Deep Learning & Applied AI

Stochastic gradient descent

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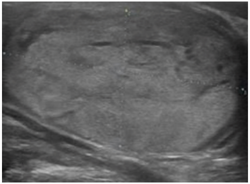
Recap

In deep learning, we deal with highly parametrized models called deep neural networks:

$$f_{\boldsymbol{\Theta}}(\mathbf{x}) = \mathbf{y}$$

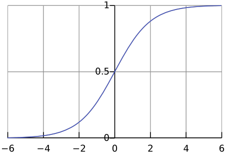
Recap: Logistic regression

What if we want to predict a category instead of a value?

$f_\Theta($  $) = \{0, 1\}$

General idea: Modify the loss to minimize over categorical values.

$$\ell_\Theta(\{x_i, y_i\}) = -\sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i)\ln(1 - \sigma(ax_i + b))$$



Recap: Logistic regression

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(ax_i + b)) = (1 - \sigma(ax_i + b))x_i$$

we see that the parameters enter the gradient in a nonlinear way.

Thus:

- $\nabla \ell_\Theta = 0$ is not a linear system that we can solve easily.
- $\nabla \ell_\Theta = 0$ is a transcendental equation $\Rightarrow$ no analytical solution.

model	**loss**	**solution**
linear regression	convex	least squares
linear regression + Tikhonov	convex	least squares
logistic regression	convex	nonlinear optimization

Gradient descent: Intuition

Gradient descent is a first-order iterative minimization algorithm.

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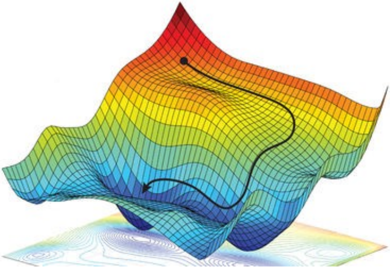
Example of a loss function $\ell_{\boldsymbol{\Theta}} : \mathbb{R}^2 \to \mathbb{R}$:



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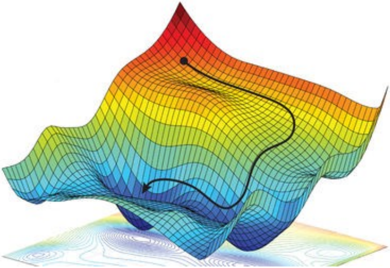

Overall idea: Move where the function decreases the most.

1. Start from some point $\boldsymbol{\Theta}^{(0)} \in \mathbb{R}^2$.

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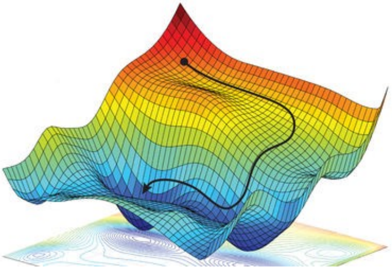

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1. Start from some point $\mathbf{\Theta}^{(0)} \in \mathbb{R}^2$.
2. Iteratively compute:

$$\mathbf{\Theta}^{(t+1)} = \mathbf{\Theta}^{(t)} - \alpha \nabla \ell_{\mathbf{\Theta}^{(t)}}$$

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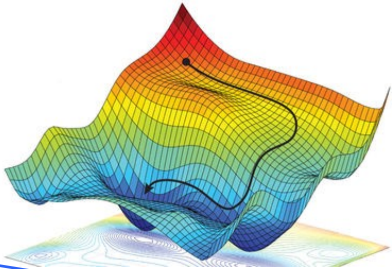
Example of a loss function $\ell_{\boldsymbol{\Theta}} : \mathbb{R}^2 \to \mathbb{R}$:

per ogni coordinata su R^2 c'è valore dove l'altezza di questo punto è proporzionale alla loss function su quel valore



la loss function

questo è R^2

Overall idea: Move where the function decreases the most.

