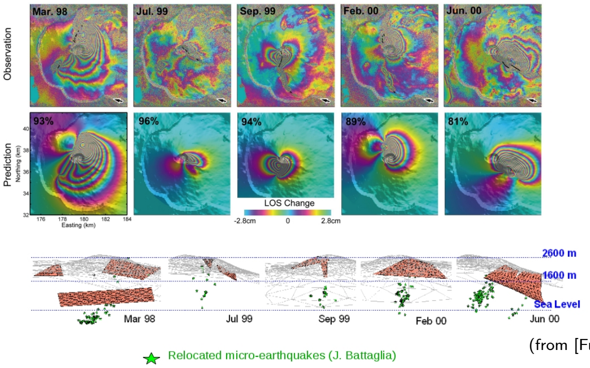
Optimization example: design



(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



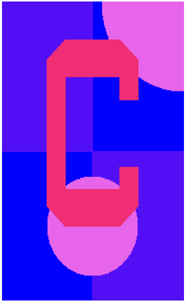
(from [Fukushima et al., 2010])

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.

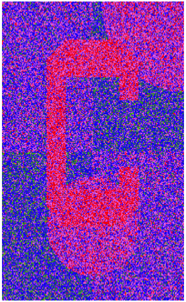
Optimization example: image denoising

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

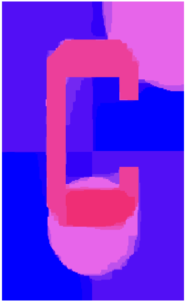
$\lambda \geq 0$ regularization constant



target image



noisy (observed)
$= y_i$'s



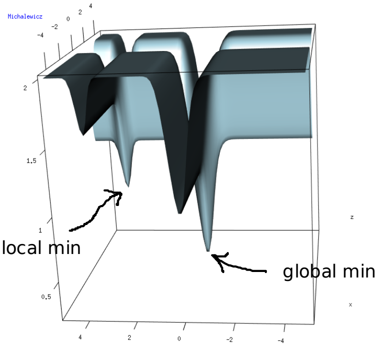
denoised (optimized)
$= x^\star$

(from [Ravikumar and Singh, 2017])

Basic mathematical concepts for optimization

Local versus global optimum

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

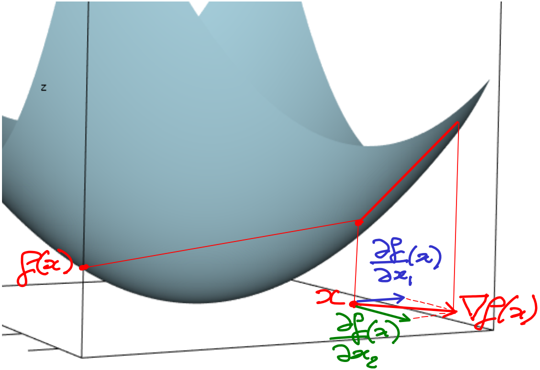


Python code to generate such a 3D plot given in the `Code` folder, `3D_plots.py`

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,

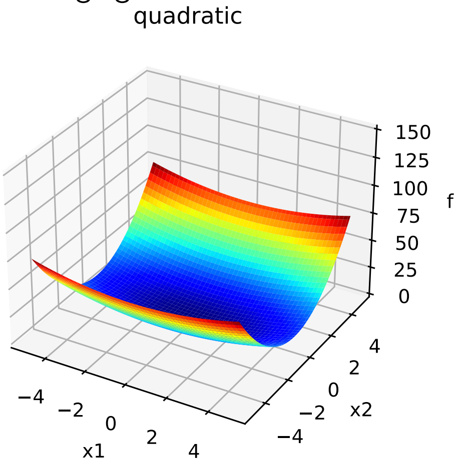
$$\nabla^2 f(x) = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} \\ \cdots & \cdots & \ddots & \cdots \\ \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix}$$

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

Quadratic function and Hessian I

$$f(x) \;=\; \frac{1}{2}x^{\top}Hx \quad , \quad \nabla^2 f(x) = H$$

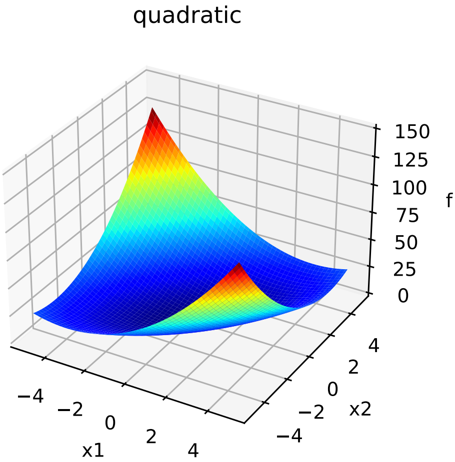
a good approximation to what happens on any function when converging



