



Deep Learning Optimisé - Jean Zay

Entraînement et large batches



INSTITUT DU
DÉVELOPPEMENT ET DES
RESSOURCES EN
INFORMATIQUE
SCIENTIFIQUE



Loss Landscape

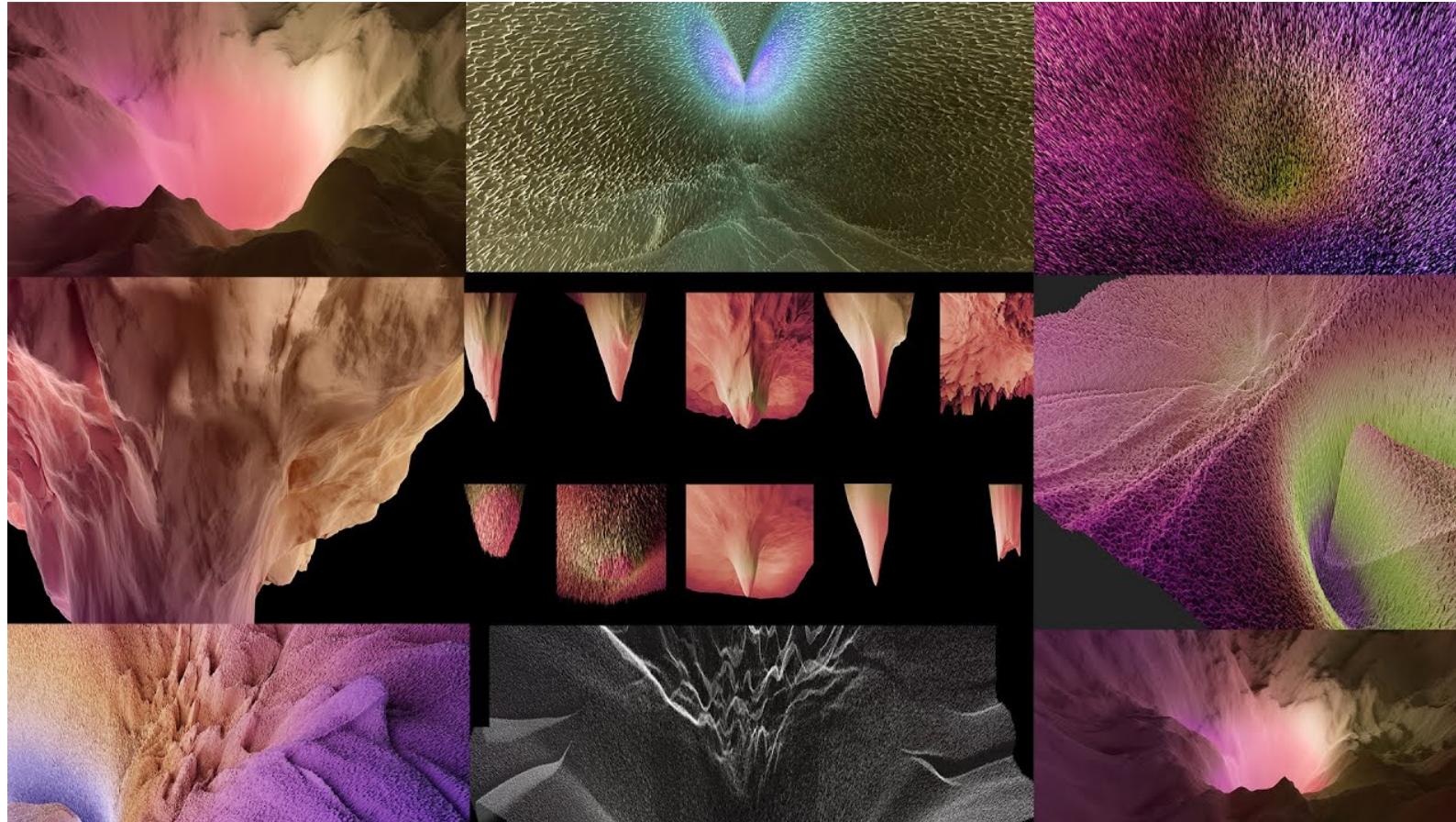
Loss Landscape ◀

Residual Learning ◀

Initialization ◀

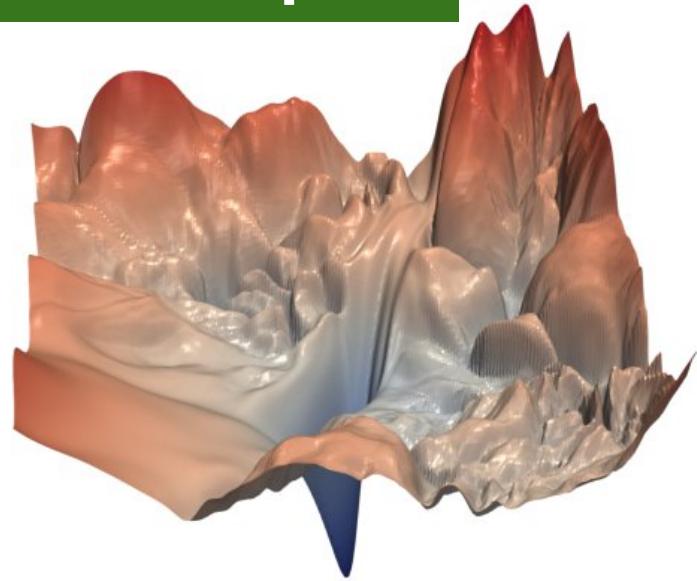
Loss Landscape

<https://losslandscape.com/>

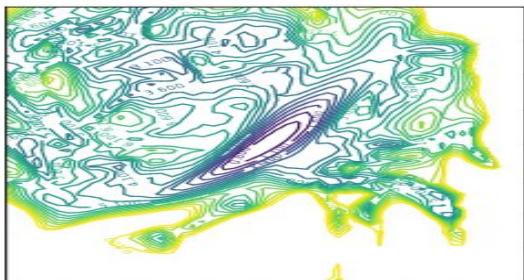


Loss Landscape

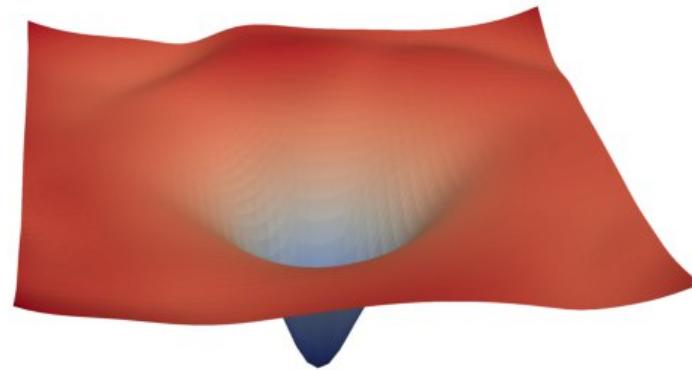
<https://arxiv.org/pdf/1712.09913.pdf>



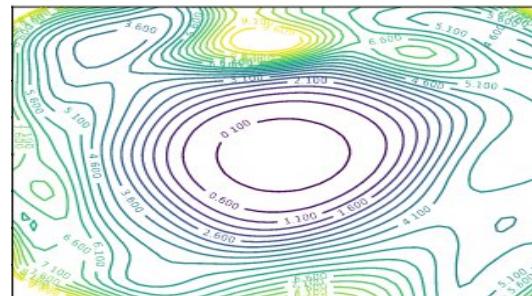
(a) without skip connections



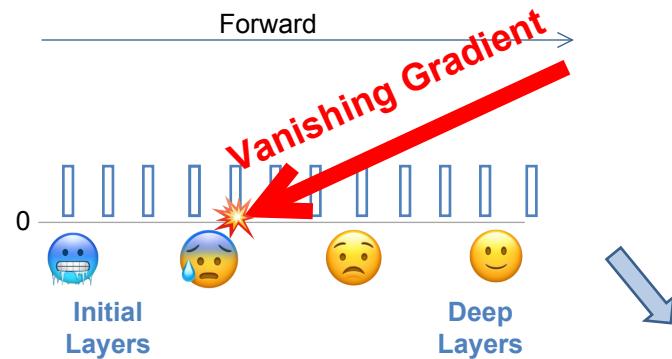
Residual Learning
Depuis les Resnets (2015) ...



(b) with skip connections

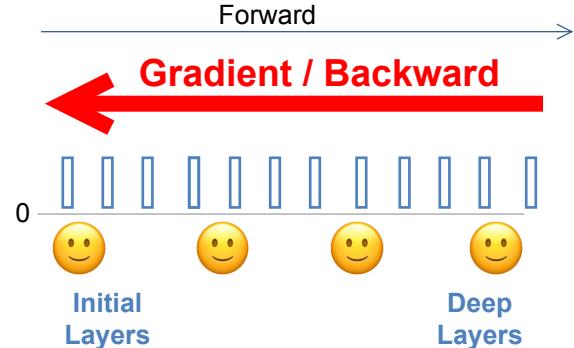


Residual Learning

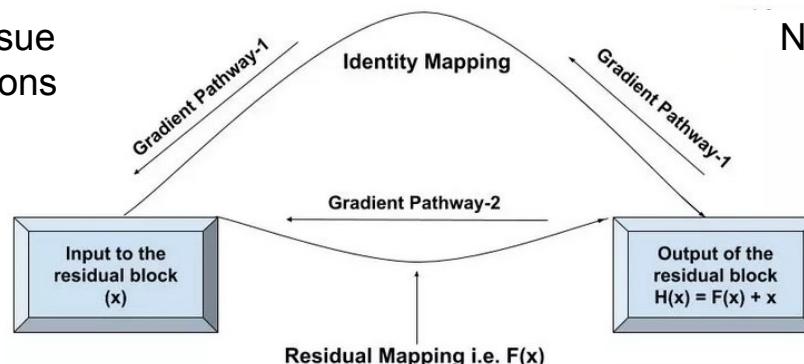


Vanishing Gradient issue
without skip connections

Residual Block
 $F(x) + x$



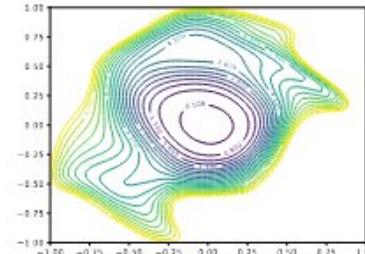
No Vanishing Gradient issue
with skip connections



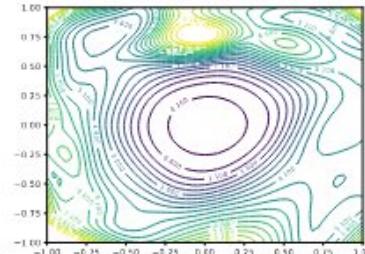
Gradient Pathways in ResNet

Residual Learning – impact sur la profondeur

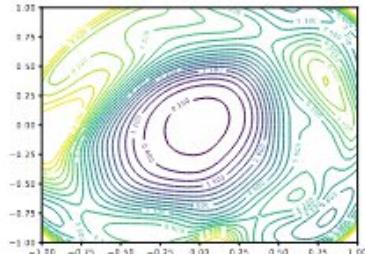
ResNet



(a) ResNet-20, 7.37%

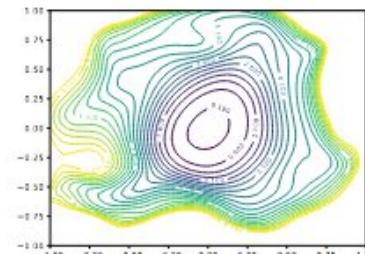


(b) ResNet-56, 5.89%

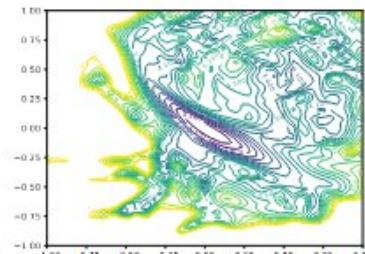


(c) ResNet-110, 5.79%

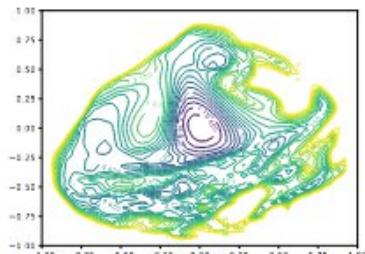
ResNet -
No Short
without skip connections