1. Start from some point $\boldsymbol{\Theta}^{(0)} \in \mathbb{R}^2$. quindi un punto nello spazio dei parametri
2. Iteratively compute:

$$\boldsymbol{\Theta}^{(t+1)} = \boldsymbol{\Theta}^{(t)} - \alpha \nabla \ell_{\boldsymbol{\Theta}^{(t)}}$$

3. Stop when a minimum is reached.

Gradient descent

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

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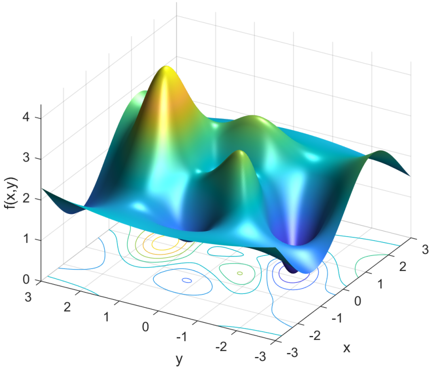
ridenominazione dei
parametri di f



Le forme disegnate sul piano sono un altro modo di rappresentare i grafici.
Queste rappresentazioni prendono il nome di **isoline representation** o **level set representation.**
Le linee che si creano prendono il nome di **isolines** e queste ci indicano che SOLO lungo il loro perimetro i valori della funzione f per quei punti del piano sono uguali

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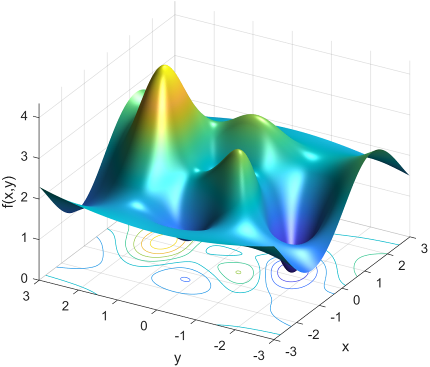

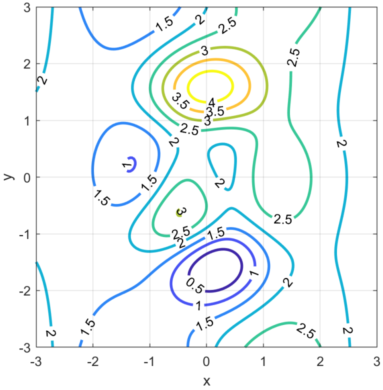

i valori qui specificati sulle isolines sono
i valori della funzione f per quei punti

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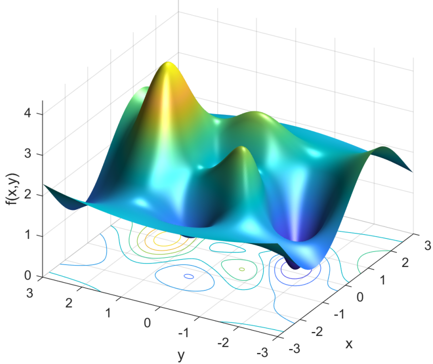

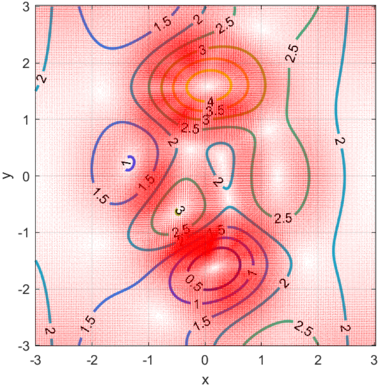

in questa immagine viene computato il gradiente negativo per ogni punto del piano. Questo, quindi si riempie di vettori che puntano verso i punti più bassi nei dintorni. (realmente viene solo computato il gradiente del parametro x)