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

(guess the eigenvalues and eigenvectors)

Quadratic function and Hessian II



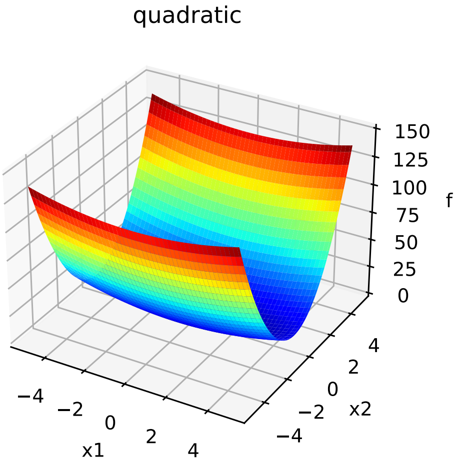
the same rotated by 45°

$$H = \begin{bmatrix} 3 & -2 \\ -2 & 3 \end{bmatrix}$$

$$\text{eig.vect} = \begin{bmatrix} \sqrt{2}/2 & -\sqrt{2}/2 \\ \sqrt{2}/2 & \sqrt{2}/2 \end{bmatrix}$$

$$\text{eig.val} = [1, 5]$$

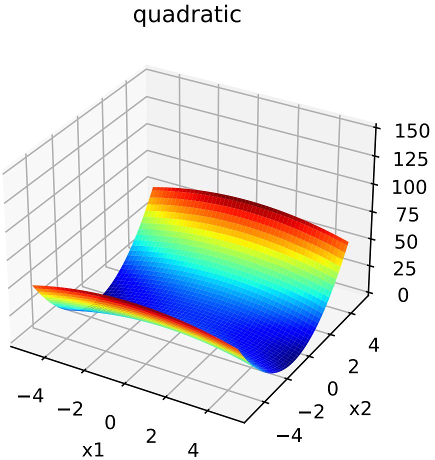
Quadratic function and Hessian III



increased curvature (condition number)

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

Quadratic function and Hessian IV



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

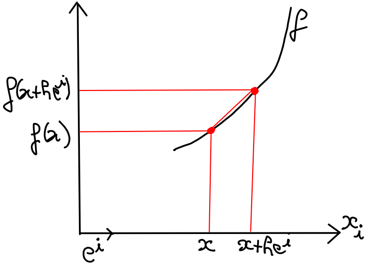
$$\frac{\partial f(x)}{\partial x_i} \approx \frac{f(x+he^i)-f(x)}{h}$$

Proof: by Taylor,

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

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

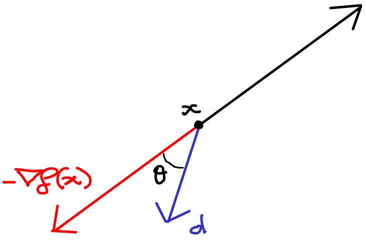
and make h very small $\square$



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!

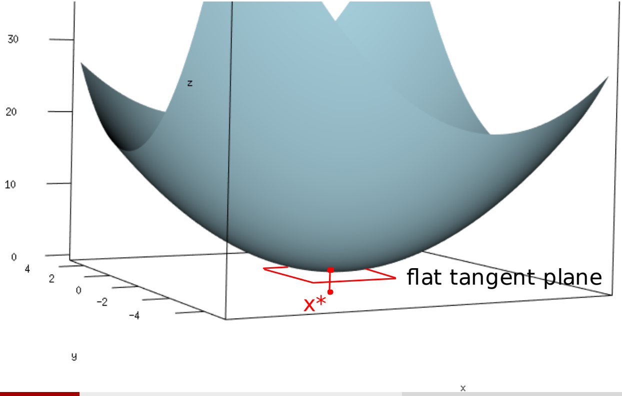


Proof: by Taylor, $\forall \alpha,\ \exists \epsilon \in [0,1]$ such that
$f(x+\alpha d) = f(x) + \alpha d^\top.\nabla f(x) + \frac{\alpha^2}{2} d^\top \nabla^2 f(x+\alpha\epsilon d) d$
$\lim_{\alpha\to 0^+} \frac{f(x+\alpha d)-f(x)}{\alpha} = d^\top.\nabla f(x) = -1 \times \|\nabla f(x)\| \cos(d, -\nabla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