(d) ResNet-20-NS, 8.18%



(e) ResNet-56-NS, 13.31%



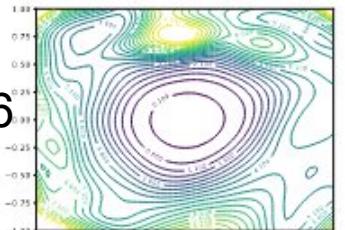
(f) ResNet-110-NS, 16.44%



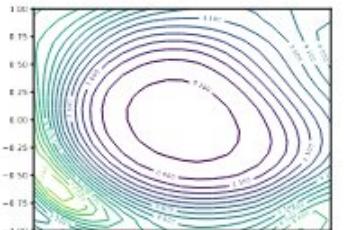
Residual Learning – impact sur la largeur



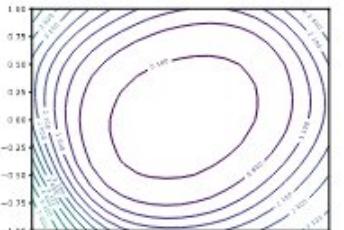
Wide-ResNet-56



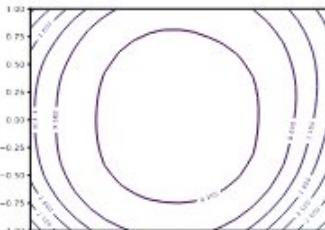
(a) $k = 1, 5.89\%$



(b) $k = 2, 5.07\%$

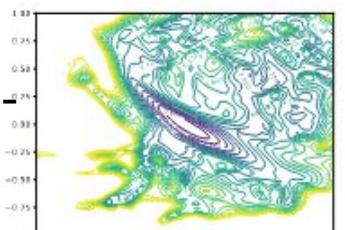


(c) $k = 4, 4.34\%$

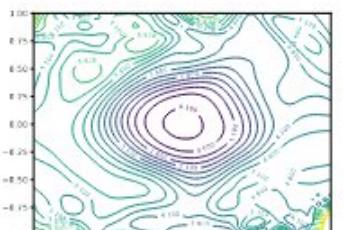


(d) $k = 8, 3.93\%$

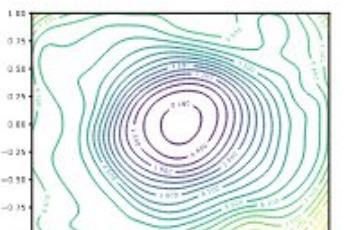
Wide-ResNet-56-
No Short
without skip connections



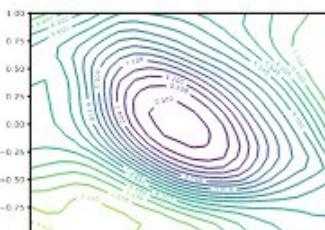
(e) $k = 1, 13.31\%$



(f) $k = 2, 10.26\%$



(g) $k = 4, 9.69\%$



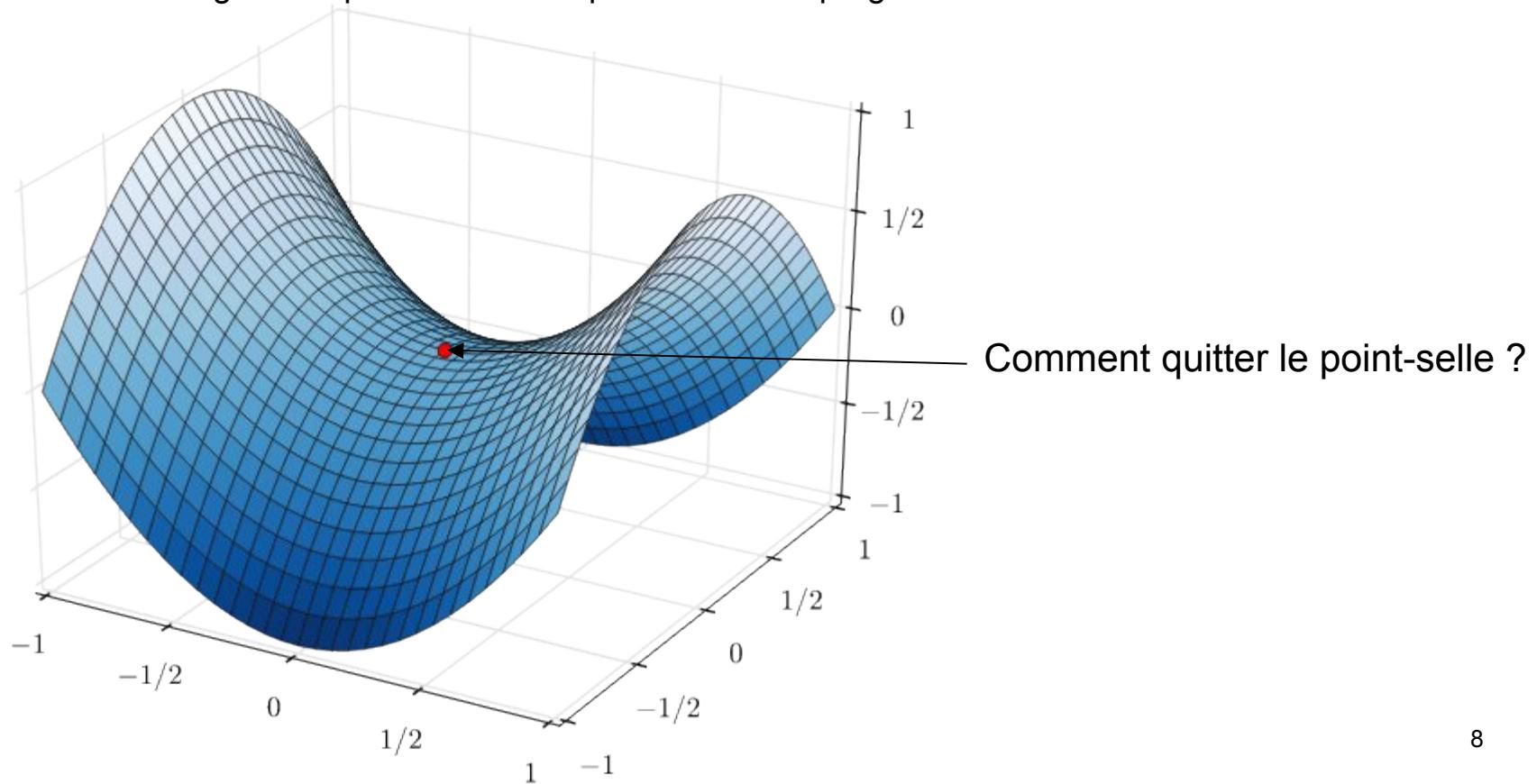
(h) $k = 8, 8.70\%$



k = coefficient largeur des channels par rapport à ResNet

Problème du point-selle

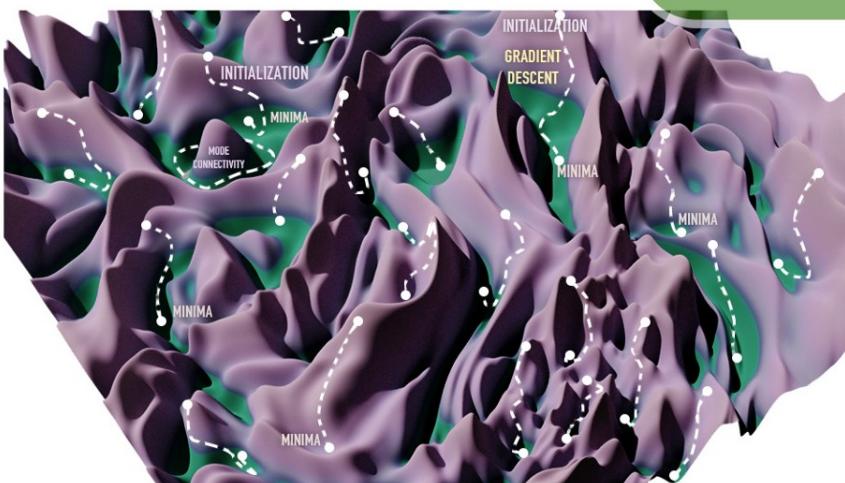
Point-selle : Un gradient proche de zéro qui va rendre la progression du modèle très lente



Initialisation des paramètres du modèle

The Blessing of Dimensionality :

Local



FINDING A MINIMA BECOMES A "LOCAL" CHALLENGE



- Xavier Initialization
 - uniform
 - normal
- Kaiming Initialization
 - uniform
 - normal

Par défaut dans *PyTorch* :

- Meilleur algorithme d'initialisation selon le type de couche (linéaire, convolutionnel, transformer, ...).
- Aujourd'hui, il n'est plus nécessaire de chercher à optimiser l'initialisation.

Learning rate scheduler

Learning rate scheduler ◀

Cyclic scheduler ◀

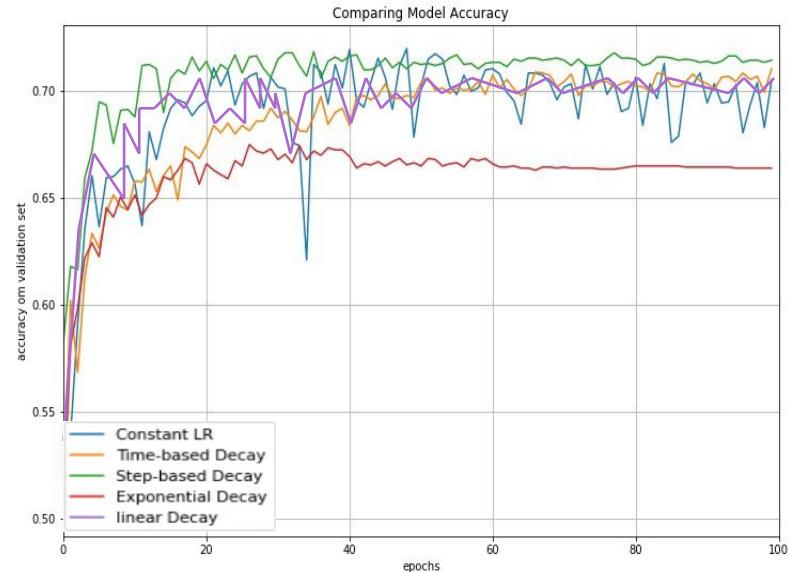
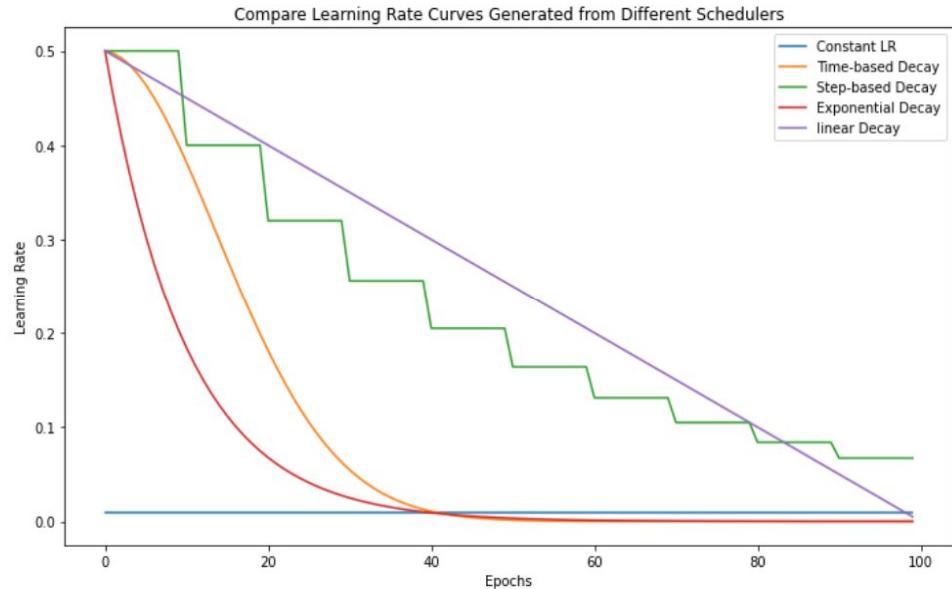
One cycle scheduler ◀