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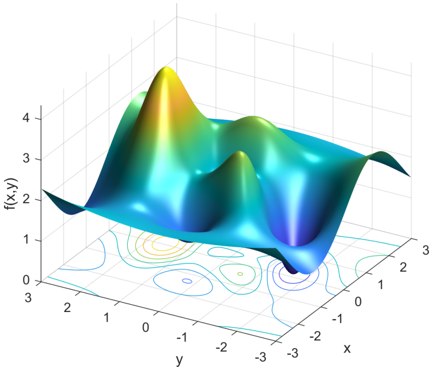

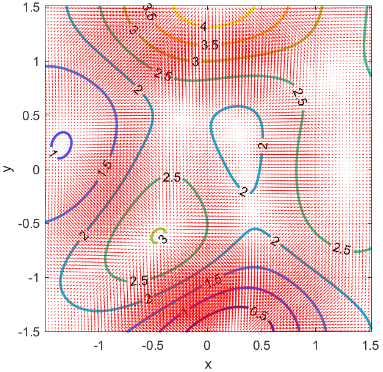

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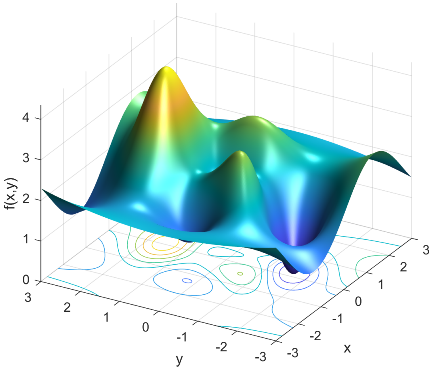

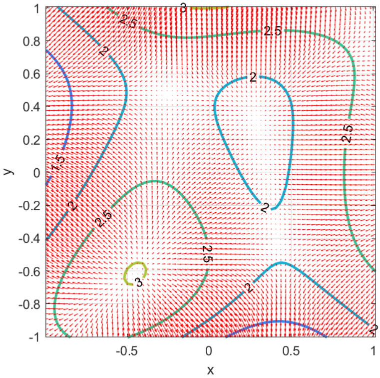

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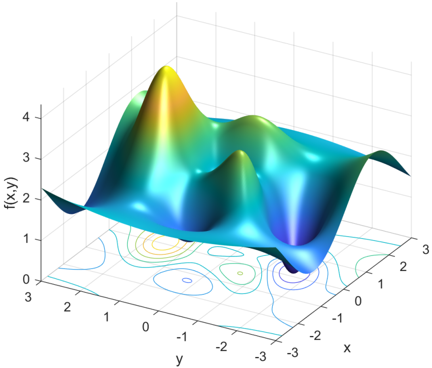

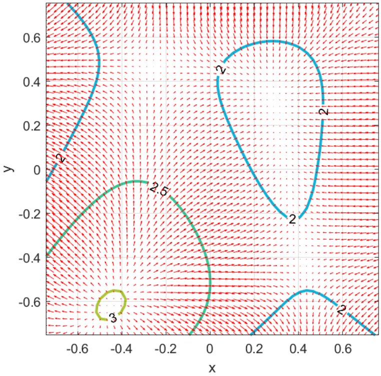

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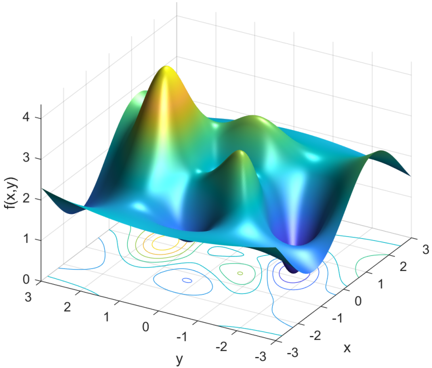

