Introduction aux réseaux de neurones : La descente de gradient

Matériel de cours rédigé par Pascal Germain, 2019

Out[1]: voir/cacher le code.

Régression linéaire

Considérons un ensemble d'apprentissage $S = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_n, y_n)\}$,

avec $\mathbf{x} \in \mathbb{R}^d$ et $y \in \mathbb{R}$.

Considérons un préficteur $f_{\mathbf{w}}$ *linéaire* et sans biais,

$$f_{\mathbf{w}}(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x}\,,$$

La minimisation de la *fonction de perte quadratique* revient à résoudre problème d'opimisation des *moindres carrés*:

$$\min_{\mathbf{w}} \left[\frac{1}{n} \sum_{i=1}^{n} (\mathbf{w} \cdot \mathbf{x}_i - y_i)^2 \right].$$

Nous désirons trouver le minimum de la **fonction objectif** $F(\mathbf{w})$ suivante:

$$F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} (\mathbf{w} \cdot \mathbf{x}_i - y_i)^2.$$

Calculons la **dérivée partielle** de $F(\mathbf{w})$ selon un élément w_k du vecteur $\mathbf{w}$

$$\begin{aligned}
\frac{\partial F(\mathbf{w})}{\partial w_k} &= \frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial w_k} (\mathbf{w} \cdot \mathbf{x}_i - y_i)^2 \\
&= \frac{1}{n} \sum_{i=1}^{n} 2\,(\mathbf{w} \cdot \mathbf{x}_i - y_i) \frac{\partial}{\partial w_k} (\mathbf{w} \cdot \mathbf{x}_i - y_i) \\
&= \frac{1}{n} \sum_{i=1}^{n} 2\,(\mathbf{w} \cdot \mathbf{x}_i - y_i) \frac{\partial}{\partial w_k} (w_k\, x_{i,k}) \\
&= \frac{1}{n} \sum_{i=1}^{n} 2\,(\mathbf{w} \cdot \mathbf{x}_i - y_i)\, x_{i,k}\,.
\end{aligned}$$

Le **gradient** de $F(\mathbf{w})$, noté $\nabla F(\mathbf{w})$, est le vecteur de toute les dérivées partielles au point $\mathbf{w}$:

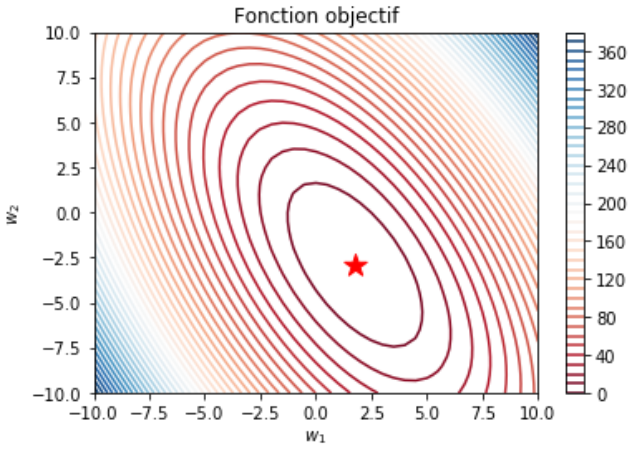
$$\nabla F(\mathbf{w}) = \begin{bmatrix} \frac{\partial}{\partial w_1} \\ \vdots \\ \frac{\partial}{\partial w_d} \end{bmatrix} = \frac{2}{n} \sum_{i=1}^{n} (\mathbf{w} \cdot \mathbf{x}_i - y_i)\, \mathbf{x}_i\,.$$

Le minimum d'une fonction convexe est atteint lorsque $\nabla F(\mathbf{w}) = 0$.