LR finder ◀

LR large batch ◀

Learning Rate Scheduler

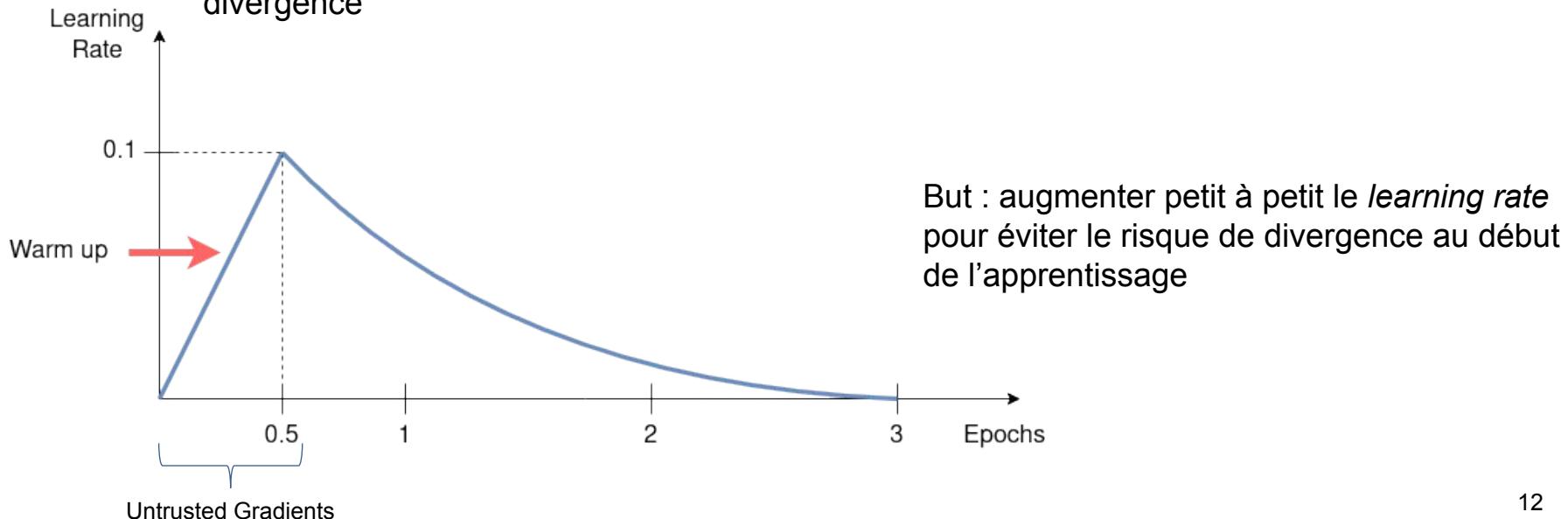
Learning rate decay



Learning Rate Scheduler

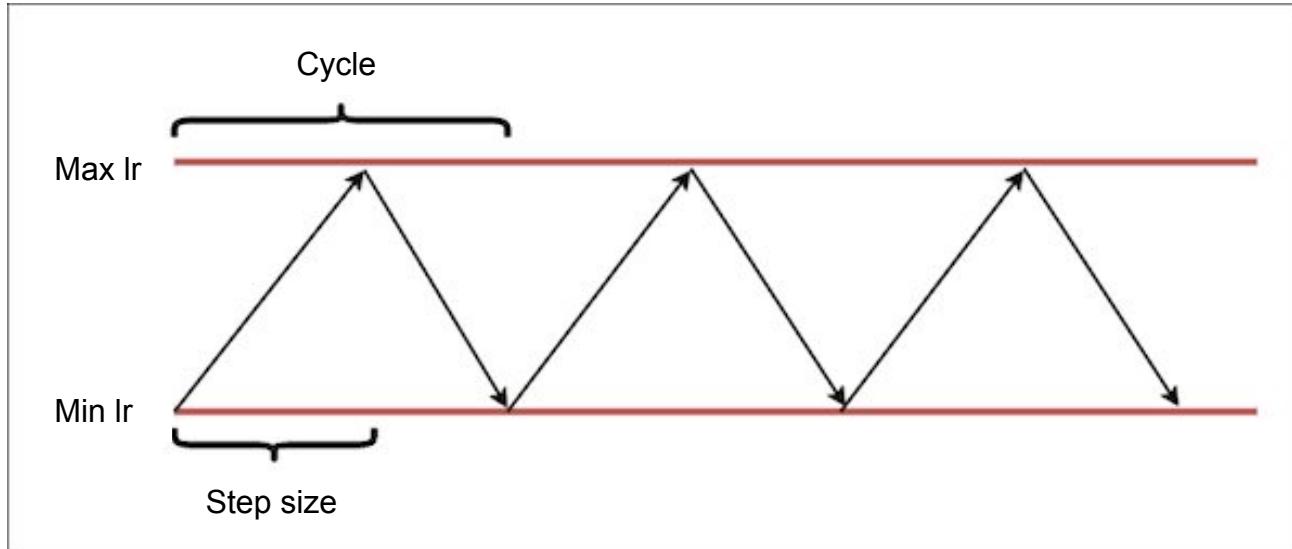
WARMUP pour *large batches*

Problèmes : Les premières itérations ont trop d'effet sur le modèle (loss importantes, gradients élevés, biais, ...), un *learning rate* élevé peut provoquer une forte instabilité ou une divergence



Cyclic Learning Rate Scheduler

Cyclical Learning Rates for Training Neural Networks - Leslie N. Smith 2017

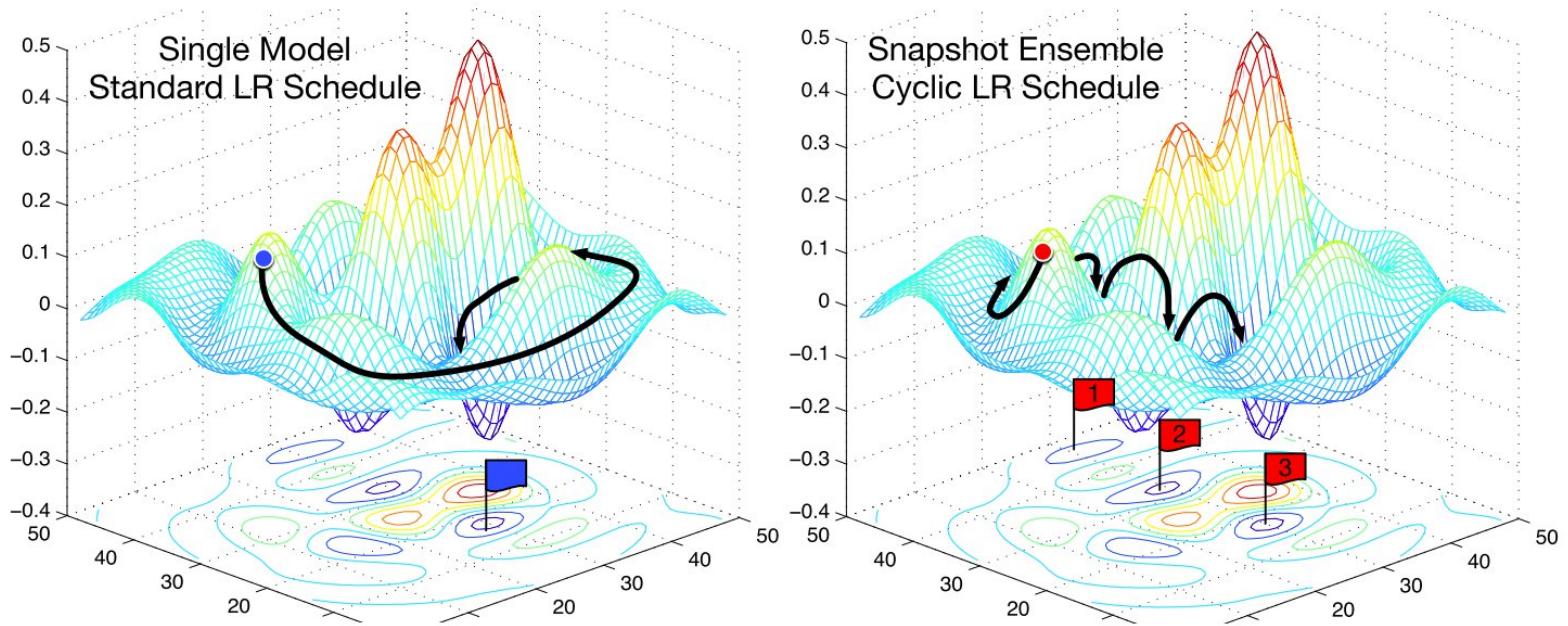


Paramètres :

- Step_size = $x * \text{epoch}$ ($2 \leq x \leq 10$)
- Base_lr -> valeur minimum de convergence
- max_lr -> valeur maximale avant divergence

Succession de *warmups* et de *learning rate decays*

Cyclic Learning Rate Scheduler



SNAPSHOT ENSEMBLES: TRAIN 1, GET M FOR FREE

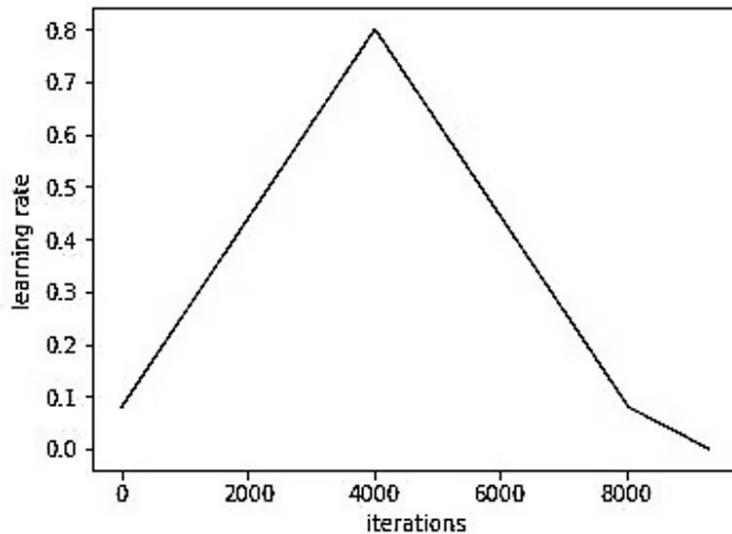
Gao Huang, Yixuan Li, Geoff Pleiss

One Cycle Learning Rate

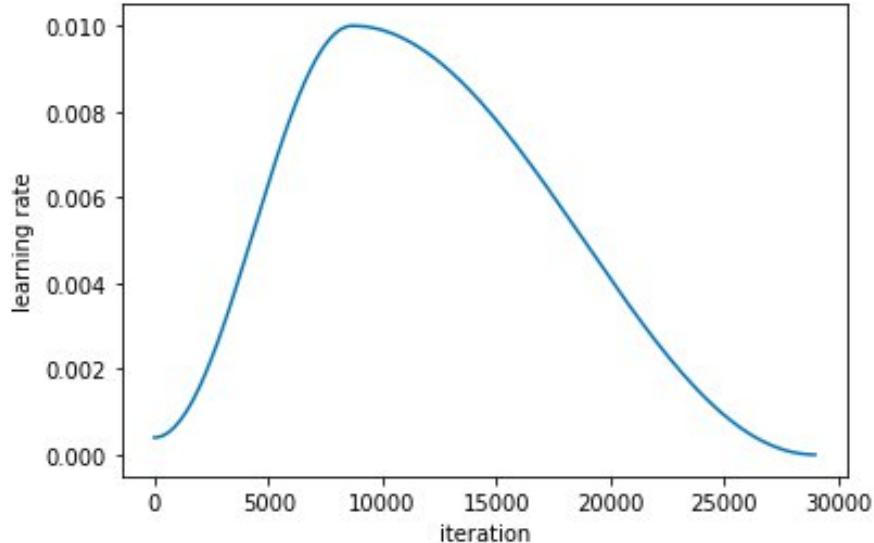
Un seul cycle suffit !

