An introduction to optimization for machine learning

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July 2021
Ecole d'Eté en Intelligence Artificielle
fondation Vallet
Cotonou, Bénin

Course outline

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

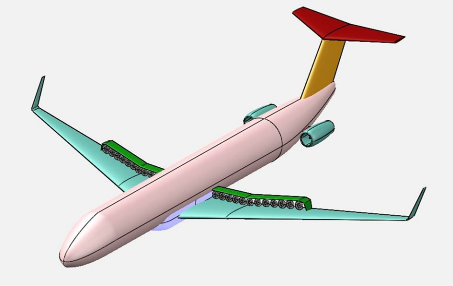
Optimization is a[1] way of mathematically modeling decision.

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

- 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

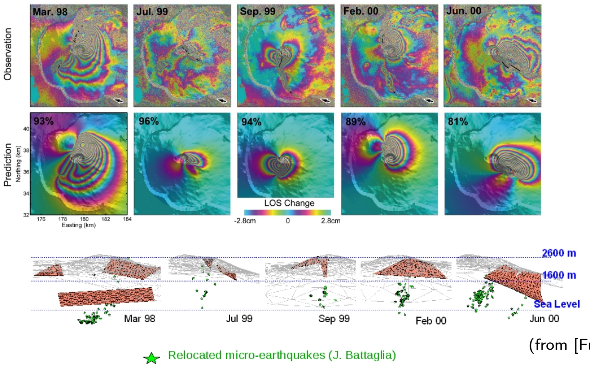
Optimization example: design



(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])

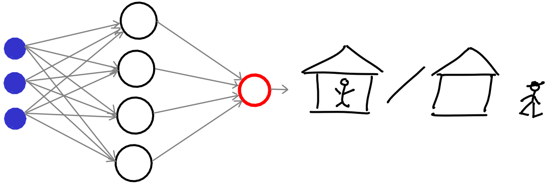
x = dike position, geometry, internal pressure

$f()$ = 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):

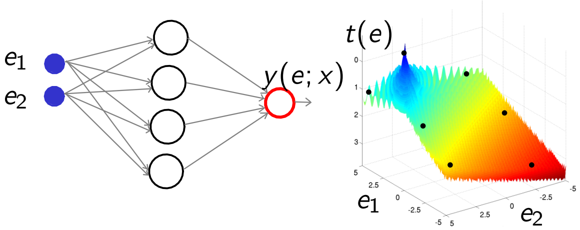
- e entries: e_1 longitude, e_2 latitude, e_3 temperature
- $t = 1$ if person stays, $t = 0$ otherwise
- Observed data set: (e^i, t^i), $i = 1, \ldots, N$
- $y(e; x)$: output of the NN, the probability that $t(e) = 1$
- $f(x) = -\sum_{i=1}^{N} \{t^i \log(y(e^i; x)) + (1 - t^i) \log(1 - y(e^i; x))\}$

- 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 $y(e;x)^t + (1 - y(e;x))^{1-t}$
- The likelihood of the N i.i.d observations is $\prod_{i=1}^{N} \left[y(e^i;x)^{t^i} + (1 - y(e^i;x))^{1-t^i} \right]$, 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: neural net regression

learn a function from a discrete limited set of observations



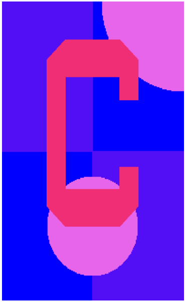
x = neural network (NN) weights and biases
$f()$ = an error of the NN predictions (sum-of-squares error):

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

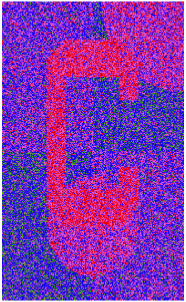
Optimization example: image denoising

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

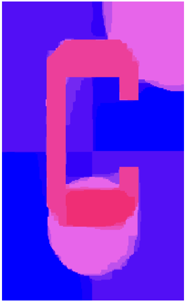
$\lambda \geq 0$ regularization constant



target image



noisy (observed) $= y_i$'s



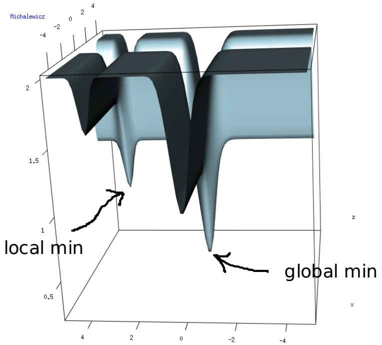
denoised (optimized) $= x^\star$

(from [Ravikumar and Singh, 2017])

Basic mathematical concepts for optimization

Local versus global optimum

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

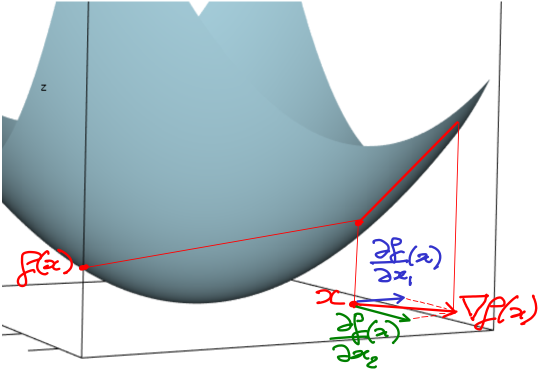


R code to generate the plot given in the project folder

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

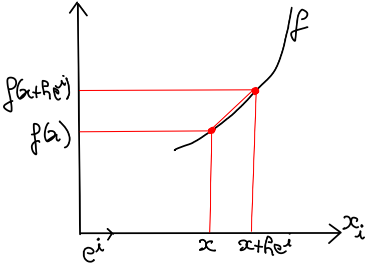
$$\frac{\partial f}{\partial x_i} f(x) \approx \frac{f(x + he^i) - f(x)}{h}$$

Proof: by Taylor,

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

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

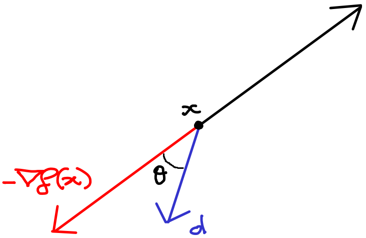
and make h very small $\square$



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!