Illustrons la fonction objectif pour un sensemble de donnnés tel que:

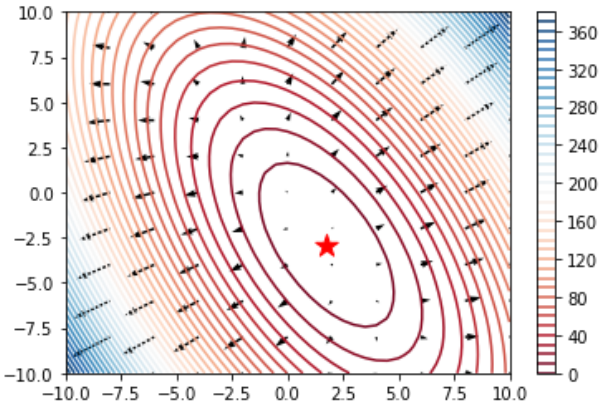
$$\mathbf{X} = \begin{bmatrix} 1 & 1 \\ 0 & -1 \\ 2 & \frac{1}{2} \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} -1 \\ 3 \\ 2 \end{bmatrix}$$

Out[2]: voir/cacher le code.



Illustrons maintenant les gradients de la fonction objectif.

Out[3]: voir/cacher le code.



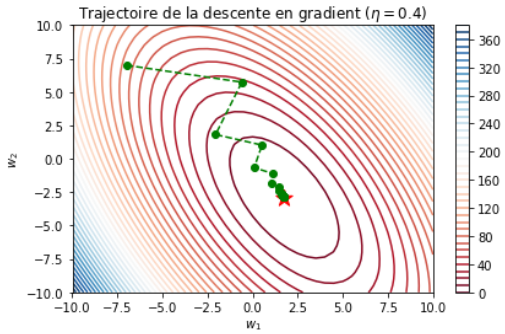
Descente en gradient

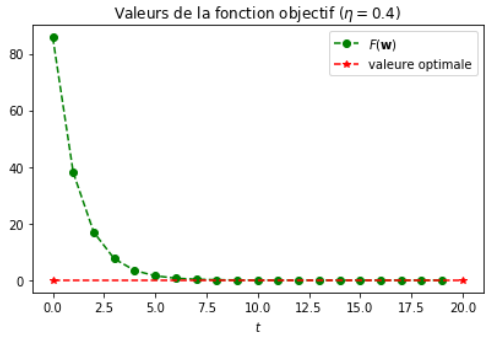
Algorithme (pour un *pas de gradient* η et un nombre d'itérations T)

- Initialiser $\mathbf{z}_0 \in \mathbb{R}^d$ aléatoirement
- Pour t de 1 à T:
  - $\mathbf{g}_t = \nabla F(\mathbf{z}_{t-1})$
  - $\mathbf{z}_t = \mathbf{z}_{t-1} - \eta\, \mathbf{g}_t$
- Retourner $\mathbf{z}_T$

Exemple avec $\eta = 0.4$ et $T = 20$

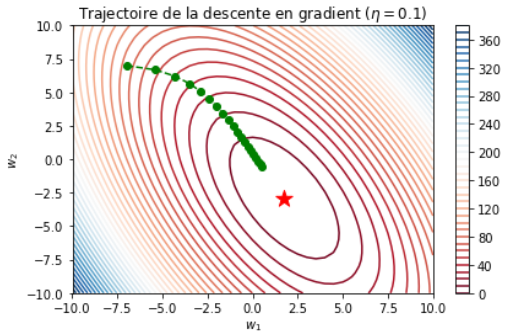
Out[4]: voir/cacher le code.