A disciplined approach to neural network hyper-parameters -
[Leslie N. Smith](#)

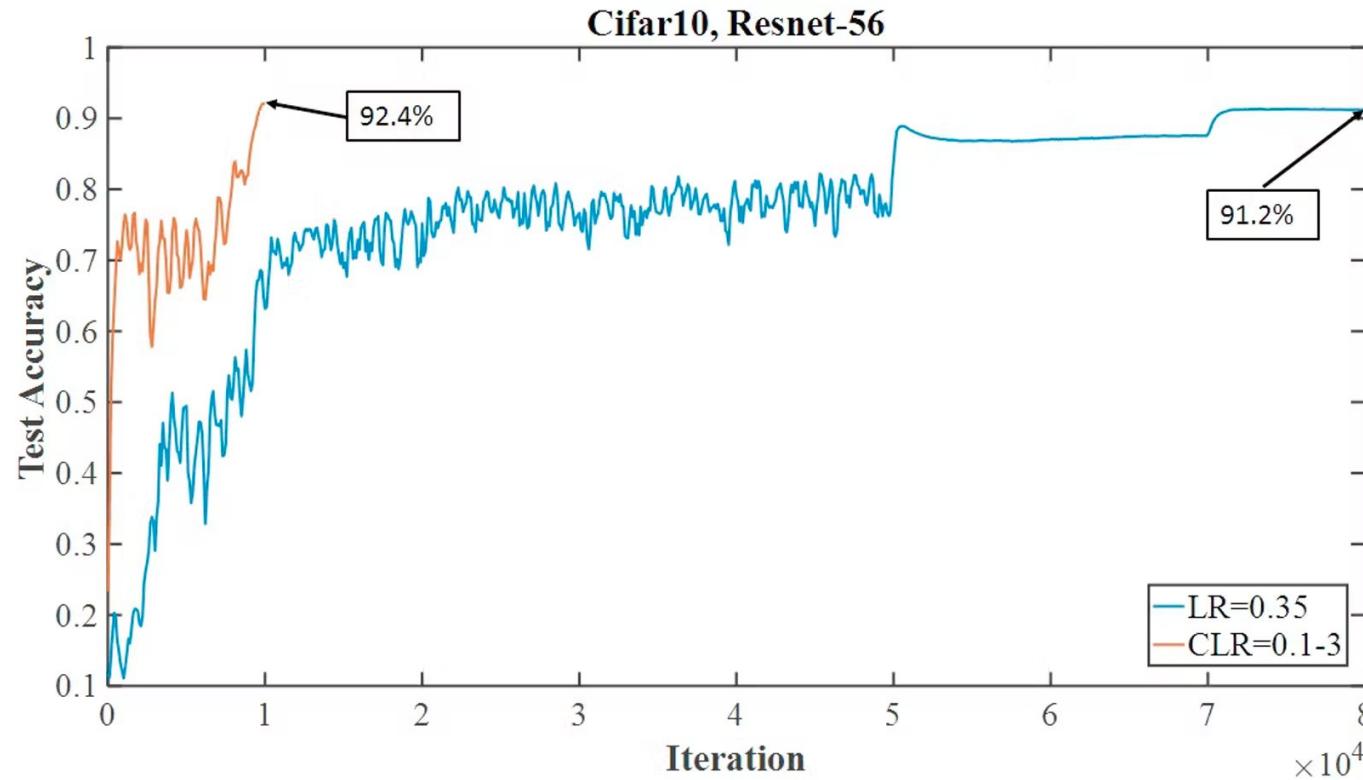
Proposition initiale



cosine annealing : Recommandation par FastAI



One Cycle Learning Rate - Super convergence

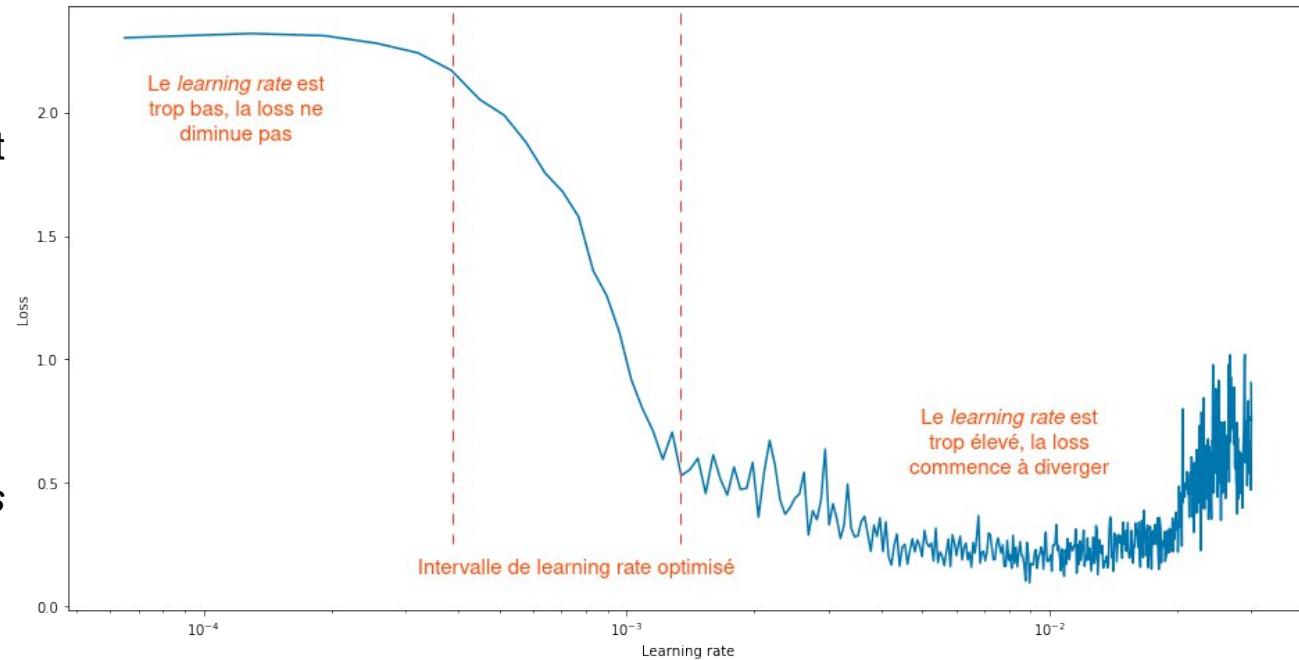


Une convergence plus rapide pour une précision finale équivalente

Learning Rate Finder

But : Trouver les valeurs de *learning rate* optimales pour son modèle, particulièrement pour la valeur maximale d'un *cyclic scheduler*

- Faire tourner son modèle sur quelques *epochs* en faisant augmenter son *learning rate*
- Début de baisse de la *loss*
→ *Learning rate minimal*
- Début de variation de la *loss*
→ *Learning rate maximal*



Learning Rate Scheduler

Chaque scheduler a ses propres paramètres

```
import torch.optim as opt
```

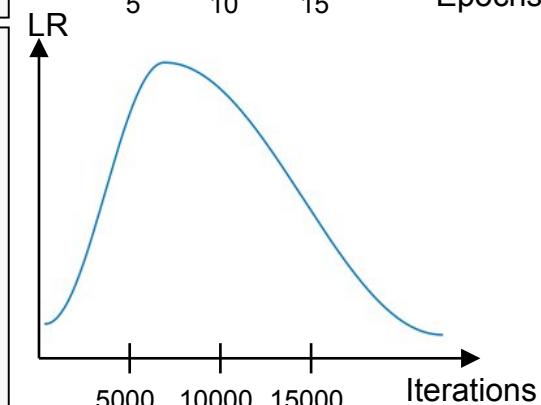
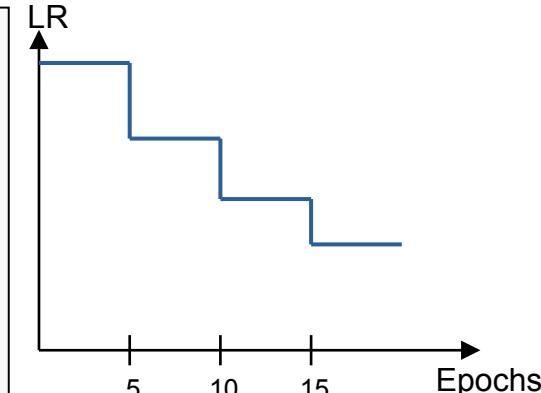
```
scheduler = opt.lr_scheduler.StepLR(optimizer, step_size=5, gamma=0.1)
```

```
for epoch in range(100):
    train(...)
    validate(...)
    scheduler.step()
```

```
import torch.optim as opt
```

```
scheduler = opt.lr_scheduler.CyclicLR(optimizer, base_lr=0.01, max_lr=0.1)
```

```
for epoch in range(10):
    for batch in data_loader:
        train_batch(...)
        scheduler.step()
```



Optimiseur de descente de gradient

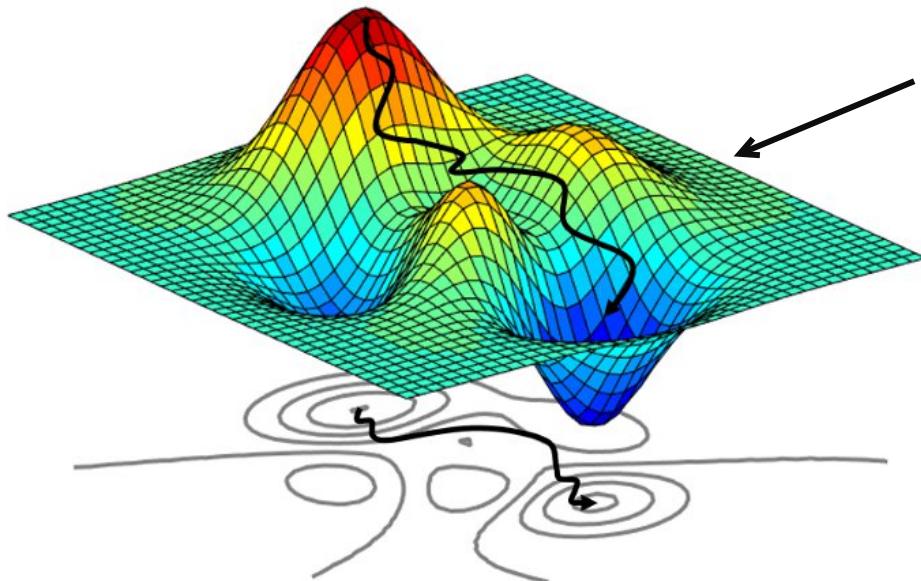
SGD ◀

ADAM ◀

ADAMW ◀

Optimiseur - SGD

L'optimiseur est l'algorithme qui pilote la descente de gradient et la recherche de minimum avec pour but d'optimiser le temps d'apprentissage et la métrique finale.