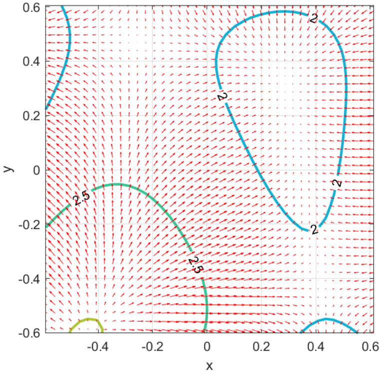

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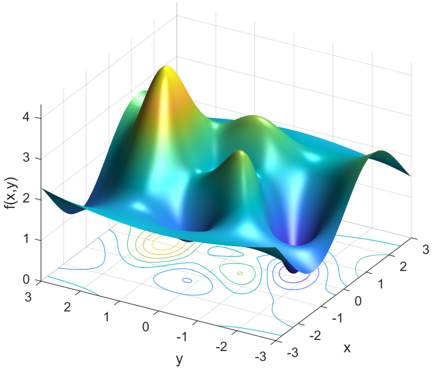
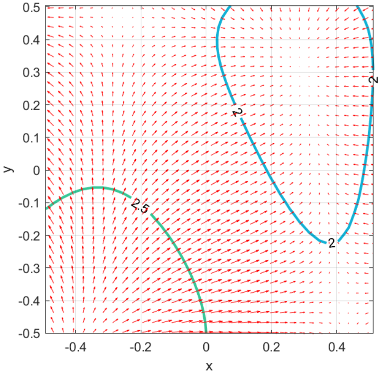
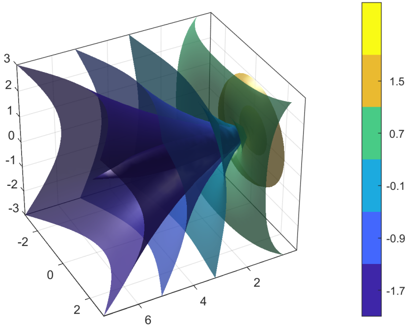


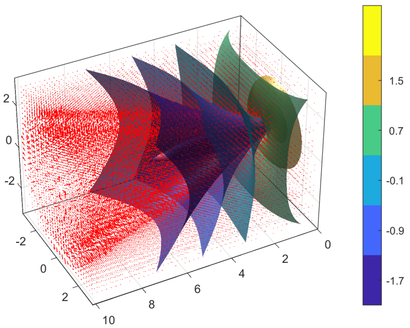


si può notare come i vettori dei gradienti sono sempre ortogonali alle isolines

Gradient descent: High dimensions

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$





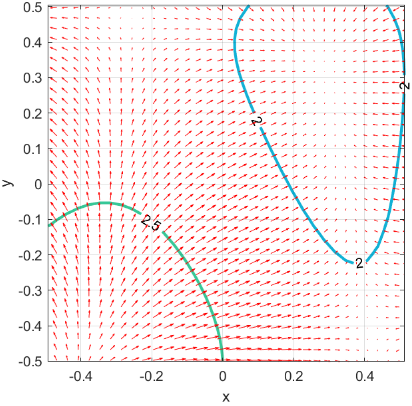
All we say is also valid in $\gg 2$ dimensions.

quindi in dimensioni > 2, si parla di **iso-surfaces** (quei fogli colorati)

Gradient descent: Orthogonality

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

The gradient is orthogonal to level curves / level surfaces.



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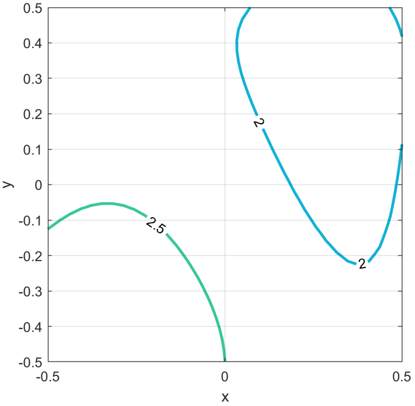