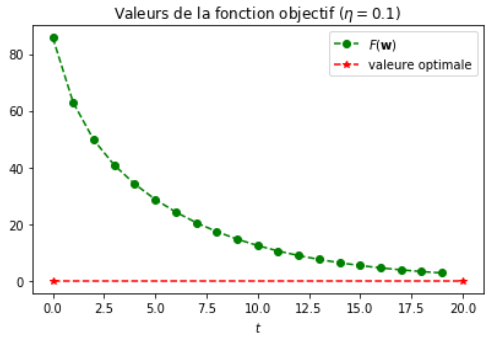




Exemple avec $\eta = 0.1$ et $T = 20$

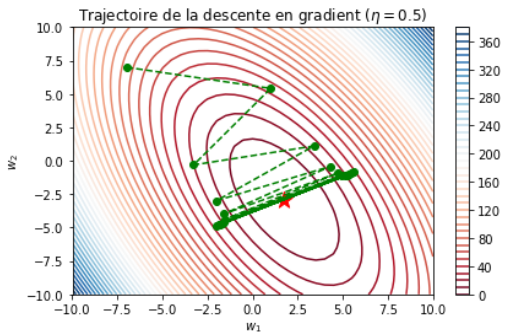
Out[5]: voir/cacher le code.

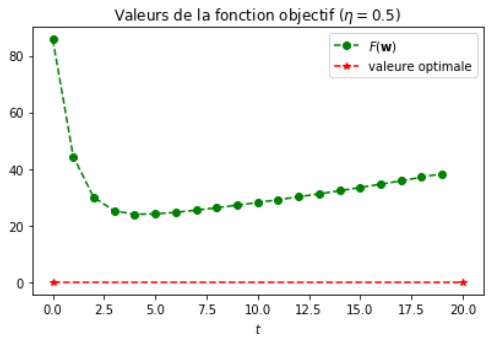




Exemple avec $\eta = 0.5$ et $T = 20$

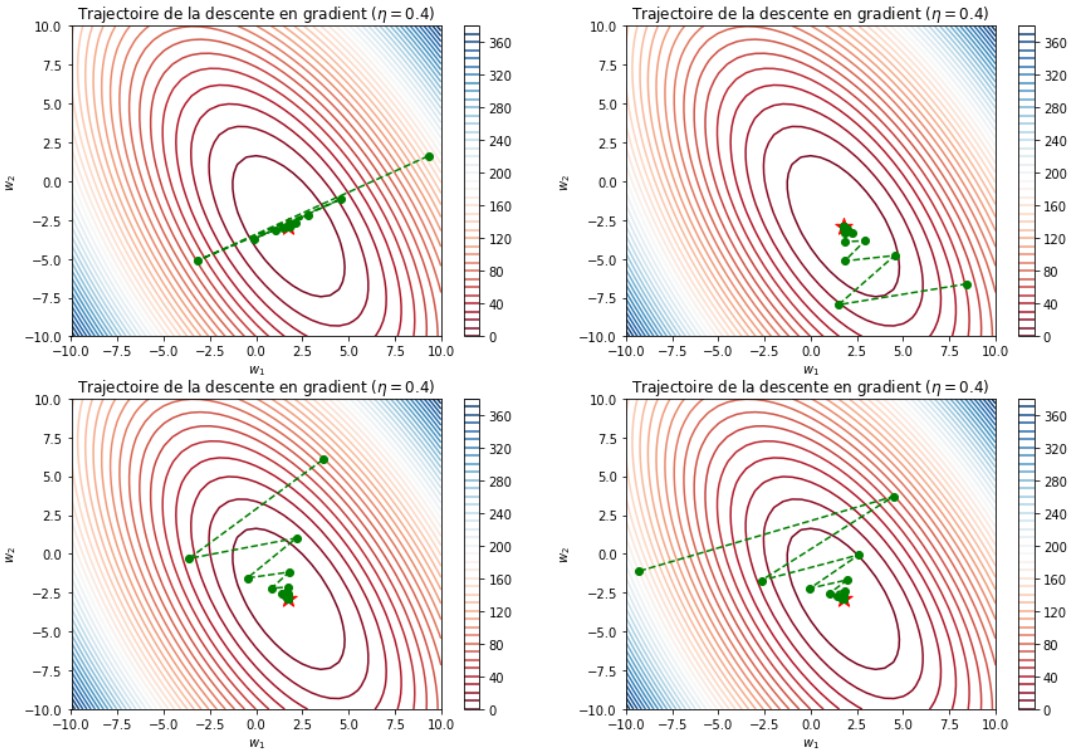
Out[6]: voir/cacher le code.