SGD = *Stochastic Gradient Descent*
Calcul du Gradient et mise à jour des poids
à chaque **batch**

- + Taille de *batch* et *learning rate* adaptables selon les besoins contradictoires :
 - D'exploration pour trouver le meilleur minimum local
 - D'accélération de la descente de gradient

SGD with Momentum

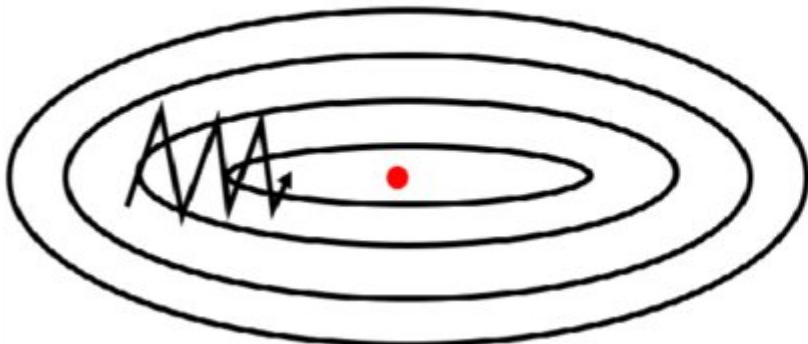
$$m_0 = 0$$

Coefficient de momentum

$$m_i = \boxed{\beta} * m_{i-1} + (1 - \beta) * g_i$$

$$\theta_i = \theta_{i-1} - \alpha * m_i$$

SGD without momentum



+ Permet de converger plus rapidement

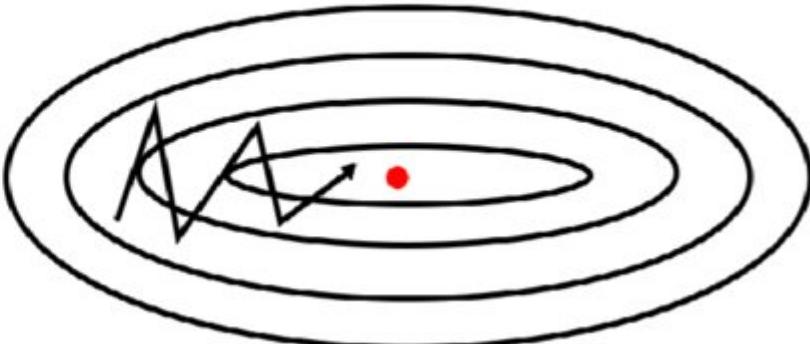
- Pas de garantie que le *momentum* nous amène dans la bonne direction

Objectif : Prendre en considération les gradients précédents pour une descente de gradient plus rapide.

Valeur initiale conseillée : 0,9

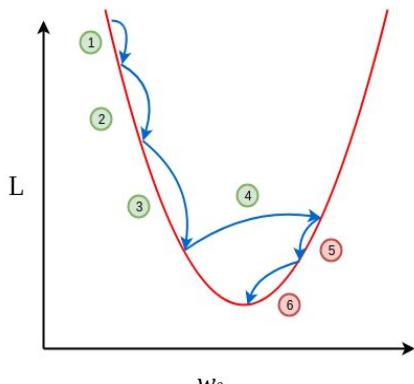
$$0.85 < \beta < 0.95$$

SGD with momentum

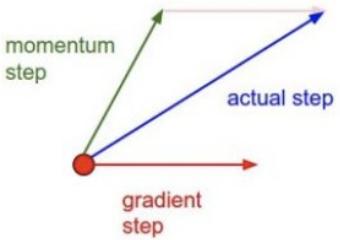


Types de Momentum

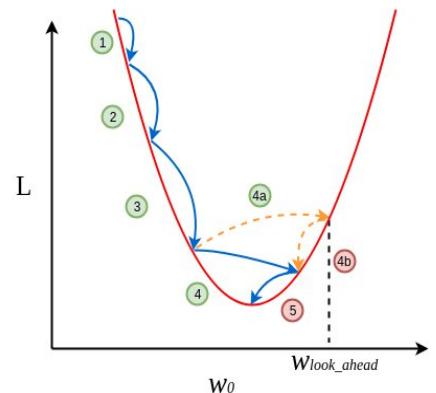
Momentum



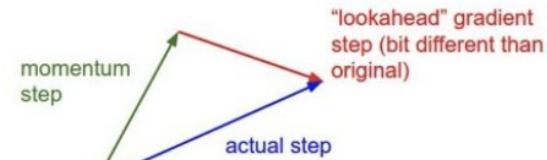
Momentum update



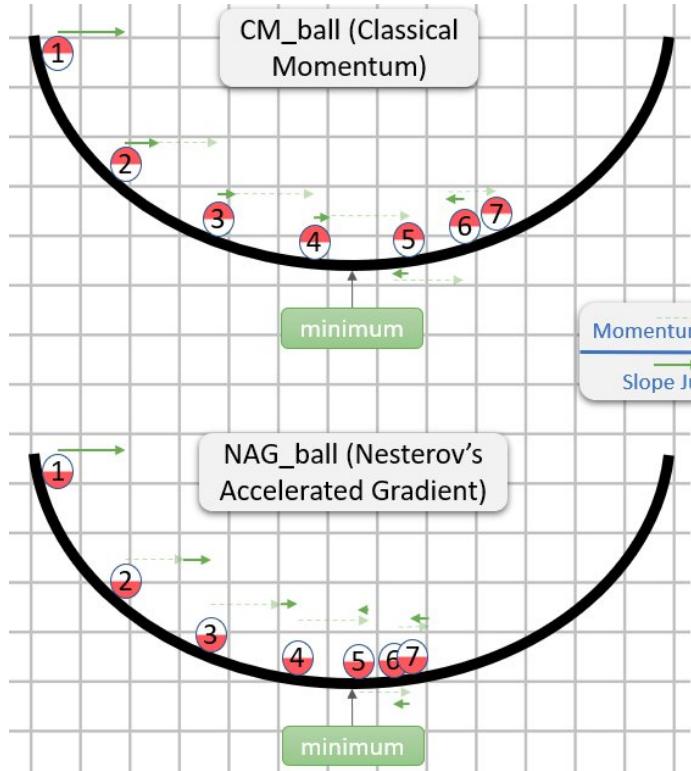
Nesterov momentum



Nesterov momentum update



CM_ball (Classical Momentum)



NAG_ball (Nesterov's Accelerated Gradient)

Optimiseurs adaptatifs

Plutôt que de piloter la descente de gradient manuellement avec le *learning rate* ...

Nous pouvons adapter le ***learning rate pour chaque poids du modèle*** en fonction du gradient, du gradient², ou de la norme des poids de la couche !!

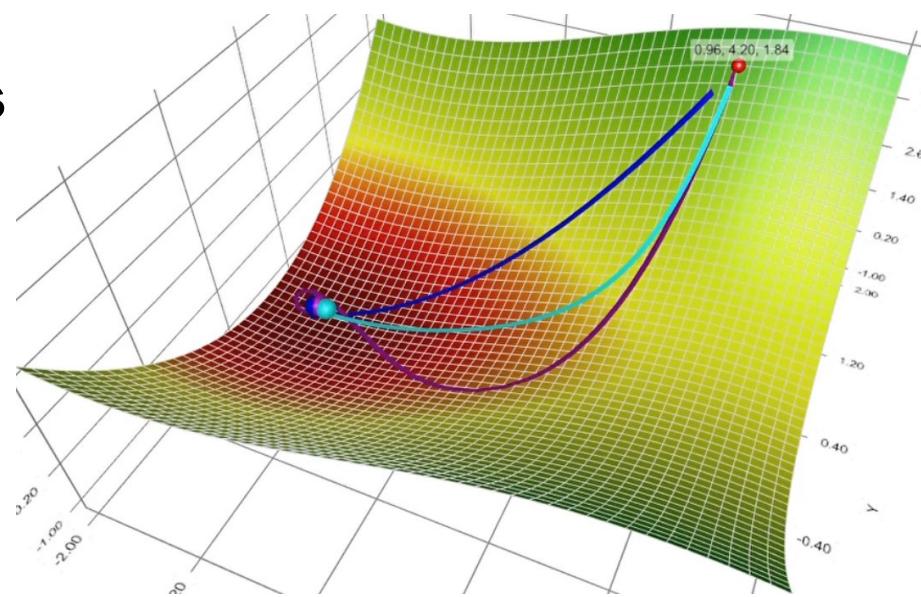
Exemples :

- AdaGrad,
- AdaDelta,
- RMSprop
- Adam

Spécialisés pour les batches larges :

- LARS
- LAMB

- SGD (no *momentum*)
- SGD (with *momentum*)
- Adam



Adam

Adam : Adaptative moment estimation

$$m_i = \beta_1 * m_{i-1} + (1 - \beta_1) * g_i \quad \text{Premier moment : moyenne glissante}$$

$$v_i = \beta_2 * v_{i-1} + (1 - \beta_2) * g_i^2 \quad \text{Second moment : variance non centrée glissante}$$

$$\hat{m}_i = \frac{m_i}{1 - \beta_1^i}$$

$$\hat{v}_i = \frac{v_i}{1 - \beta_2^i} \quad \text{Correction des biais des premières itérations}$$

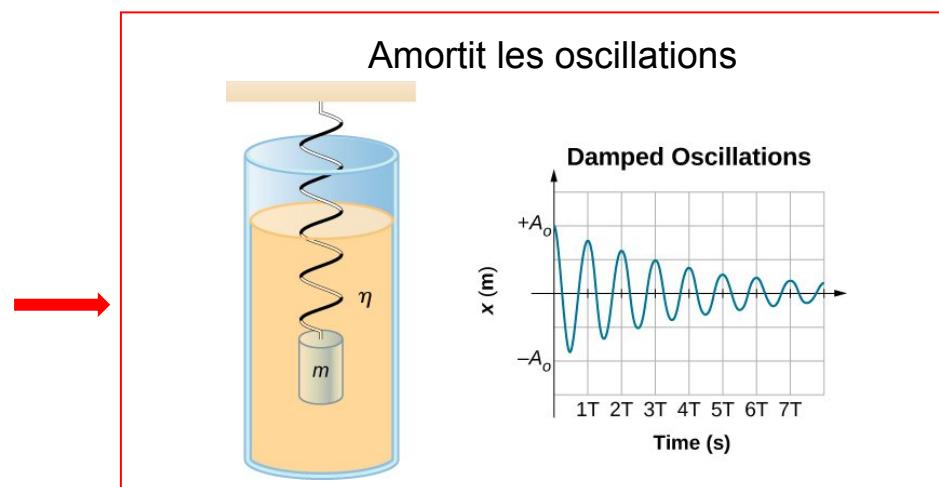
$$\theta_i = \theta_{i-1} - \frac{\alpha}{\sqrt{\hat{v}_i + \epsilon}} * \hat{m}_i$$

Paramètres :

β_1 & β_2 = Taux de régression ($\beta_1 = 0.9$ & $\beta_2 = 0.999$)

