Introduction à l'optimisation pour le machine learning

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Plan du cours

Introduction à l'optimisation pour le machine learning

Objectifs du cours

- Donner des bases pour l'optimisation numérique
- en faisant le lien avec le machine learning
- pour un public de bac+1
- avec quelques exemples de programmes en R/python codés à partir de 0.
- Limites: les algorithmes ne seront pas exactement ceux utilisés en pratique pour le deep learning, mais les principaux concepts y seront.

Bibliographie du cours

Ce cours doit beaucoup à

- [Minoux, 2008] : un classique sur l'optimisation, écrit avant l'avènement du machine learning mais une vraie base (niveau bac+3)
- [Ravikumar and Singh, 2017] : présentation détaillée des algorithmes d'optimisation utiles en machine learning (niveau bac+3)
- [Bishop, 2006] : un excellent livre d'introduction au machine learning avec quelques commentaires sur l'optimisation (niveau bac+3)
- [Schmidt et al., 2007] : techniques pour la régularisation L1 (article de recherche)
- [Sun, 2019] : panorama des méthodes d'optimisation pour les réseaux de neurones, rétro-propagation de gradient (article de recherche)

Nous en simplifierons le contenu et emprunterons des illustrations.

Optimisation = formalisation de la décision

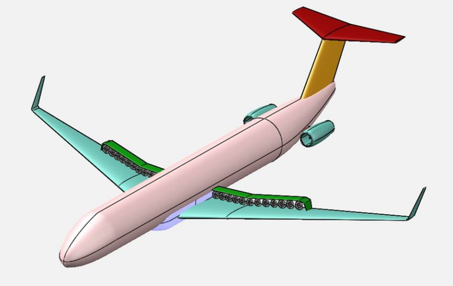
L'optimisation est une[1] formalisation mathématique de la décision

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

- x vecteur des paramètres de la décision : dimensions, somme investie, réglage d'une machine/code, ...
- $f(x)$: coût de la décision x
- $\mathcal{S}$: ensemble des valeurs possibles de x, espace de recherche

[1] non unique, contestable par rapport à l'humain et la vie

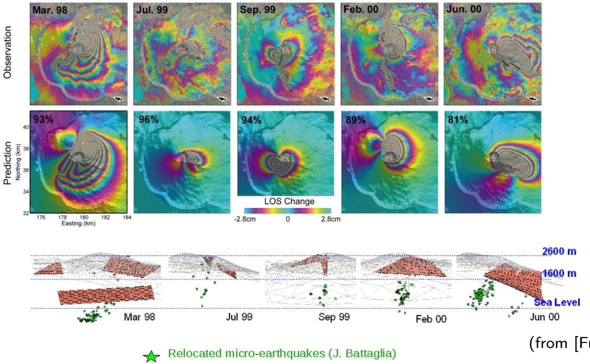
Optimization example: design



(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

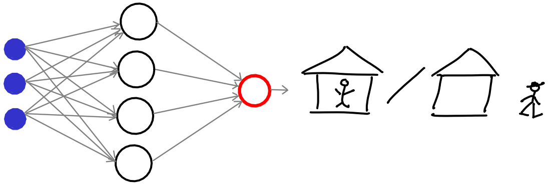


(from [Fukushima et al., 2010])

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):

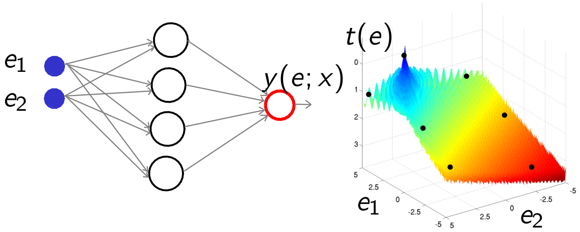
- e entries: e_1 longitude, e_2 latitude, e_3 temperature
- $t = 1$ if person stays, $t = 0$ otherwise
- Observed data set: (e^i, t^i), $i = 1, \dots, N$
- $y(e; x)$: output of the NN, the probability that $t(e) = 1$
- $f(x) = -\sum_{i=1}^{N} \{t^i \log(y(e^i; x)) + (1 - t^i) \log(1 - y(e^i; x))\}$

- 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



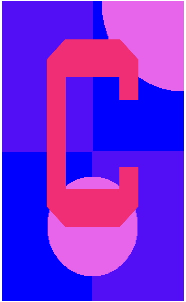
x = neural network (NN) weights and biases
$f()$ = an error of the NN predictions (sum-of-squares error):

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

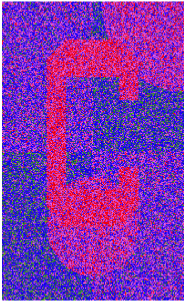
Optimization example: image denoising

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

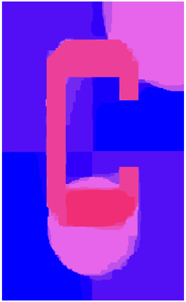
$\lambda \geq 0$ regularization constant



target image



noisy (observed) $= y_i$'s



denoised (optimized) $= x^\star$

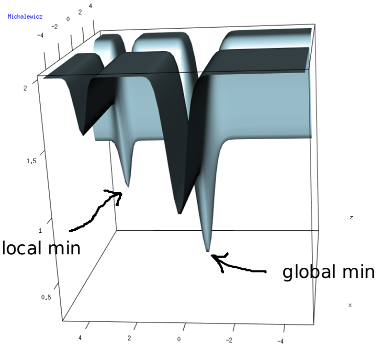
(from [Ravikumar and Singh, 2017])