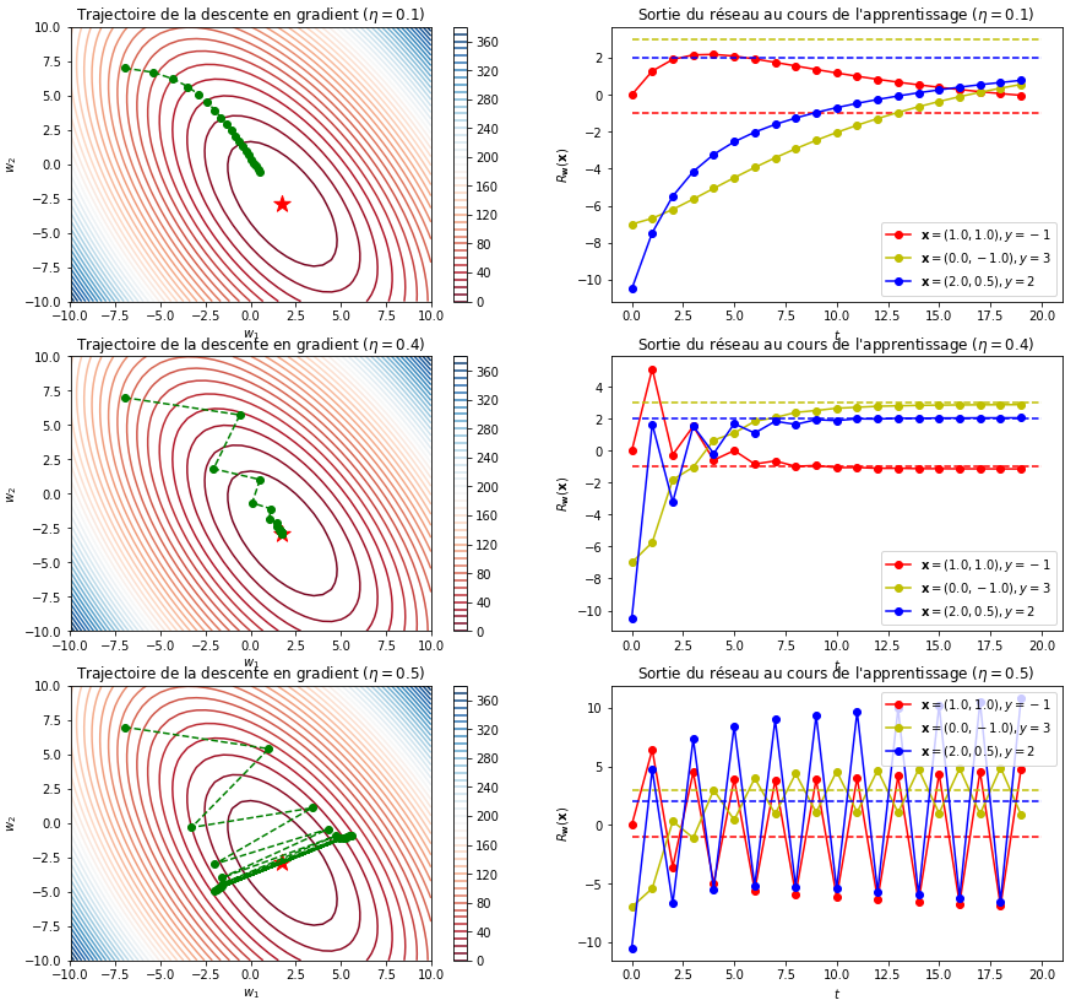


Exemple avec $\eta = 0.4$ et $T = 20$, différentes initialisation aléatoires

Out[7]: voir/cacher le code.



Out[8]: voir/cacher le code.