ϵ — Très petite valeur pour éviter une division par zéro

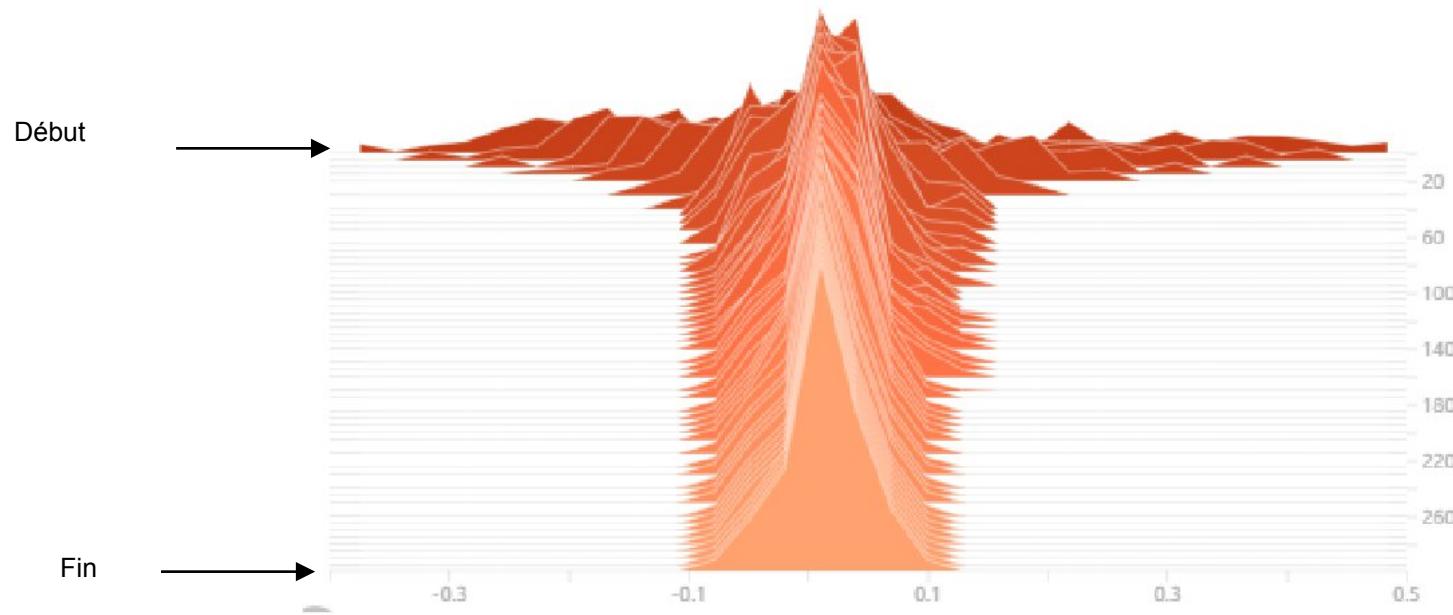
But : Adapter l'importance des mise à jours de poids en fonction des précédents gradients et de la variabilité du gradient.



Weight decay

Un réseau de neurones qui converge et généralise correctement (ni sous-apprentissage ni sur-apprentissage) a généralement **des poids qui tendent vers 0**.

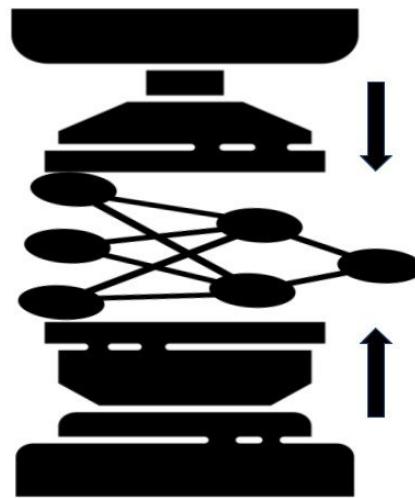
Distribution des poids durant l'apprentissage :



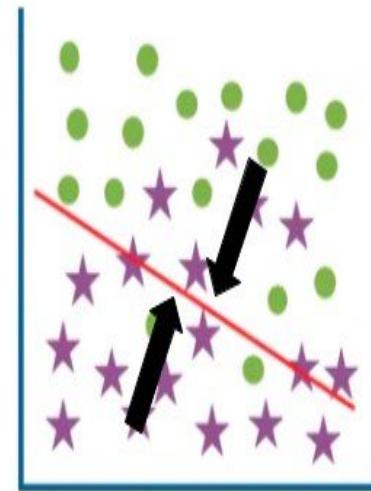
Weight decay

Préférable à la régularisation L2 standard définie dans la fonction de perte

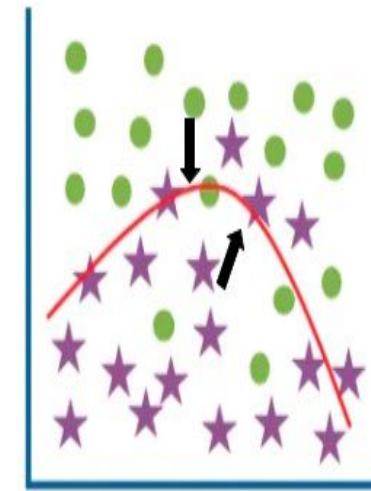
λ : paramètre du *weight decay* (généralement entre 0 et 0.1)



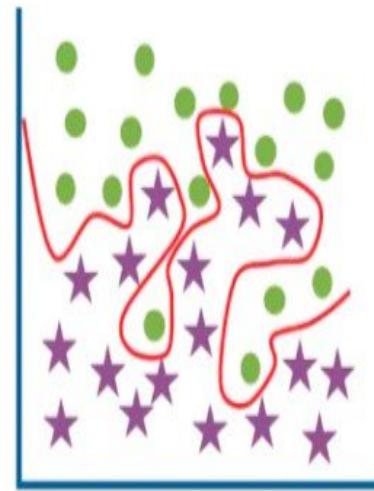
Underfitting
(λ trop élevé)



Weight decay correct
(Valeur idéal de λ)



Overfitting
(λ trop faible ou nul)



La technique de *weight decay*, définie dans *l'optimizer* permet de forcer les poids à converger vers des valeurs proches de zéro.

Weight decay and decoupled weight decay

ADAM

ADAMW

For i = 1 to ...

$$g_i = \nabla_{\theta} f_i(\theta_{i-1}) + \lambda \theta_{i-1}$$

$$m_i = \beta_1 * m_{i-1} + (1 - \beta_1) * g_i$$

$$v_i = \beta_2 * v_{i-1} + (1 - \beta_2) * g_i^2$$

$$\hat{m}_i = \frac{m_i}{1 - \beta_1^i}$$

$$\hat{v}_i = \frac{v_i}{1 - \beta_2^i}$$

$$\theta_i = \theta_{i-1} - \frac{\alpha}{\sqrt{\hat{v}_i + \epsilon}} * \hat{m}_i$$

Return θ_i

Weight decay

For i = 1 to ...

$$g_i = \nabla_{\theta} f_i(\theta_{i-1})$$

$$m_i = \beta_1 * m_{i-1} + (1 - \beta_1) * g_i$$

$$v_i = \beta_2 * v_{i-1} + (1 - \beta_2) * g_i^2$$

$$\hat{m}_i = \frac{m_i}{1 - \beta_1^i}$$

$$\hat{v}_i = \frac{v_i}{1 - \beta_2^i}$$

$$\theta_i = \theta_{i-1} - \frac{\alpha}{\sqrt{\hat{v}_i + \epsilon}} * \hat{m}_i - \alpha \lambda \theta_{i-1}$$

Return θ_i

Decoupled weight decay

Évolution du *weight decay*: *Decoupled weight decay* (découplé du momentum !!)

- SGD et Adam avec le *weight decay*
- SGDW et AdamW avec le *decoupled weight decay*

SGD et SGDW sont à peu près équivalents en performance.

Cependant AdamW est notablement meilleur que Adam !!

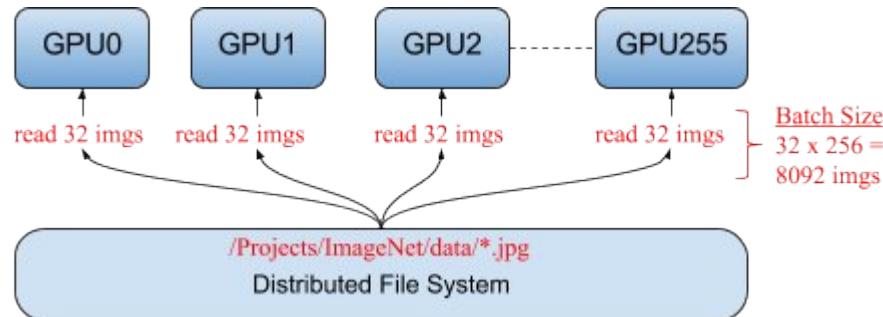
Optimisation des larges batch

Problématiques larges batches ◀

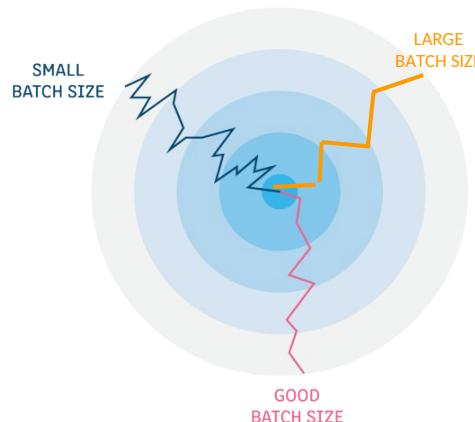
Learning Rate Scaling & Batch Schedulers ◀

Optimiseurs larges batches ◀

Large Batches avec le parallélisme de données



Parallélisme de données : La parallélisation implique une grande taille de *batch*



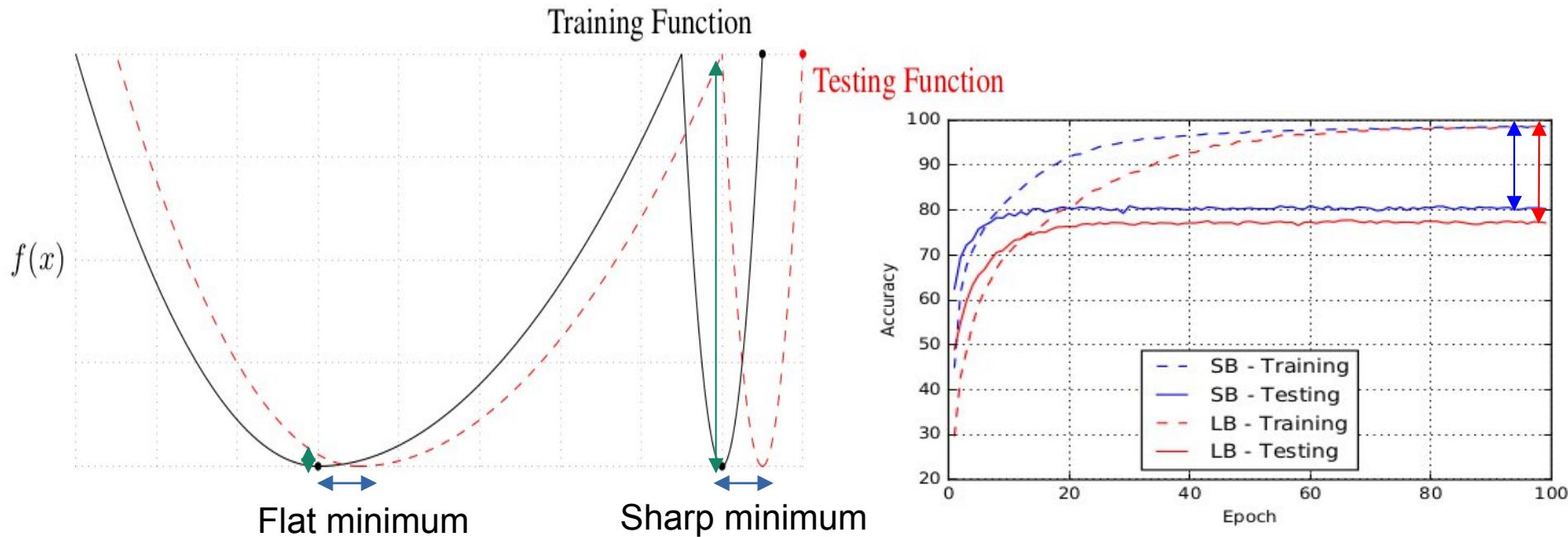
Problème : Les *batches* trop grands (> 512) ont tendance à engendrer de moins bonnes performances



Large Batches

On Large-Batch Training for Deep Learning: Generalization Gap and Sharp Minima

Nitish Shirish Keskar, Dheevatsa Mudigere, Jorge Nocedal, Mikhail Smelyanskiy, Ping Tak Peter Tang



Comparaison d'entraînement d'un réseau convolutionnel avec des petits batch (SB) et large batch (LB) sur CIFAR 10

Plus le *batch* est grand, plus le modèle a tendance à converger vers des minimums pentus et étroits.