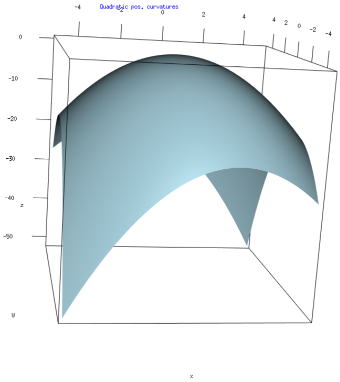
Necessary optimality condition (1)

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

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

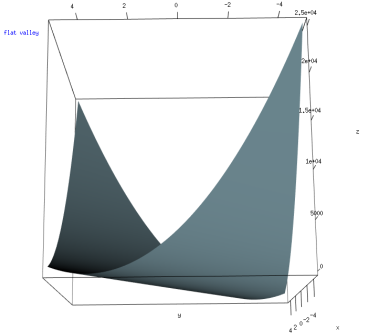


Necessary optimality condition (2)



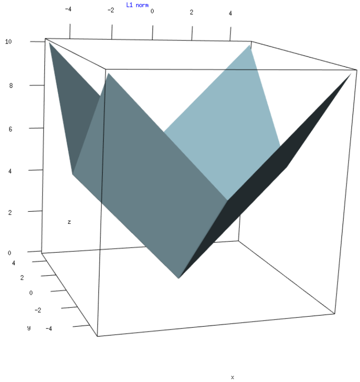
necessary is not sufficient (works with a max)

Necessary optimality condition (3)



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

Necessary optimality condition (4)



$\nabla f()$ not defined everywhere, example with L1 norm $= \sum_i^n |x_i|$

Course outline

An introduction to optimization for machine learning

Optimizers as iterative algorithms

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

- Except for special cases (e.g., convex quadratic problems), the solution is not obtained analytically through the optimality conditions ($\nabla f(x^\star) = 0$ + 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, ϵ^{step}, ϵ^{grad}, $i^{\max}$

  $i \leftarrow 0$, $f^{\text{bestSoFar}} \leftarrow$ `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 $i > i^{\max}$ **or** $\|x^i - x^{i-1}\| \leq \epsilon^{\text{step}}$ **or** $\|\nabla f(x^i)\| / \sqrt{n} \leq \epsilon^{\text{grad}}$

  return $x^{\text{bestSoFar}}$ and $f^{\text{bestSoFar}}$

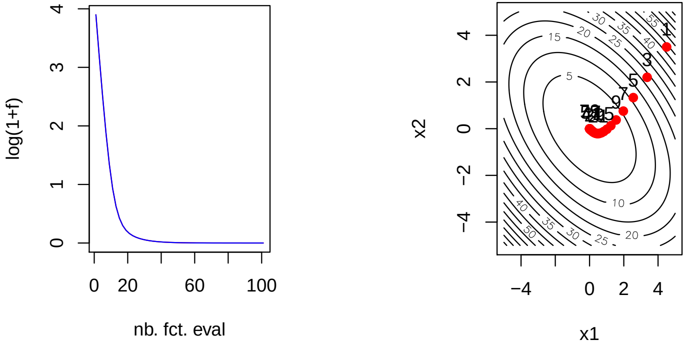
(code organization)

- `main_optim.py`: main script for starting the descent algorithms.
- `gradient_descent.py`: gradient-based descent algorithms; the current gradient fixed-step version, and the ones coming up (other direction, with a line search).
- `random_search.py`: a random search algorithm.
- `test_functions.py`: a collection of test functions.
- `3D_plots.py`: plots a 2 dimensional function in a 3D dynamic plot + contour plot.
- `optim_utilities.py`: additional routines.

Fixed step steepest descent algorithm (2)

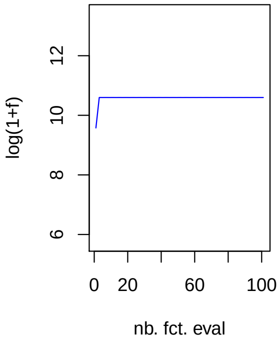
- The choice of the step size factor $\bar{\alpha}$ is critical : the steeper the function, the smaller $\bar{\alpha}$. Default value $= 0.1$
- The true code (cf. `gradient_descent.R`) is a bit longer because it is necessary to record the points visited.