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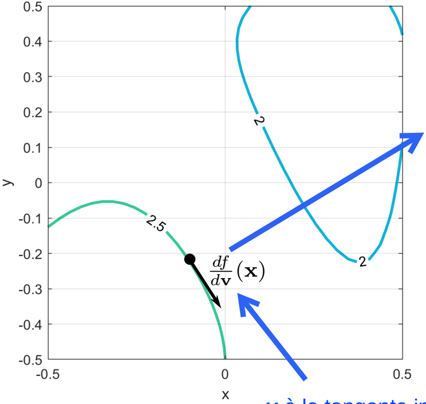

df è la **direction derivative**, che generalizza la partial derivative

v è la tangente in quel punto della curva che indica la direzione verso la quale la curva sta procedendo

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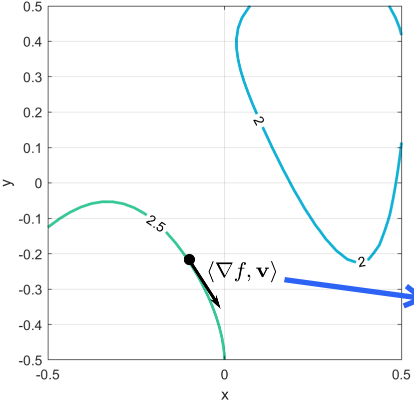

la direction derivative rispetto a v, si trova facendo questo inner product (è un altro modo di definire il gradiente)

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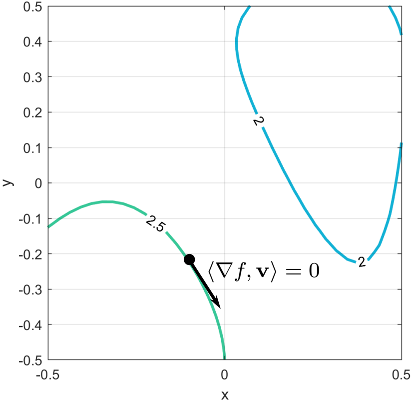

The directional derivative is zero along isocurves.

perché le iso-curves sono funzioni costanti

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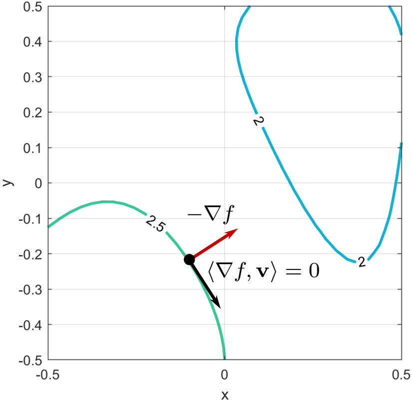

The directional derivative is zero along isocurves.

quindi, siccome l'inner product è 0, la tangente direzionale e il gradiente sono ortogonali

Gradient descent: Differentiability

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

Gradient descent requires f to be differentiable at all points.

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significa che la funzione non ha
salti o discontinuità

See examples at: `https://mathinsight.org/differentiability_multivariable_subtleties`

Gradient descent: Stationary points

A stationary point is such that:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \underbrace{\cancel{\nabla f(\mathbf{x}^{(t)})}}_{0}$$

Gradient descent "gets stuck" at stationary points.

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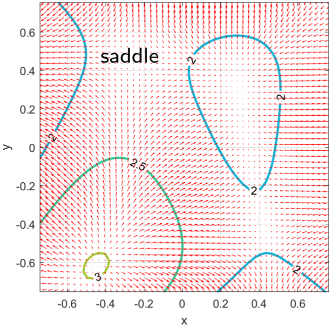

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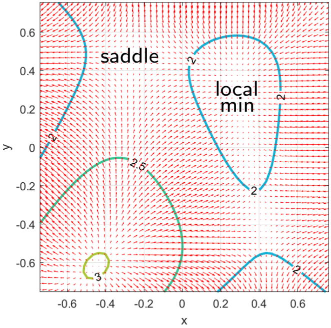

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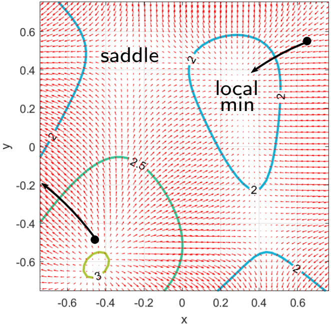
- Stationary point $\not\Rightarrow$ local minimum $\not\Rightarrow$ global minimum.
- Which stationary point depends on the initialization.