Large Batches : Learning rate scaling

Lorsqu'on augmente considérablement la taille du *batch* global, il est souvent nécessaire de mettre le *learning rate* à l'échelle :

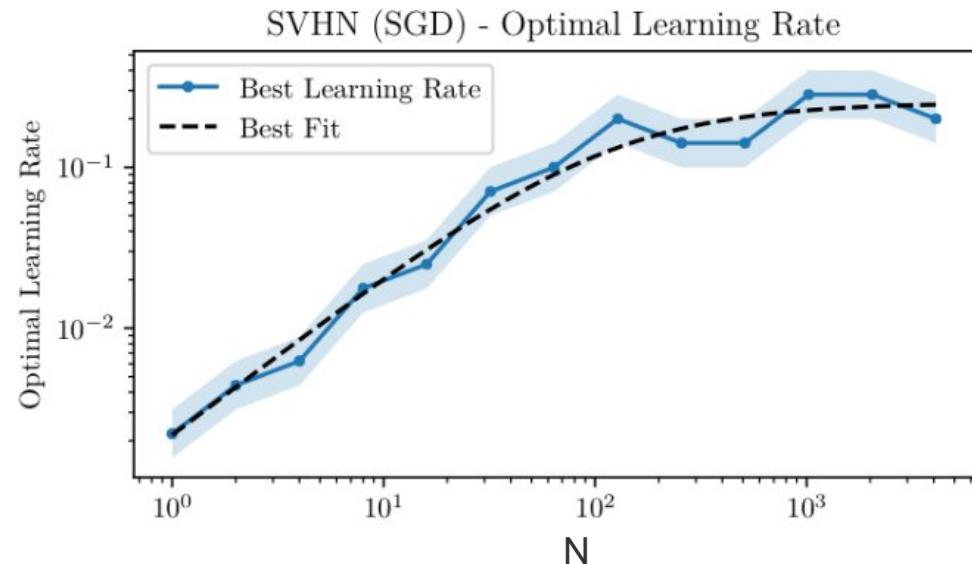
N = Nombre de processus parallèles

Croissance linéaire du *learning rate* :

$$\alpha \rightarrow N * \alpha$$

Croissance en racine carrée du *learning rate* :

$$\alpha \rightarrow \sqrt{N} * \alpha$$



An Empirical Model of Large-Batch Training
Sam McCandlish, Jared Kaplan, Dario Amodei

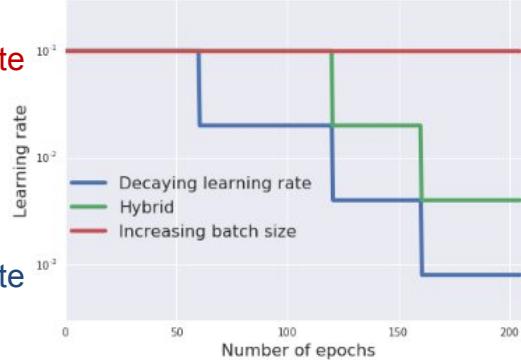
Optimal : croissance linéaire au début puis en racine carrée (recommandé par OpenAI)

Batch Size Scheduler

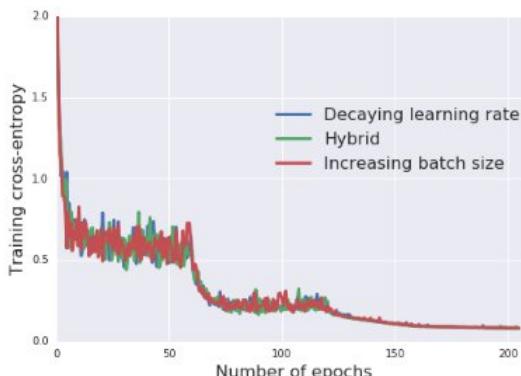
=> Alternative au *Learning Rate Scheduler*

DON'T DECAY THE LEARNING RATE, INCREASE THE BATCH SIZE

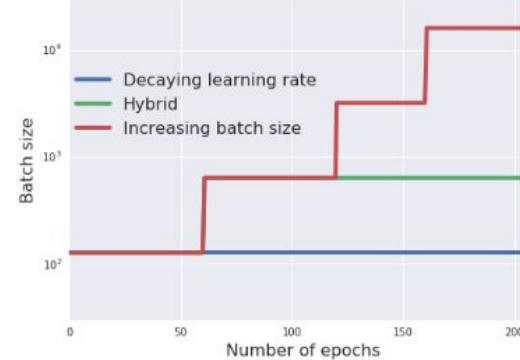
High Learning Rate



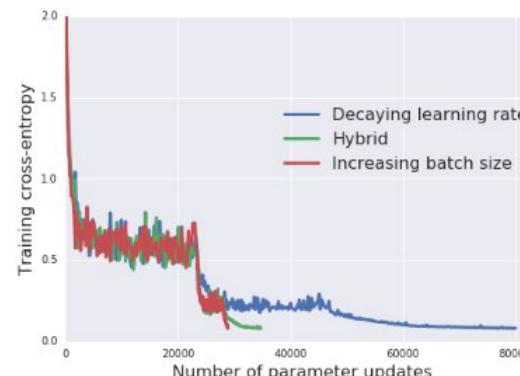
Low Learning Rate



Large Batch



Small Batch



Large Batches

Tendances :

Flat Minimum | **Sharp Minimum**

- Test Loss

Slow Descent

+ Test Loss

Fast Descent

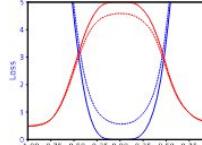
Small Batch Large Batch

SGD ADAM

Weight Decay Sans W Decay

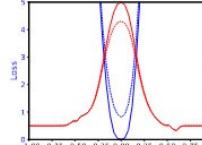
SGD

Small Batch

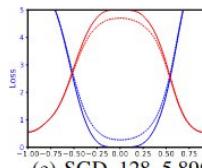


(a) SGD, 128, 8.26%

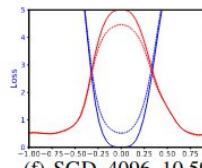
Large Batch



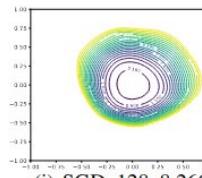
(b) SGD, 4096, 13.93%



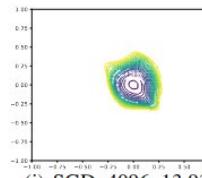
(e) SGD, 128, 5.89%



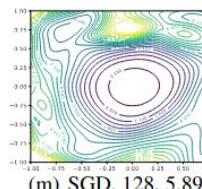
(f) SGD, 4096, 10.59%



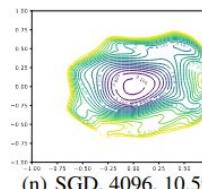
(i) SGD, 128, 8.26%



(j) SGD, 4096, 13.93%



(m) SGD, 128, 5.89%

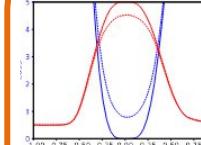


(n) SGD, 4096, 10.59%

Weight Decay
= 0

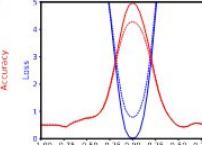
Adam

Small Batch

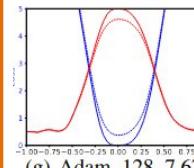


(c) Adam, 128, 9.55%

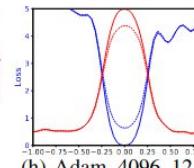
Large Batch



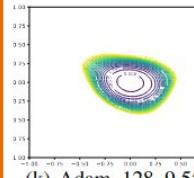
(d) Adam, 4096, 14.30%



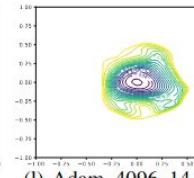
(g) Adam, 128, 7.67%



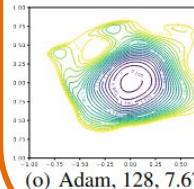
(h) Adam, 4096, 12.36%



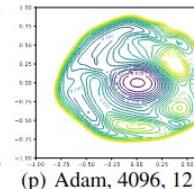
(k) Adam, 128, 9.55%



(l) Adam, 4096, 14.30%



(o) Adam, 128, 7.67%



(p) Adam, 4096, 12.36%

Weight Decay
= $5e^{-4}$

Optimiseurs Large Batches - LARS

LARS pour “Layer-wise Adaptive Rate Scaling.”

Adaptation de *SGD with momentum* avec l'ajout d'un trust ratio pour chaque couche qui dépend de l'évolution du gradient de la couche

r = Trust ratio

l = Numéro de couche

$$m_i = \beta * m_{i-1} + (1 - \beta) * (g_i + \lambda \theta_{i-1})$$

$$r_1 = \|\theta_{i-1}^l\|_2$$

$$r_2 = \|m_i^l\|_2$$

$$r = r_1 / r_2$$

$$\alpha^l = r * \alpha$$

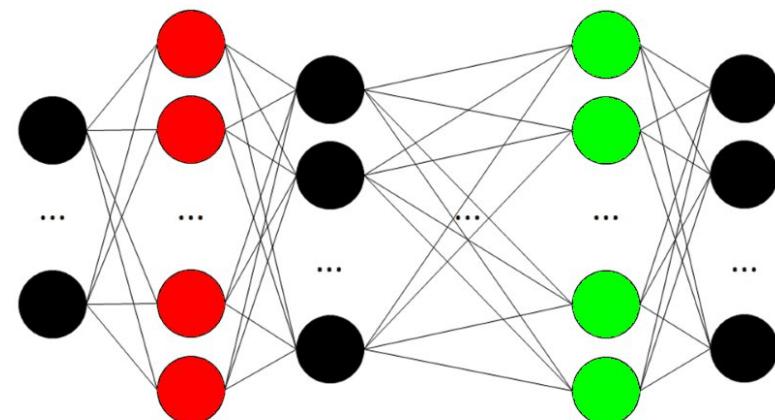
$$\theta_i^l = \theta_{i-1}^l - \alpha^l * m_i^l$$

Weight decay



Peu de confiance
Valeur faible de r

Beaucoup de confiance
Valeur élevée de r



But : Adapter l'importance des mise à jours des poids en fonction d'un *trust ratio* calculé pour chaque couche du réseau.