Descente en gradient stochastique

Nous désirons trouver le minimum de la **fonction objectif** $F(\mathbf{w})$ suivante:

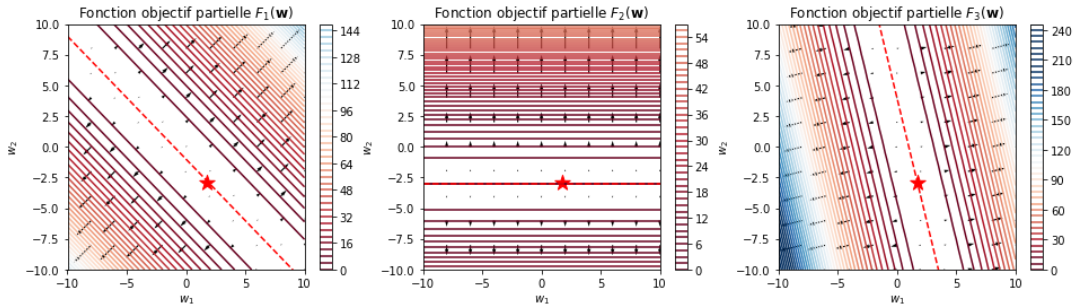
$$F(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{w}\cdot\mathbf{x}_i - y_i)^2 = \frac{1}{n}\sum_{i=1}^{n} F_i(\mathbf{w})\,,$$

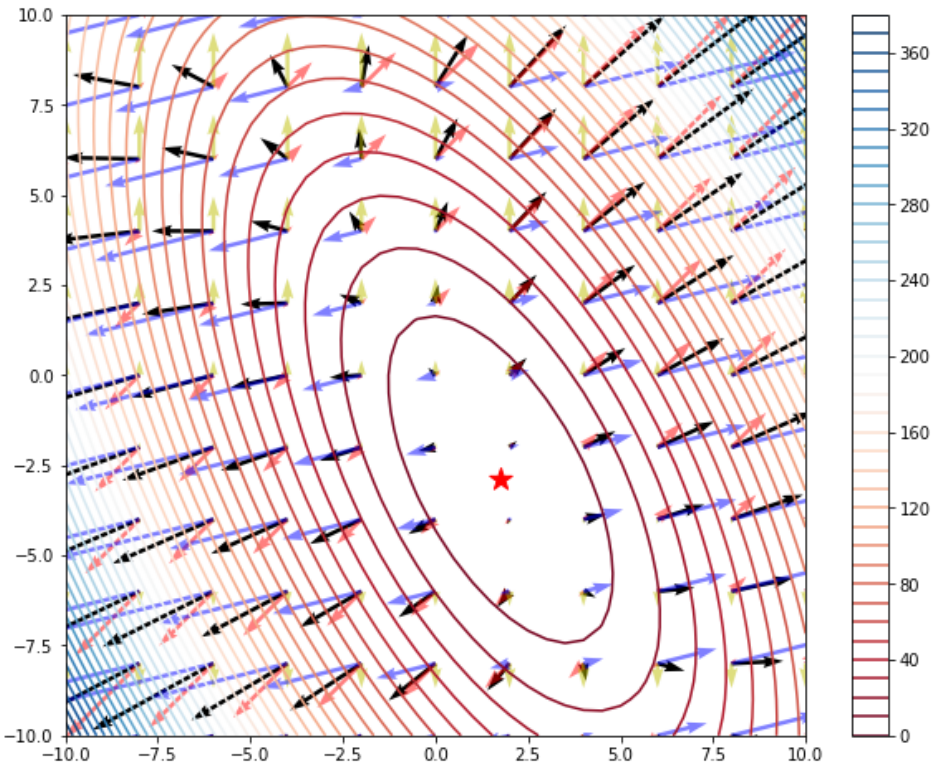
avec $F_i(\mathbf{w}) = (\mathbf{w}\cdot\mathbf{x}_i - y_i)^2$ et donc $\nabla F_i(\mathbf{w}) = 2\,(\mathbf{w}\cdot\mathbf{x}_i - y_i)\,\mathbf{x}_i$.