Gradient descent: Learning rate

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The parameter $\alpha > 0$ is also called learning rate in ML.

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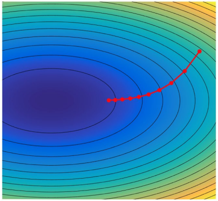

small α

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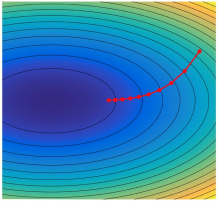
- Too big: risk of overshooting



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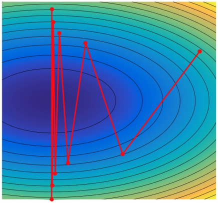

large α

Gradient descent: Learning rate

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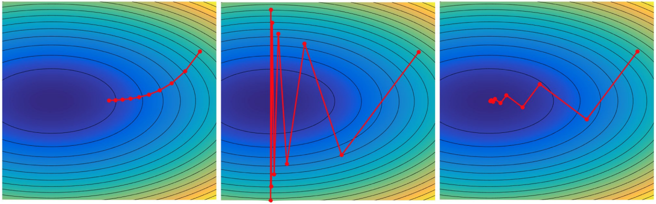
The parameter $\alpha > 0$ is also called learning rate in ML.

Remark: The length of a step is not simply α, but $\alpha \|\nabla f\|$. questa è la lunghezza del gradiente

- Too small: slow convergence speed
- Too big: risk of overshooting
- Optimal values can be found via line search algorithms



small α large α optimal α

$\arg\min_\alpha f(\mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)}))$

Decay and momentum

The learning rate can be adaptive or follow a schedule.

Decay and momentum

The learning rate can be adaptive or follow a schedule.

- Decrease α according to a decay parameter ρ:
  Examples:

$$\alpha^{(t+1)} = (1-\frac{t}{\rho})\alpha^{(0)}+\frac{t}{\rho}\alpha^{(\rho)}\,, \quad \alpha^{(t+1)} = \frac{\alpha^{(t)}}{1+\rho t}\,, \quad \alpha^{(t+1)} = \alpha^{(0)}e^{-\rho t}$$

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- Accumulate past gradients and keep moving in their direction:

$$\begin{aligned} \mathbf{v}^{(t+1)} &= \lambda\mathbf{v}^{(t)} - \alpha\nabla f(\mathbf{x}^{(t)}) \quad \text{momentum} \\ \mathbf{x}^{(t+1)} &= \mathbf{x}^{(t)} + \mathbf{v}^{(t+1)} \end{aligned}$$

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linear decay lr

$$lr_{\text{linear}} = k\left(1 - \frac{i}{n}\right)$$

declino

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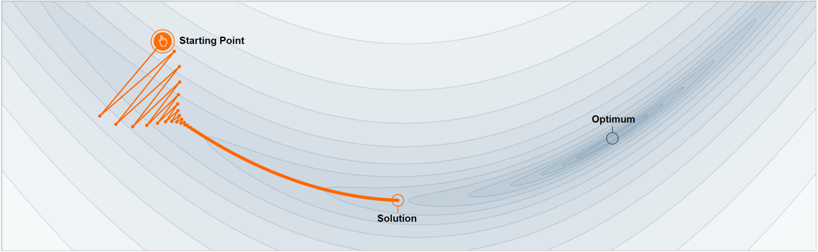
  Step length $\propto$ how aligned is the sequence of gradients.

