

An introduction to optimization for machine learning

Rodolphe Le Riche¹, Dédji Brian Whannou², Espéran Padonou³

¹ CNRS LIMOS at Mines Saint-Etienne, France

² KPMG France

³ Fondation Vallet

July 2021

Ecole d'Eté en Intelligence Artificielle
fondation Vallet
Cotonou, Bénin

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 - Objectives, acknowledgements
 - Optimization problem formulation
 - Examples of optimization usages
 - Basic mathematical concepts for optimization
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 - Fixed step steepest descent algorithm
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Objectives of this 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 R/python from scratch.
- Limitation: the algorithms are not exactly those used in state-of-the-art deep learning, but the main concepts will be presented.

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 for tuning neural nets, gradient backpropagation (research article)

The content of these references will be simplified for this class.

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
- \mathcal{S} : set of possible values for x , search space

¹non unique, incomplete when considering human beings or life

Optimization example: design



(from [Sgueglia et al., 2018])

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

At the minimum, the design is “optimal”.

Optimization example: model identification



(from [Fukushima et al., 2010])

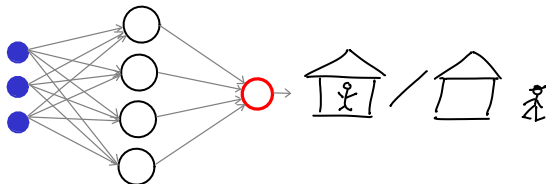
x = dike position, geometry, internal pressure

$f()$ = 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: 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) , $i = 1, \dots, N$
- $y(e; x)$: output of the NN, the probability that $t(e) = 1$
- $f(x) = - \sum_{i=1}^N \{ t^i \log(y(e^i; x)) + (1 - t^i) \log(1 - y(e^i; x)) \}$

(a word on the classification cross-entropy error)

- 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 $y(e; x)^t + (1 - y(e; x))^{1-t}$
- The likelihood of the N i.i.d observations is $\prod_{i=1}^N [y(e^i; x)^{t^i} + (1 - y(e^i; x))^{1-t^i}]$, 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: 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) , $i = 1, \dots, N$
- $y(e; x)$: output of the NN, the expected value of $t(e)$
- $f(x) = 1/2 \sum_{i=1}^N (t^i - y(e^i; x))^2$

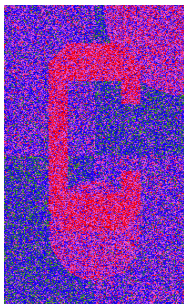
Optimization example: image denoising

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

$\lambda \geq 0$ regularization constant



target image



noisy (observed)
 $= y_i$'s



denoised (optimized)
 $= x^*$

(from [Ravikumar and Singh, 2017])

Basic mathematical concepts for optimization

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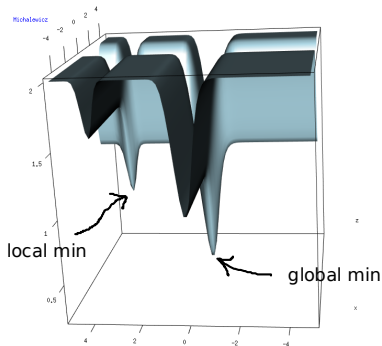
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Local versus global optimum

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

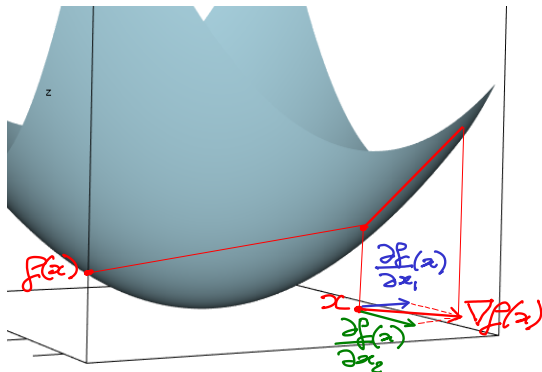


R code to generate the plot given in the project folder

Gradient of a function

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

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



Numerical approximation of the gradient

By forward finite differences

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

Proof: by Taylor,

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

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

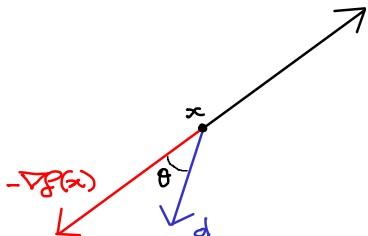
and make h very small \square



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, $\forall \alpha \leq 0, \exists \epsilon \in [0, 1]$ such that

$$f(x + \alpha d) = f(x) + \alpha d^\top \cdot \nabla f(x) + \frac{\alpha^2}{2} d^\top \nabla^2 f(x + \alpha \epsilon d) d$$