Algorithme (pour un *pas de gradient* η et un nombre d'itérations T)

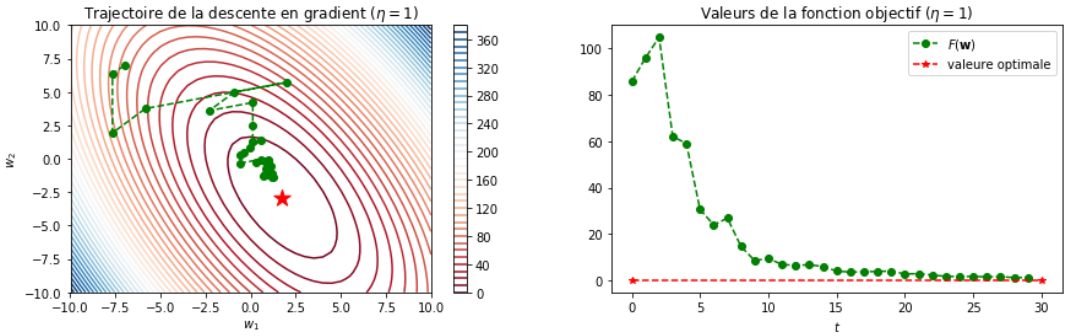
- Initialiser $\mathbf{z}_0 \in \mathbb{R}^d$ aléatoirement
- Pour t de 1 à T:
  - Choisir aléatoirement $i \in \{1,\ldots,n\}$
  - $\mathbf{g}_t = \nabla F_i(\mathbf{z}_{t-1})$
  - $\mathbf{z}_t = \mathbf{z}_{t-1} - \dfrac{\eta}{\sqrt{t}}\,\mathbf{g}_t$
- Retourner $\mathbf{z}_T$

Out[9]: voir/cacher le code.





Out[11]: voir/cacher le code.

