An introduction to optimization for machine learning

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Course outline

An introduction to optimization for machine learning

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

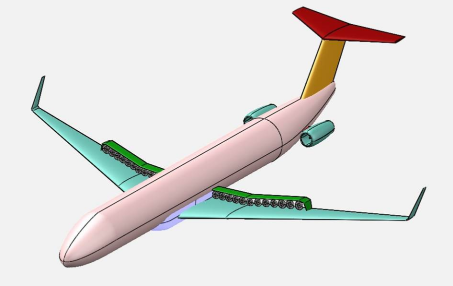
Optimization is a[1] way of mathematically modeling decision.

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

- 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

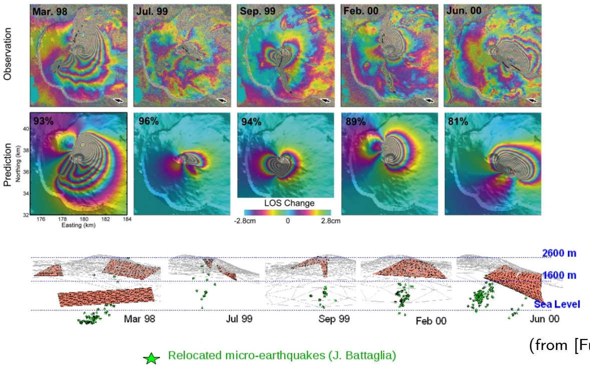
Optimization example: design



(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

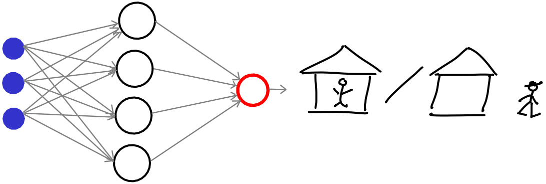


(from [Fukushima et al., 2010])

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):

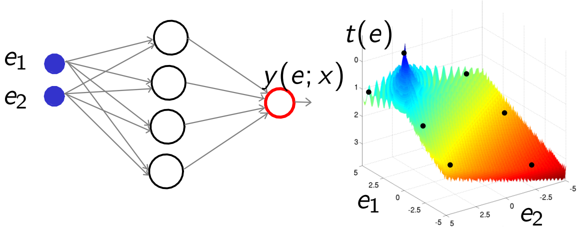
- e entries: e_1 longitude, e_2 latitude, e_3 temperature
- $t = 1$ if person stays, $t = 0$ otherwise
- Observed data set: (e^i, t^i), $i = 1, \ldots, N$
- $y(e; x)$: output of the NN, the probability that $t(e) = 1$
- $f(x) = -\sum_{i=1}^{N} \{t^i \log(y(e^i; x)) + (1 - t^i) \log(1 - y(e^i; x))\}$

- 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



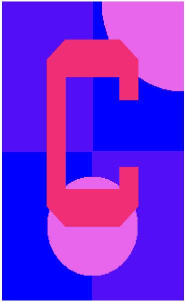
x = neural network (NN) weights and biases
$f()$ = an error of the NN predictions (sum-of-squares error):

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

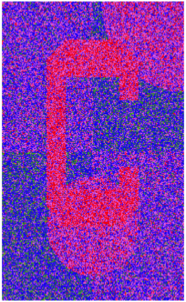
Optimization example: image denoising

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

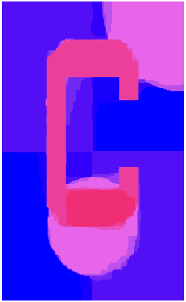
$\lambda \geq 0$ regularization constant



target image



noisy (observed) $= y_i$'s

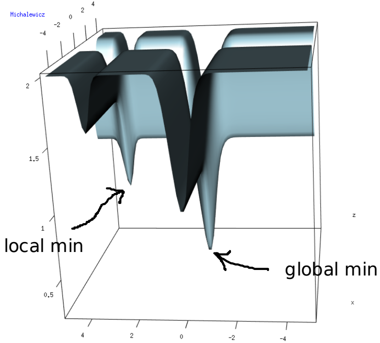


denoised (optimized) $= x^\star$

(from [Ravikumar and Singh, 2017])

Local versus global optimum

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

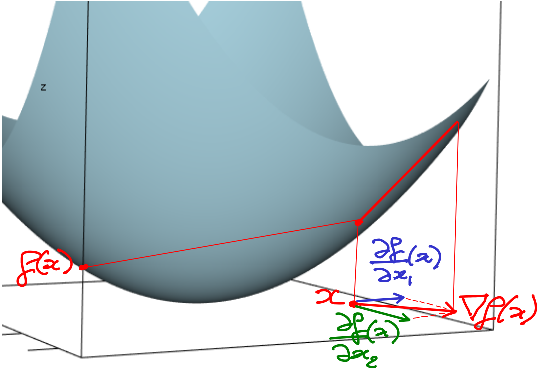


R code to generate the plot given in the project folder

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

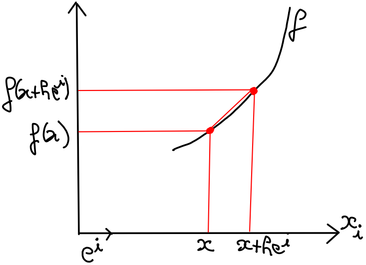
$$\frac{\partial f}{\partial x_i} f(x) \approx \frac{f(x + he^i) - f(x)}{h}$$