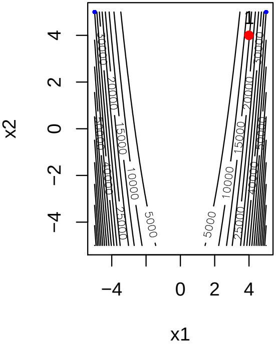
$f(x) = 1/2x^\top Hx$, H positive definite



Fixed step steepest descent algorithm (3)

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





$$x^\star = (1,1)\ ,\ \ f(x^\star) = 0$$

Descent with line search

At each iteration, search for the best step size in the descent[2] 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 α 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

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

Approximate line search (1)

Notation: during line search i,

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

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

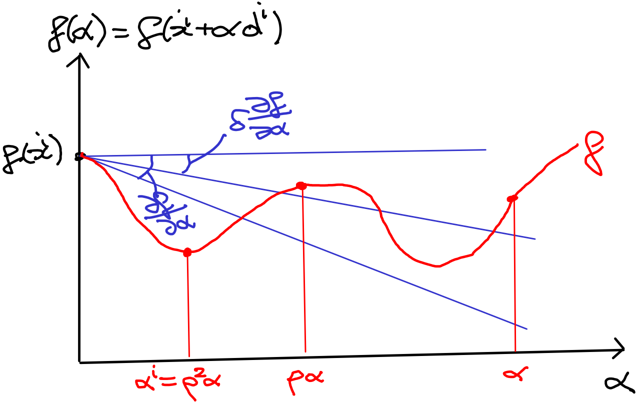
$$\text{find } \alpha^i \text{ such that } f(x^i + \alpha^i d^i) < f(x^i) + \delta \alpha^i \nabla f(x^i)^\top . d^i$$

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

Approximate line search (2)

Sufficient decrease condition rewritten with line search notation:

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



Approximate line search (3)

At iteration i:

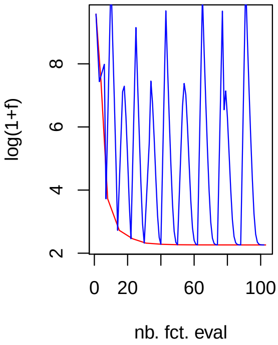
Backtracking line search (Armijo)

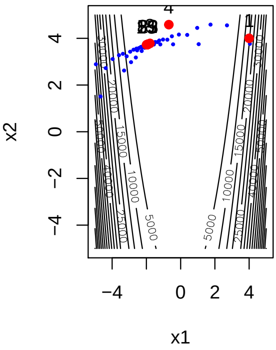
Require: d^i a descent direction, x^i, $\delta \in [0,1]$, $\rho \in]0,1[$, $C > 0$
(defaults: $\delta = 0.1$, $\rho = 0.5$, $C = 1$)
initialize step size: $\alpha = \max(C \times \|\nabla f(x^i)\|\ ,\ \sqrt{n}/100)$
while $f(x^i + \alpha d^i) \geq f(x^i) + \delta\alpha\nabla f(x^i)^\top d^i$ **do**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

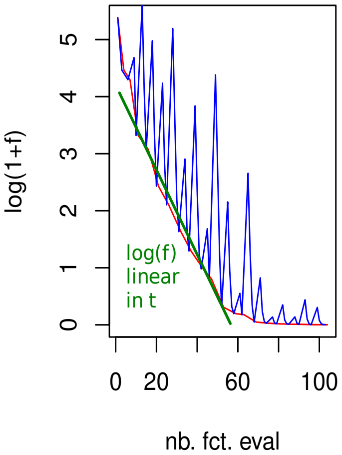




Better, but not perfect: oscillations make progress very slow.

Gradient convergence speed

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



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 $f(x^t) < \varepsilon$, $t > \mathcal{O}(\log(1/\varepsilon))$

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

$\xi\gamma^t < \varepsilon \Leftrightarrow t > \frac{\log(\varepsilon) - \log(\xi)}{\log(\gamma)} = \frac{-1}{\log(\gamma)} \log(\xi/\varepsilon)$

$\Rightarrow \; t > \mathcal{O}(\log(1/\varepsilon))$.