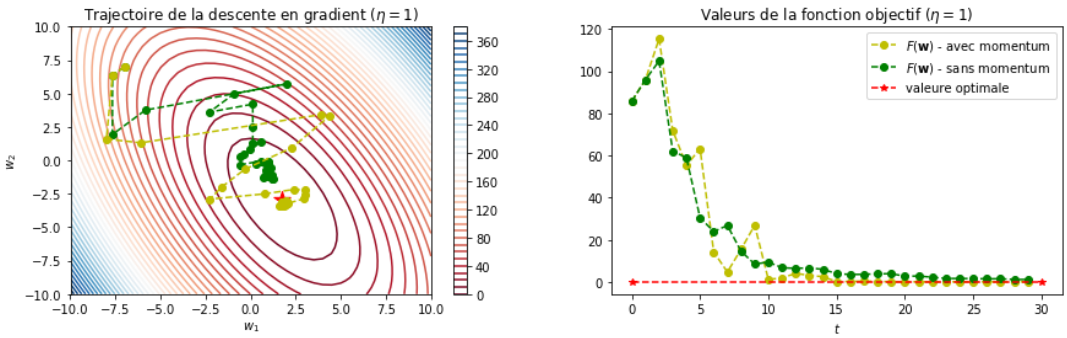


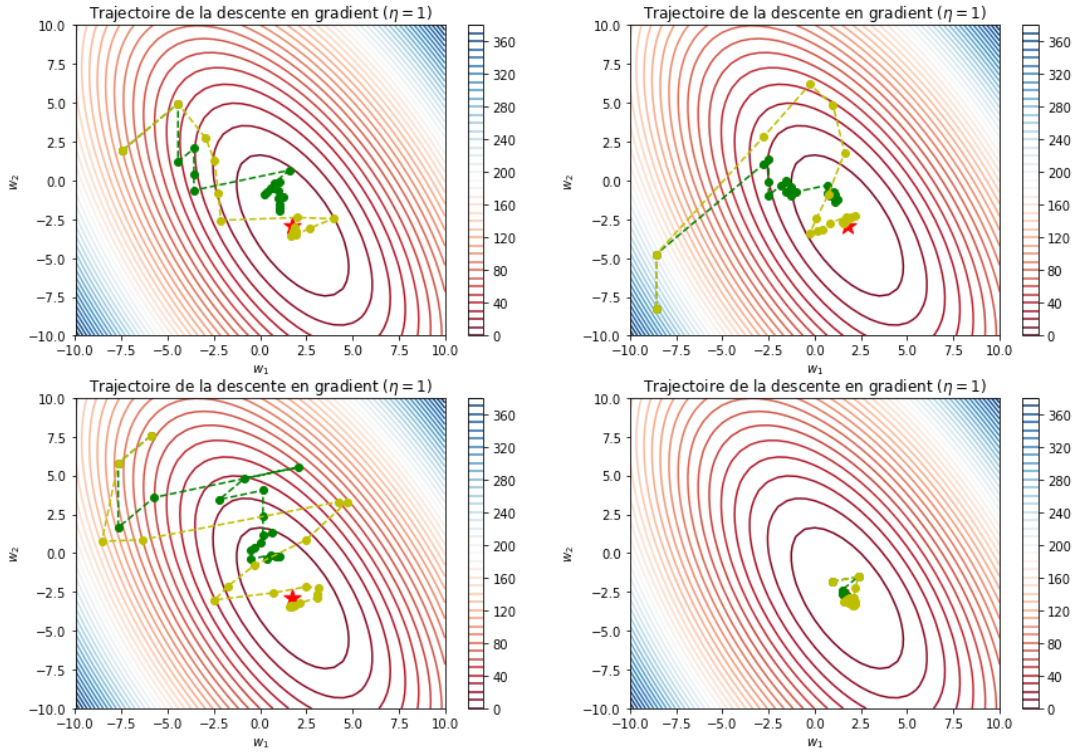
Descente en gradient stochastique avec momentum

Algorithme (pour un *pas de gradient* η, une vélocité α et un nombre d'itérations T)

- Initialiser $\mathbf{z}_0 \in \mathbb{R}^d$ aléatoirement
- $\mathbf{v}_0 = 0$
- Pour t de 1 à T:
  - Choisir aléatoirement $i \in \{1, \ldots, n\}$
  - $\mathbf{g}_t = \nabla F_i(\mathbf{z}_{t-1})$
  - $\mathbf{v}_t = \alpha\, \mathbf{v}_{t-1} - \dfrac{\eta}{\sqrt{t}} \mathbf{g}_t$
  - $\mathbf{z}_t = \mathbf{z}_{t-1} + \mathbf{v}_t$
- Retourner $\mathbf{z}_T$

Out[12]: voir/cacher le code.



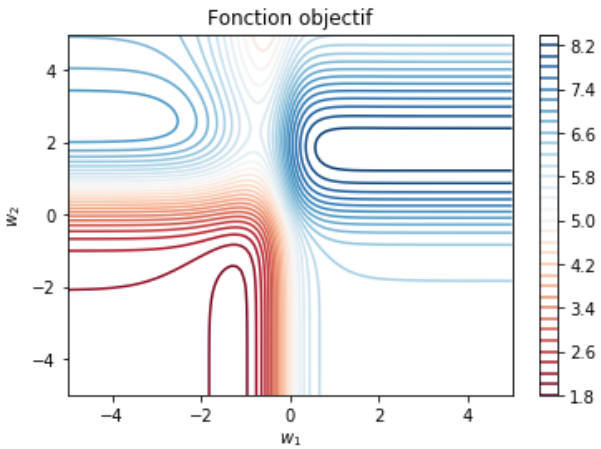


Les réseaux de neurones génèrent des fonctions d'optimisation non-convexes

$$R_{\mathbf{w}}(\mathbf{x}) = \mathbf{v} \cdot \tanh\left(\begin{bmatrix} w_1 & -1 \\ 1 & w_2 \end{bmatrix} \mathbf{x}\right), \quad \text{avec } \mathbf{v} = [-1, 1]\,.$$

$$F(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} (R_{\mathbf{w}}(\mathbf{x}_i) - y_i)^2.$$

Out[101]: voir/cacher le code.