Proof: by Taylor,

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

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

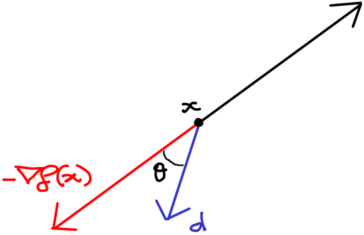
and make h very small $\square$



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!

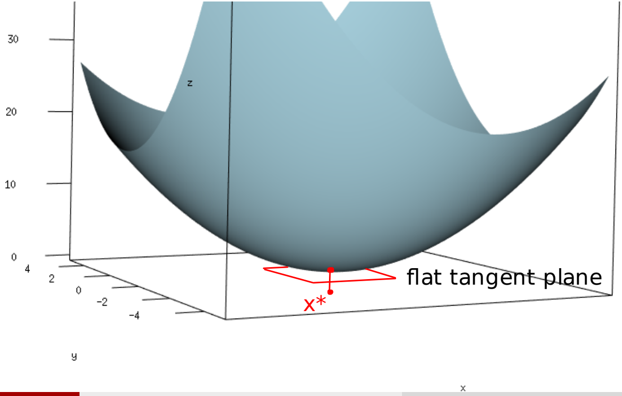


Proof: by Taylor, $\forall \alpha \leq 0$, $\exists \epsilon \in [0,1]$ such that
$f(x+\alpha d) = f(x) + \alpha d^\top . \nabla f(x) + \frac{\alpha^2}{2} d^\top \nabla^2 f(x + \alpha\epsilon d) d$
$\lim_{\alpha \to 0^+} \frac{f(x+\alpha d) - f(x)}{\alpha} = d^\top . \nabla f(x) = -1 \times \|\nabla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

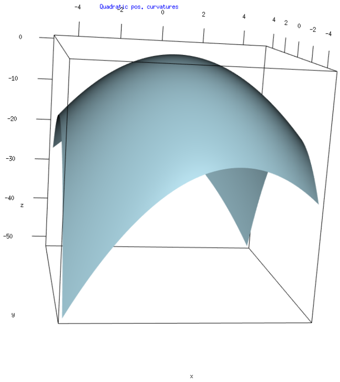
Necessary optimality condition (1)

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

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

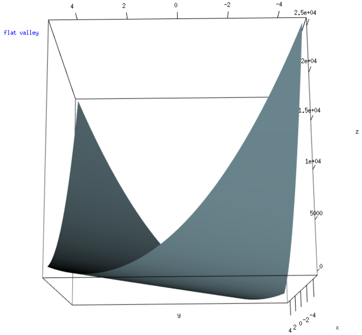


Necessary optimality condition (2)



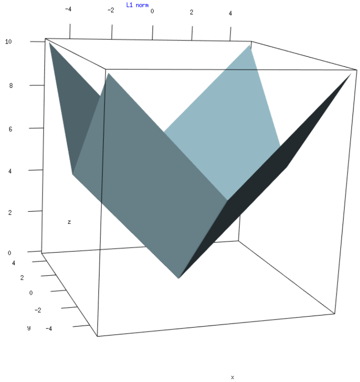
necessary is not sufficient (works with a max)

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^{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. Often have to strike a compromise between them.

Fixed step steepest descent algorithm (1)

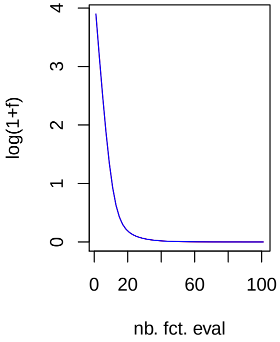
Repeat steps along the steepest descent direction, $-\nabla f(x^t)$.
The size of the steps is proportional to the gradient norm.

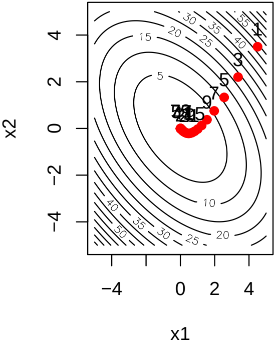
Require: $f()$, $\alpha \in]0,1]$, x^1, ϵ^{step}, ϵ^{grad}, $i^{\max}$
  $i \leftarrow 0$, $f^{\text{best so far}} \leftarrow$ `max_double`
  repeat
    $i \leftarrow i+1$
    calculate $f(x^i)$ and $\nabla f(x^i)$
    if $f(x^i) < f^{\text{best so far}}$ **then**
      update $x^{\text{best so far}}$ 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 $i > i^{\max}$ **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.