questa formula funziona perché lambda è un valore < 1

$$\frac{1}{1-\lambda}\alpha\|\nabla f\|$$

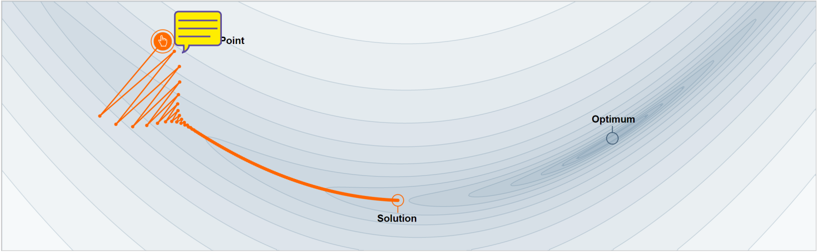
Acceleration effect for big λ + escape from local minima.

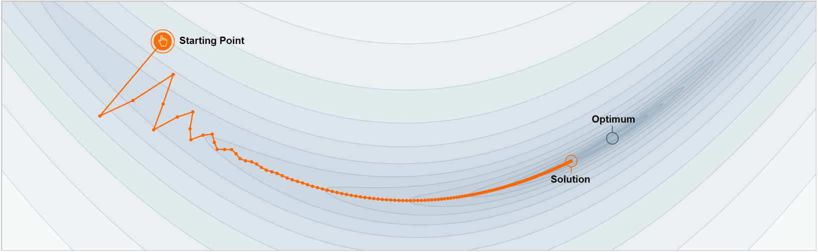
Momentum



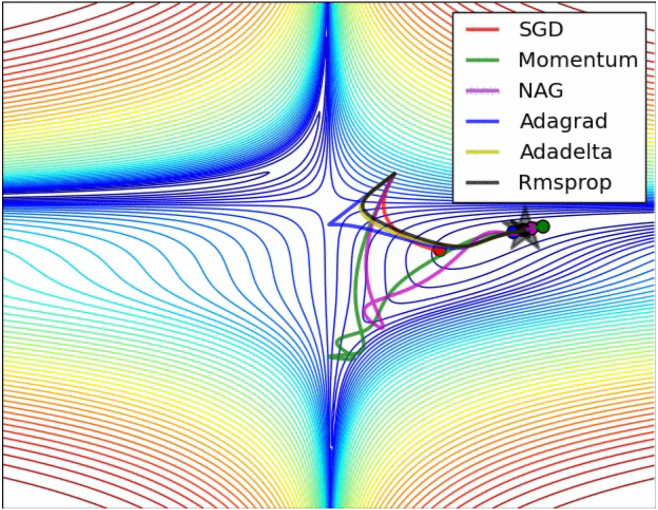
Goh, "Why momentum really works", Distill 2017

Momentum





Goh, “Why momentum really works”, Distill 2017



tutti questi sono first-order acceleration methods

First-order acceleration methods

Let us try to unroll gradient descent:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

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&= \mathbf{x}^{(0)} - \alpha \nabla f(\mathbf{x}^{(0)}) - \alpha \nabla f(\mathbf{x}^{(1)})
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The more general form:

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dovrebbe essere t

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generalizes optimization algorithms like ADAM, AdaGrad, etc.

Gradient descent for deep learning

Gradient descent can be applied to nonconvex problems, without optimality guarantees.

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We are rarely interested in the global optimum.

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We get more efficient and numerically stable solutions.

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perché si rischia overfitting

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- Linear regression ($\mathbf{X}$ can be huge and must be inverted/factorized)
- Logistic regression (no closed form solution)

We get more efficient and numerically stable solutions.

Gradient descent for deep learning

In the general DL setting:

Each parameter gets updated so as to decrease the loss:

$$\boldsymbol{\theta}_i \leftarrow \boldsymbol{\theta}_i - \alpha \frac{\partial \ell}{\partial \boldsymbol{\theta}_i}$$

The gradient tells us how to modify the parameters.