Optimization basics

1. Introduction
   - Objectifs, remerciements
   - Formulation d'un problème d'optimisation
   - Examples of optimization usages
   - Optimization basics
2. Steepest descent
   - Algorithm
   - Application neural network
3. Improved gradient searches
4. Prise en compte des contraintes d'optimisation
5. Conclusions
6. Bibliography

Local versus global optimum

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

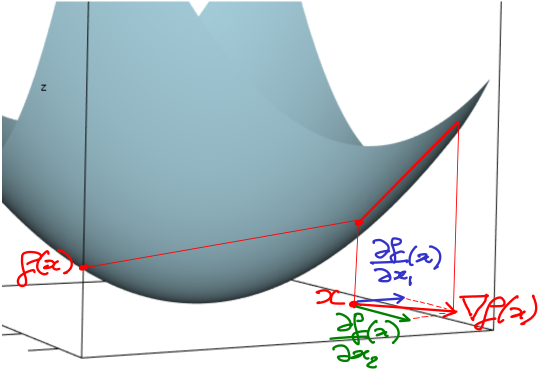


R code to generate the plot given in the project folder

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

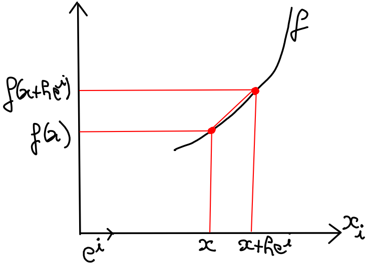
$$\frac{\partial f}{\partial x_i} f(x) \approx \frac{f(x+he^i) - f(x)}{h}$$

Proof: by Taylor,

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

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

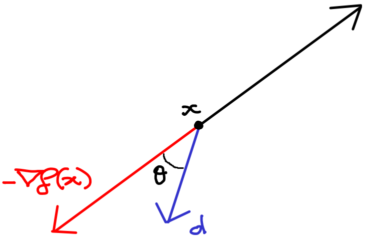
and make h very small $\square$



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!

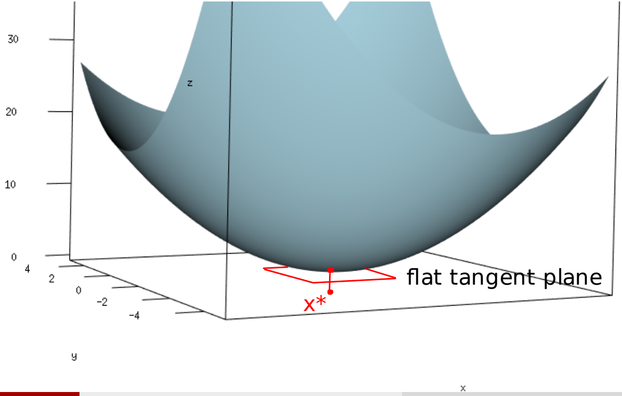


Proof: by Taylor, $\forall \alpha \leq 0,\ \exists \epsilon \in [0,1]$ such that
$f(x+\alpha d) = f(x) + \alpha d^\top \nabla f(x) + \frac{\alpha^2}{2} d^\top \nabla^2 f(x+\alpha\epsilon d) d$
$\lim_{\alpha \to 0^+} \frac{f(x+\alpha d)-f(x)}{\alpha} = d^\top \nabla f(x) = -1 \times \|\nabla f(x)\| \cos(d,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

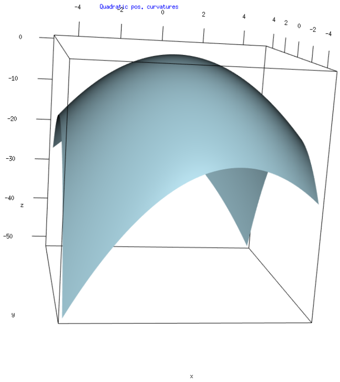
Necessary optimality condition (1)

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

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

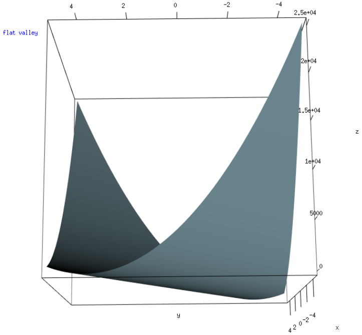


Necessary optimality condition (2)



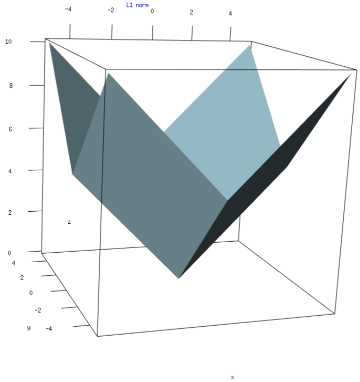
necessary is not sufficient (works with a max)

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 $= \sum_i^d |x_i|$

Plan du cours

An introduction to optimization for machine learning

Steepest descent algorithm

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

(work in progress)present algo

Comments on steepest descent

(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

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An introduction to optimization for machine learning

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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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