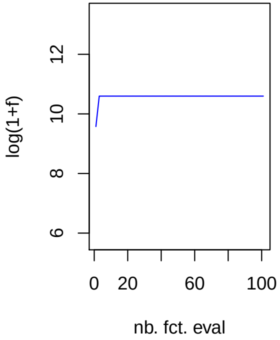
$f(x) = 1/2x^\top Hx$, H positive definite

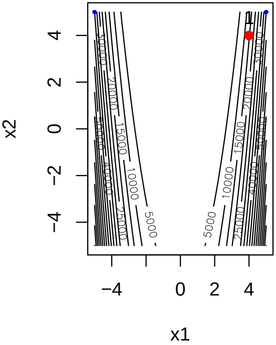




Fixed step steepest descent algorithm (3)

$\alpha = 0.1$ 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 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,

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

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

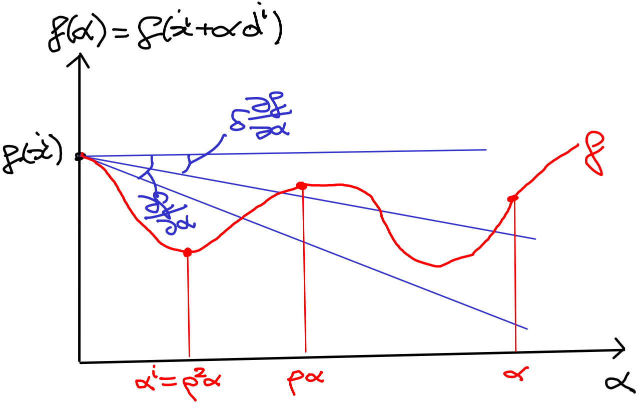
$$
\text{find } \alpha^i \text{ such that } f(x^i + \alpha^i d^i) < f(x^i) + \delta \alpha^i \nabla f(x^i)^\top . d^i
$$

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:

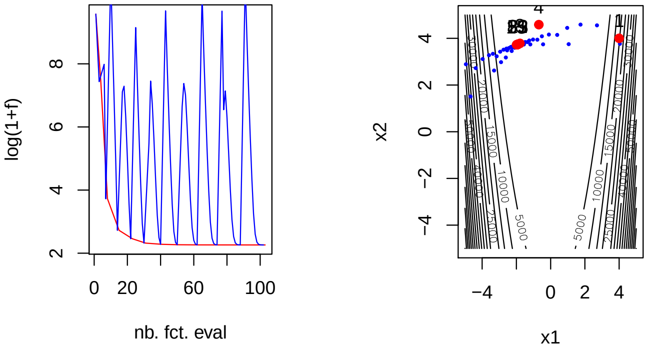
Backtracking line search (Armijo)

Require: d 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 $f(x^i + \alpha d^i) \geq f(x) + \delta \alpha \nabla f(x^i)^\top . d$ **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)

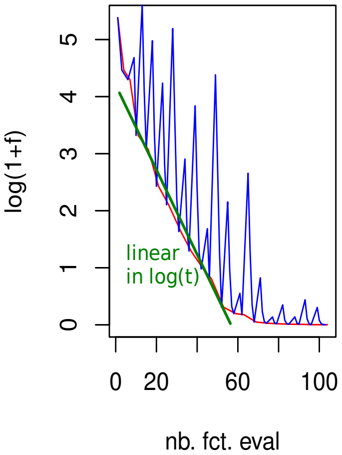
Look at what line search does to $f(x) =$ Rosenbrock where fixed step size diverged



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

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

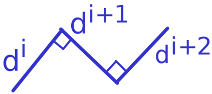
Necessary conditions of optimal step size:

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

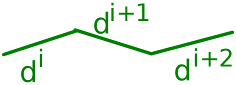
If the direction is the gradient,

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

gradient does



less oscillations seems better



Course outline

An introduction to optimization for machine learning

Gradient with momentum

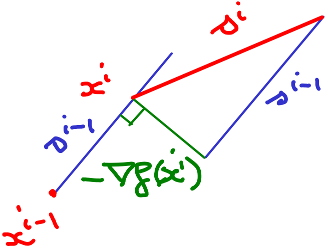
Recall fixed step gradient descent,

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

s^i, the step, corrected by a fixed or optimized (line search) α.
Introduce a momentum (i.e., a memory) in the search step,

$$s^i = -\nabla f(x^i) + \beta s^{i-1}$$

where[3] $\beta = 0.9$.
This should contribute to avoid the oscillations occuring at the botton of valleys:



[3] alternatively, for iteration varying momentum, $\beta^i = (i-2)/(i+1)$

Nesterov accelerated gradient (NAG)

(work in progress)

Course outline

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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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