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GD riscritto

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- The loss may be non-convex and non-differentiable
- Be aware of computational aspects (e.g. $\nabla \|\mathbf{0}\|_1$?)

Stochastic gradient descent

Recall that the loss is usually defined over n training examples:

$$\ell_\Theta(\{x_i, y_i\}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - f_\Theta(x_i))^2$$

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Two bottlenecks make gradient descent impractical:

- Number of examples
- Number of parameters

Wilson and Martinez, "The general inefficiency of batch training for gradient descent learning", Neural Networks 2003

Mini-batches

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$$\nabla \ell_\Theta(\mathcal{T}) = \frac{1}{n} \sum_{i=1}^{n} \nabla \hat{\ell}_\Theta(\mathcal{T})$$

Compute $\nabla \ell_\Theta$ for a small representative subset of $m \ll n$ examples:

$$\frac{1}{m} \sum_{i=1}^{m} \nabla \hat{\ell}_\Theta(\mathcal{B}) \approx \frac{1}{n} \sum_{i=1}^{n} \nabla \hat{\ell}_\Theta(\mathcal{T})$$

The mini-batch $\mathcal{B} \subset \mathcal{T}$ is drawn uniformly.

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T indica il training set.
é solo una ridenominazione
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The true gradient $\nabla \ell_\Theta$ is approximated, but with a significant speed-up.

Example: MNIST dataset

$$n = 60,000\,,\ m = 10 \quad \Rightarrow \quad 6,000 \times \ \text{speedup}$$

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Remark: The update cost is constant regardless of the size of $\mathcal{T}$.

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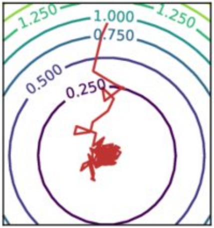

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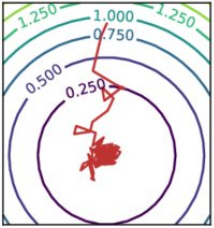

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Oscillations are due to the noise induced by the random sampling.

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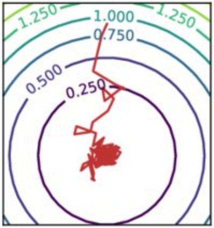

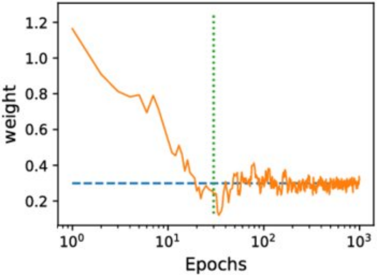

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Asymptotic upper bounds

For a convex problem, there is a true minimizer:

$$f^* = \arg\min_f \ell(f)$$

f * è la funzione ground-truth

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$$|\underbrace{\ell(f_\Theta)}_{\text{GD/SGD}} - \underbrace{\ell(f^*)}_{\text{true}}| < \underbrace{\rho}_{\text{accuracy}}$$

Bottou and Bousquet, "The Tradeoffs of Large Scale Learning", NIPS 2008

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n training examples
d parameters
κ, ν are constants related to the conditioning of the problem

	cost per iteration	**iterations to reach ρ**
GD	$O(nd)$	$O(\kappa \log \frac{1}{\rho})$
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SGD does not depend on the number of examples, implying better generalization

Bottou and Bousquet, "The Tradeoffs of Large Scale Learning", NIPS 2008

Suggested reading

Distill article on why momentum really works:
`https://distill.pub/2017/momentum/`

Seminal paper on using mini-batches for training:
`http://axon.cs.byu.edu/papers/Wilson.nn03.batch.pdf`

Seminal paper on GD vs. SGD performance:
`https://papers.nips.cc/paper/3323-the-tradeoffs-of-large-scale-learning.pdf`