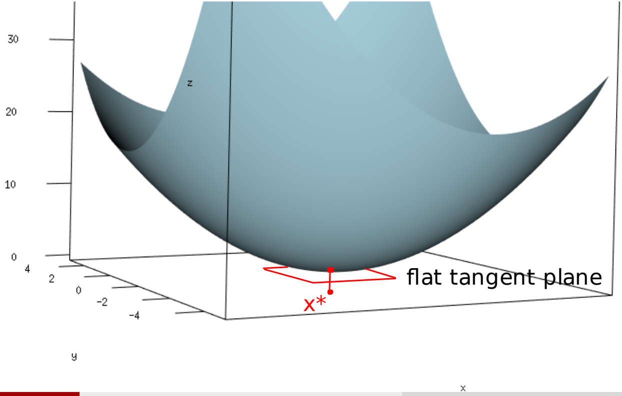


Proof: by Taylor, $\forall \alpha \leq 0,\ \exists \epsilon \in [0,1]$ such that
$f(x+\alpha d) = f(x) + \alpha d^\top \nabla f(x) + \frac{\alpha^2}{2} d^\top \nabla^2 f(x + \alpha\epsilon d) d$
$\lim_{\alpha \to 0^+} \frac{f(x+\alpha d) - f(x)}{\alpha} = d^\top \nabla f(x) = -1 \times \|\nabla f(x)\|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

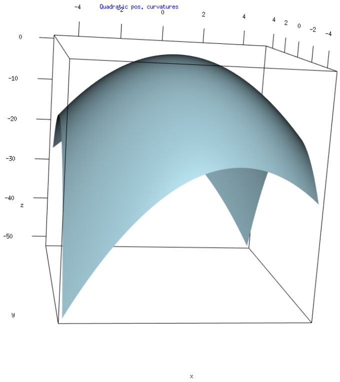
Necessary optimality condition (1)

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

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

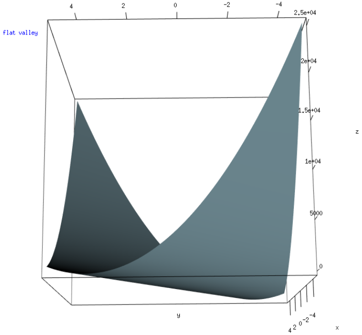


Necessary optimality condition (2)



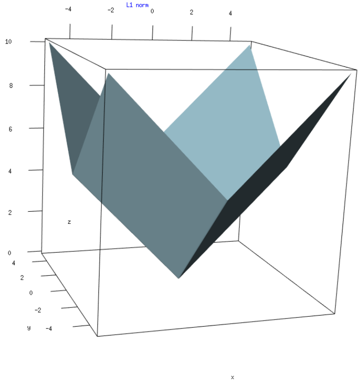
necessary is not sufficient (works with a max)

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 $= \sum_i^d |x_i|$

Course outline

An introduction to optimization for machine learning

Optimizers as iterative algorithms

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

- 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^{t+1} depends on previous iterates, $x^1, \ldots, x^t$ and their f's.
- t as a reference to computing time, because often calculating $f(x^t)$ 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}, $t^{\max}$

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

repeat

$t \leftarrow t + 1$

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

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

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

end if

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

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

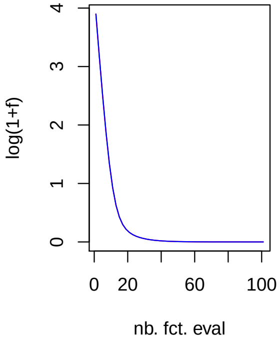
until $t > t^{\max}$ **or** $\|x^t - x^{t-1}\| \leq \epsilon^{\text{step}}$ **or** $\|\nabla f(x^t)\| \leq \epsilon^{\text{grad}}$

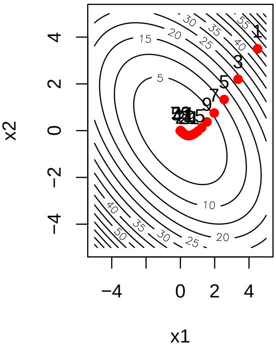
return $x^{\text{best so far}}$ and $f^{\text{best so far}}$

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.

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





Steepest descent with line search

oscillations thus need better directions (work in progress)

Course outline

Gradient with momentum

(work in progress)

Nesterov accelerated gradient (NAG)

(work in progress)

Restarted local searches

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

Course outline

An introduction to optimization for machine learning

Bound constraints

(work in progress)

Constraints handling by penalization

(work in progress)

Comments on gradient based descent algorithms

(work in progress)comment on bound limits, handled with gradient projection
show that (with perfect line search) consecutive search directions are perpendicular: tendency to oscillate, sensitive to bad conditionning
other flaws: no convergence on nondifferentiable functions, gets trapped in local minima

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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