Gradient descent oscillations

Perfect line search solves

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

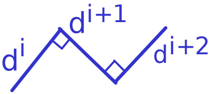
Necessary conditions of optimal step size:

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

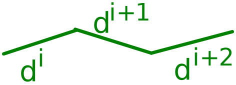
If the direction is the gradient,

$$-{d^{i+1}}^\top . d^i = 0 \quad \text{i.e. } d^{i+1} \text{ and } d^i \text{ perpendicular}$$

gradient
does



less oscillations
seems better



Course outline

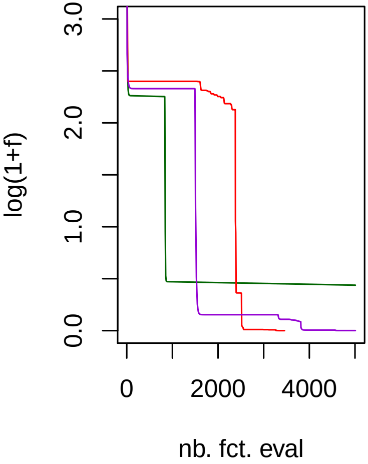
Changing the search direction

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



green=gradient, red=momentum, violet=NAG

Course outline

An introduction to optimization for machine learning

A word about constraints

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

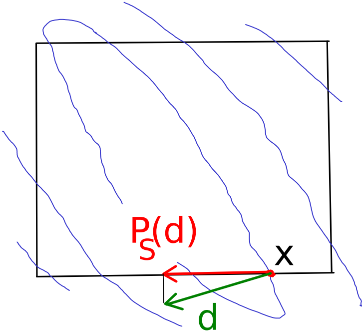
Bound constraints

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

It could be described by constraints, $g_{2i-1}(x) := LB_i - x_i \leq 0$, $g_{2i}(x) := x_i - UB_i \leq 0$, $i = 1, \ldots, d$ 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[a] $\mathcal{S} = [LB, UB]$, project the search direction vector onto the active bound.

Exercise: how to code this?



[a]This can even happen for a convex function in a convex $\mathcal{S}$, 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

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

- 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 gap[3], e.g., convex problems, there exists Lagrange multipliers $\lambda^\star$ such that

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

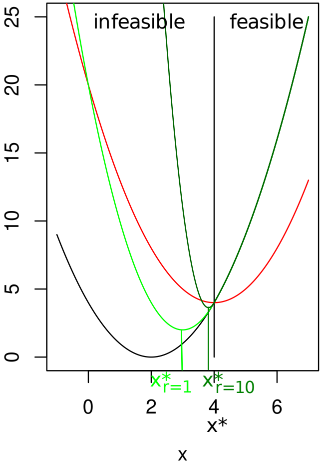
The Lagrangian $L(;\lambda^\star)$ is (when no duality gap) a valid penalty function.

- Pros: duality provides a way to calculate $\lambda^\star$, yields a feasible solution.
- Cons: estimating $\lambda^\star$ has a numerical cost. For most problems with local optima there is a duality gap $\Rightarrow$ rely on augmented Lagrangians[4].

[3]cf. duality, out of scope for this course

Constraints handling by penalizations (3)

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



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

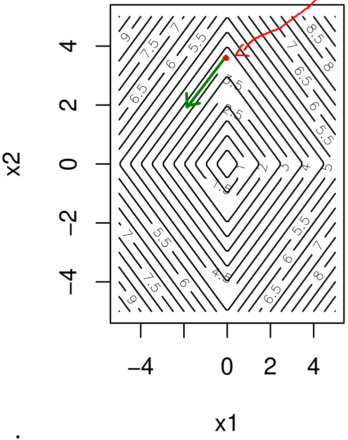
The Lagrangian is a valid penalty here.

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.

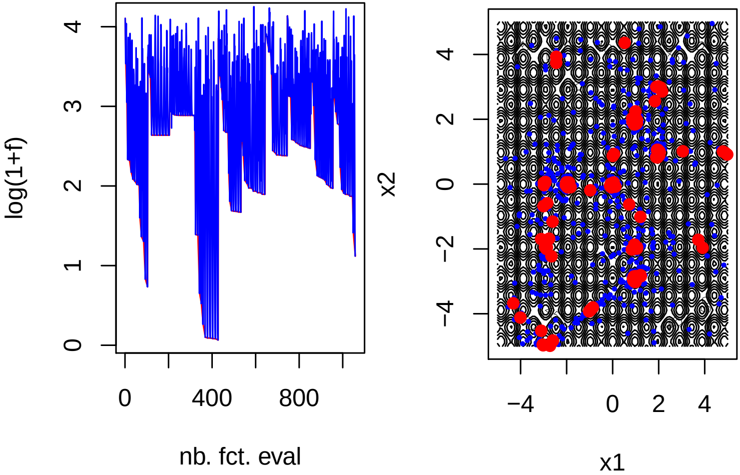
Restarted local searches

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

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/blob/main/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].

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