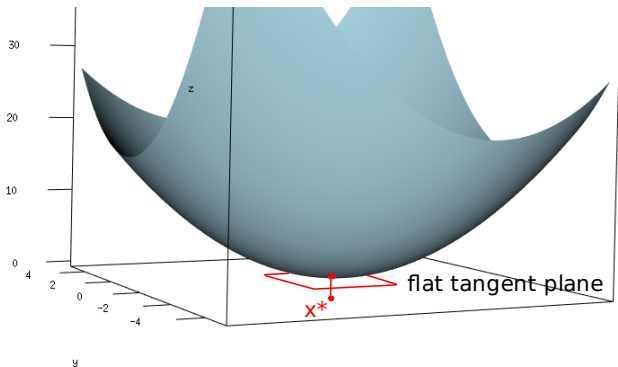
$$\lim_{\alpha \rightarrow 0^+} \frac{f(x + \alpha d) - f(x)}{\alpha} = d^\top \cdot \nabla f(x) = -1 \times \|\nabla f(x)\| \cos(d, -\nabla f(x))$$

is negative if the cosine is positive \square

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

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

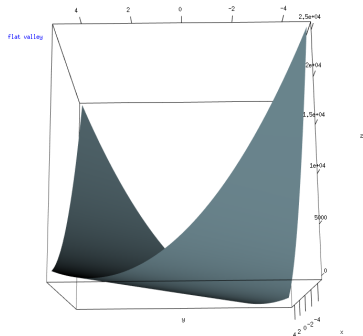


Necessary optimality condition (2)



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 $= \sum_i^d |x_i|$

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Optimizers as iterative algorithms

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

- 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, \dots, 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. Often have to strike a compromise between them.

Fixed step steepest descent algorithm (1)

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

Require: $f()$, $\alpha \in]0, 1]$, x^1 , ϵ^{step} , ϵ^{grad} , i^{max}

$i \leftarrow 0$, $f^{\text{best so far}} \leftarrow \text{max_double}$

repeat

$i \leftarrow i + 1$

calculate $f(x^i)$ and $\nabla f(x^i)$

if $f(x^i) < f^{\text{best so far}}$ **then**

 update $x^{\text{best so far}}$ and $f^{\text{best so far}}$ with current iterate

end if

direction: $d^i = -\nabla f(x^i) / \|\nabla f(x^i)\|$

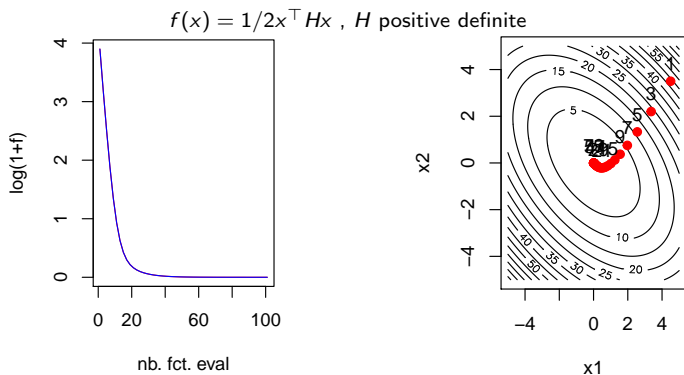
step: $x^{i+1} = x^i + \alpha \|\nabla f(x^i)\| d^i$

until $i > i^{\text{max}}$ **or** $\|x^i - x^{i-1}\| \leq \epsilon^{\text{step}}$ **or** $\|\nabla f(x^i)\| \leq \epsilon^{\text{grad}}$

return $x^{\text{best so far}}$ and $f^{\text{best so far}}$

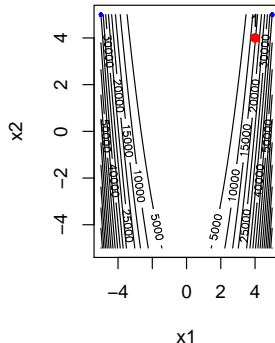
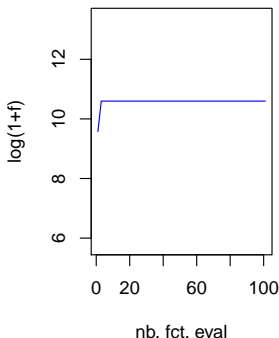
Fixed step steepest descent algorithm (2)

- The choice of the step size factor α is critical : the steeper the function, the smaller α . Default value = 0.1
- The true code (cf. project) is much longer and filled with instructions for reporting the points visited and doing plots afterwards.