Implémentation dans `pytorch` : Descente en gradient stochastique avec momentum

```
torch.optim.SGD?
```

```
Implements stochastic gradient descent (optionally with momentum).

    Nesterov momentum is based on the formula from
    `On the importance of initialization and momentum in deep learning`__.

    Args:
        params (iterable): iterable of parameters to optimize or dicts defini
ng
            parameter groups
        lr (float): learning rate
        momentum (float, optional): momentum factor (default: 0)
        weight_decay (float, optional): weight decay (L2 penalty) (default:
0)
        dampening (float, optional): dampening for momentum (default: 0)
        nesterov (bool, optional): enables Nesterov momentum (default: False)

    Example:
        >>> optimizer = torch.optim.SGD(model.parameters(), lr=0.1, momentum=
0.9)
        >>> optimizer.zero_grad()
        >>> loss_fn(model(input), target).backward()
        >>> optimizer.step()

    __ http://www.cs.toronto.edu/%7Ehinton/absps/momentum.pdf

    .. note::
        The implementation of SGD with Momentum/Nesterov subtly differs from
        Sutskever et. al. and implementations in some other frameworks.

        Considering the specific case of Momentum, the update can be written
as

        .. math::
                  v = \rho * v + g \\
                  p = p - lr * v

        where p, g, v and :math:`\rho` denote the parameters, gradient,
        velocity, and momentum respectively.

        This is in contrast to Sutskever et. al. and
        other frameworks which employ an update of the form

        .. math::
             v = \rho * v + lr * g \\
             p = p - v

        The Nesterov version is analogously modified.
```

Autre algorithme de descente de gradient

Implémentation dans `pytorch` : RMSprop

```
torch.optim.RMSprop?
```

```
Implements RMSprop algorithm.

    Proposed by G. Hinton in his
    `course <http://www.cs.toronto.edu/~tijmen/csc321/slides/lecture_slides_l
ec6.pdf>`_.

    The centered version first appears in `Generating Sequences
    With Recurrent Neural Networks <https://arxiv.org/pdf/1308.0850v5.pdf>`_.

    Arguments:
        params (iterable): iterable of parameters to optimize or dicts defini
ng
            parameter groups
        lr (float, optional): learning rate (default: 1e-2)
        momentum (float, optional): momentum factor (default: 0)
        alpha (float, optional): smoothing constant (default: 0.99)
        eps (float, optional): term added to the denominator to improve
            numerical stability (default: 1e-8)
        centered (bool, optional) : if ``True``, compute the centered RMSPro
p,
            the gradient is normalized by an estimation of its variance
        weight_decay (float, optional): weight decay (L2 penalty) (default:
0)
```

Autre algorithme de descente de gradient

Implémentation dans `pytorch` : ADAM

```
torch.optim.Adam?
```

```
Implements Adam algorithm.

    It has been proposed in `Adam: A Method for Stochastic Optimization`_.

    Arguments:
        params (iterable): iterable of parameters to optimize or dicts defini
ng
            parameter groups
        lr (float, optional): learning rate (default: 1e-3)
        betas (Tuple[float, float], optional): coefficients used for computin
g
            running averages of gradient and its square (default: (0.9, 0.99
9))
        eps (float, optional): term added to the denominator to improve
            numerical stability (default: 1e-8)
        weight_decay (float, optional): weight decay (L2 penalty) (default:
0)
        amsgrad (boolean, optional): whether to use the AMSGrad variant of th
is
            algorithm from the paper `On the Convergence of Adam and Beyond`_
            (default: False)

    .. _Adam\: A Method for Stochastic Optimization:
        https://arxiv.org/abs/1412.6980
    .. _On the Convergence of Adam and Beyond:
        https://openreview.net/forum?id=ryQu7f-RZ
```