Fixed step steepest descent algorithm (3)

$\alpha = 0.1$ 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 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

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

Approximate line search (1)

Notation: during line search i ,

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

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

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

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

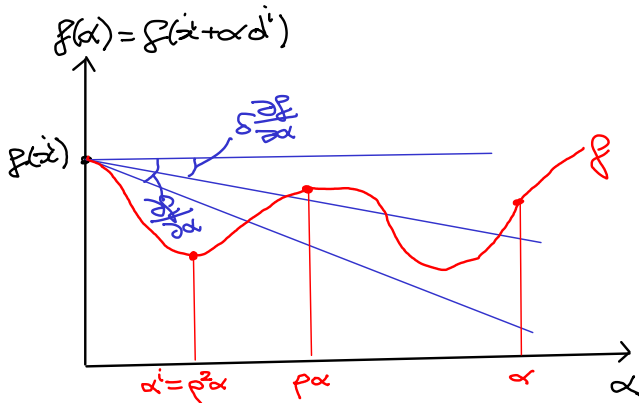
$$\text{find } \alpha^i \text{ such that } f(x^i + \alpha^i d^i) < f(x^i) + \delta \alpha^i \nabla f(x^i)^\top \cdot d^i$$

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 :

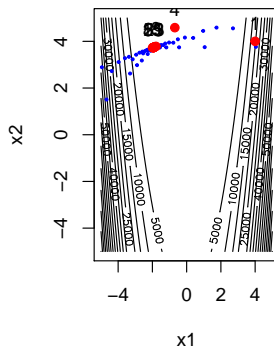
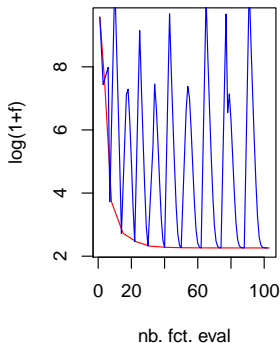
Backtracking line search (Armijo)

Require: d 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: $\alpha = \max(C \times \|\nabla f(x^i)\|, \sqrt{d}/100)$
while $f(x^i + \alpha d^i) \geq f(x) + \delta \alpha \nabla f(x^i)^\top \cdot d$ **do**
 decrease step size: $\alpha \leftarrow \rho \times \alpha$
end while
return $\alpha^i \leftarrow \alpha$

Note: 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)

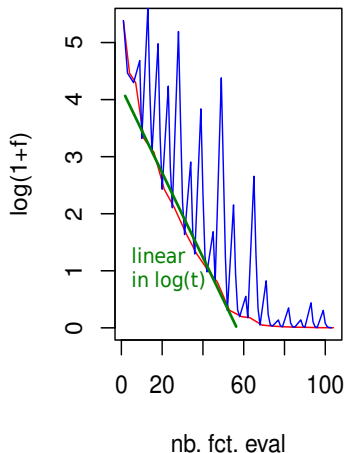
Look at what line search does to $f(x) = \text{Rosenbrock}$ where fixed step size diverged



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

Gradient convergence speed

$f(x) = \frac{1}{2}x^\top Hx$ in $d = 10$ dimensions, $H \geq 0$, 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:

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

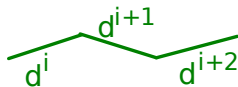
If the direction is the gradient,

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

gradient
does



less oscillations
seems better



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Gradient with momentum

Recall gradient descent,

$$x^{i+1} = x^i + \alpha^i d^i \quad \text{where} \quad d^i = -\nabla f(x^i) / \|\nabla f(x^i)\|$$

(work in progress)

Nesterov accelerated gradient (NAG)

(work in progress)

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Bound constraints

(work in progress)

Constraints handling by penalization

(work in progress)

Comments on gradient based descent algorithms

(work in progress) flaws: no convergence on nondifferentiable functions, gets trapped in local minima

Restarted local searches

(work in progress)(make a simple flow chart)

Conclusions

- L'optimisation numérique est une technique fondamentale associée à la décision optimale et à la modélisation statistique (machine learning).
- Avec l'enthousiasme autour du machine learning, de nombreux algorithmes ont été conçus que nous n'avons pas couverts ici: l'optimisation bayésienne (Bayesian optimization) pour le réglage des hyper-paramètres (paramètres de régularisation, nombre de couches du réseau de neurone, type de neurones, paramètres de l'algorithme d'optimisation des poids).

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