Optimiseurs Large Batches - LAMB

LAMB pour “Layer-wise Adaptive Moments optimizer for Batch training.”

Adaptation de Adam avec l'ajout d'un trust ratio pour chaque couche qui dépend de l'évolution du gradient de la couche

r = Trust ratio

l = Numéro de couche

$$r_1 = \|\theta_{i-1}^l\|_2$$

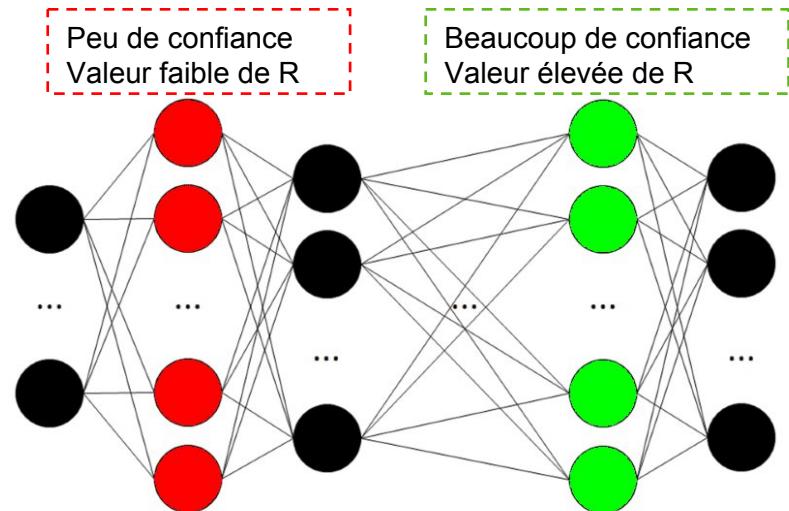
$$r_2 = \left\| \frac{\hat{m}_i^l}{\sqrt{\hat{v}_i^l + \epsilon}} + \underline{\lambda \theta_{i-1}^l} \right\|_2$$

$$r = r_1 / r_2$$

$$\alpha^l = r * \alpha$$

$$\theta_i^l = \theta_{i-1}^l - \alpha^l * \left(\frac{\hat{m}_i^l}{\sqrt{\hat{v}_i^l + \epsilon}} + \underline{\lambda \theta_{i-1}^l} \right)$$

Decoupled weight decay



But : Adapter l'importance des mise à jours des poids en fonction d'un *trust ratio* calculé pour chaque couche du réseau.

Implémentation des optimiseurs

Chaque optimiseur a ses propres paramètres

SGD

```
import torch.optim as opt  
  
SGD_optimizer = opt.SGD(params, lr, momentum=0, weight_decay=0, nesterov=False, ...)
```

ADAMW

```
import torch.optim as opt  
  
ADAM_optimizer = opt.AdamW(params, lr=0.001, betas=(0.9, 0.999), weight_decay=0.05,...)
```

LAMB

```
from apex.optimizers import FusedLamb  
  
LAMB_optimizer = FusedLamb(params, lr=0.001, betas=(0.9, 0.999), weight_decay=0,  
adam_w_mode=True)
```

LARC

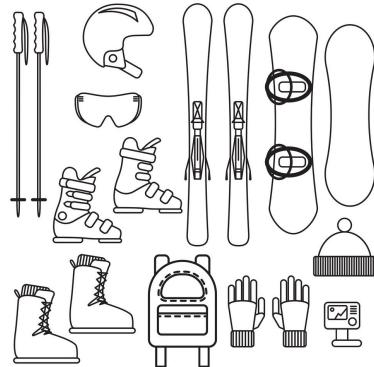
Optimisation
apex de LARS

```
import torch.optim as opt  
from apex.parallel.LARC import LARC  
  
base_optimizer = opt.SGD(params, lr=0.001, momentum=0.9, weight_decay=0)  
optimizer = LARC(base_optimizer)  
scheduler = opt.lr_scheduler.CyclicLR(base_optimizer, base_lr=0.01, max_lr=0.1)
```

Large Batches Rider

Weight Decay

SGD AdamW



Batch Scheduler

LARS
LAMB

LR Scheduler

Warmup LR scaling LR Decay



BLOOM example

95281 steps (116.8 days)

AdamW,
 $\beta_1=0.9$, $\beta_2=0.95$, $\text{eps}=1e-8$

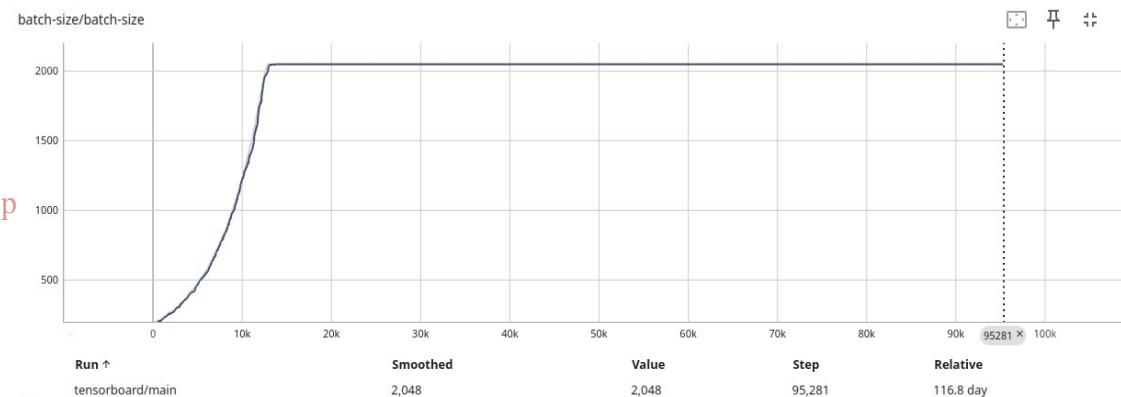
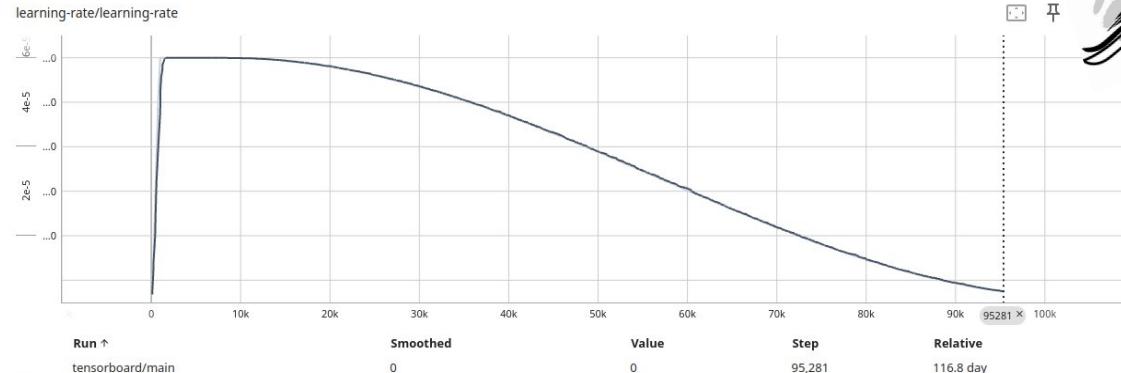
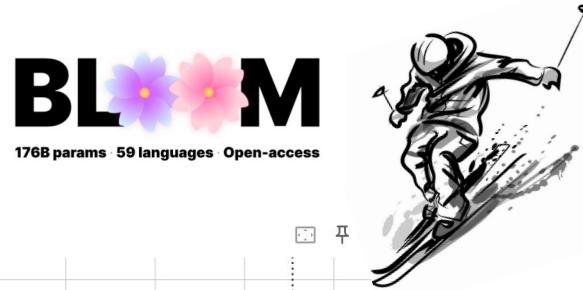
Weight Decay of 0.1

LR Scheduler

- peak=6e-5
- warmup over 375M tokens
- cosine decay for learning rate down to 10% of its value, over 410B tokens

Batch Scheduler

- start from 32k tokens (GBS=16)
- increase linearly to 4.2M tokens/step (GBS=2048) over ~20B tokens
- then continue at 4.2M tokens/step (GBS=2048) for 430B tokens



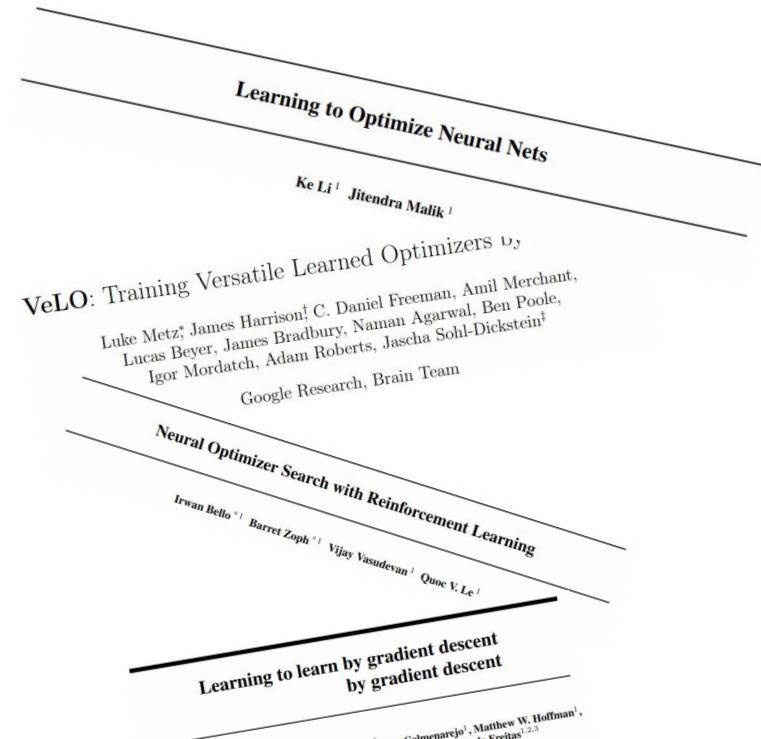
Nouveaux optimiseurs

Nouvelle tendance : l'apprentissage d'optimiseur ◀

Gouffre des nouveaux optimiseurs ◀

LION : exemple d'une nouvelle approche ◀

Nouvelle tendance : l'apprentissage d'optimiseur



Marcin Andrychowicz¹, Misha Denil¹, Sergio Gómez Colmenarinho¹, Matthew W. Hoffman¹,
David Pfau¹, Tom Schaul¹, Brendan Shillingford^{1,2}, Nando de Freitas^{1,2,3}
¹Google DeepMind ²University of Oxford ³Canadian Institute for Advanced Research
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(denil,sergomez,matthew.hoffman,pfau,schaul@google.com
brendan.shillingford@cs.ox.ac.uk, nando.defreitas@google.com

Gouffre des nouveaux optimiseurs

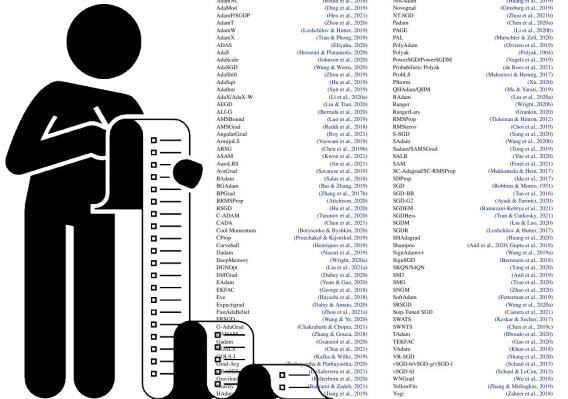
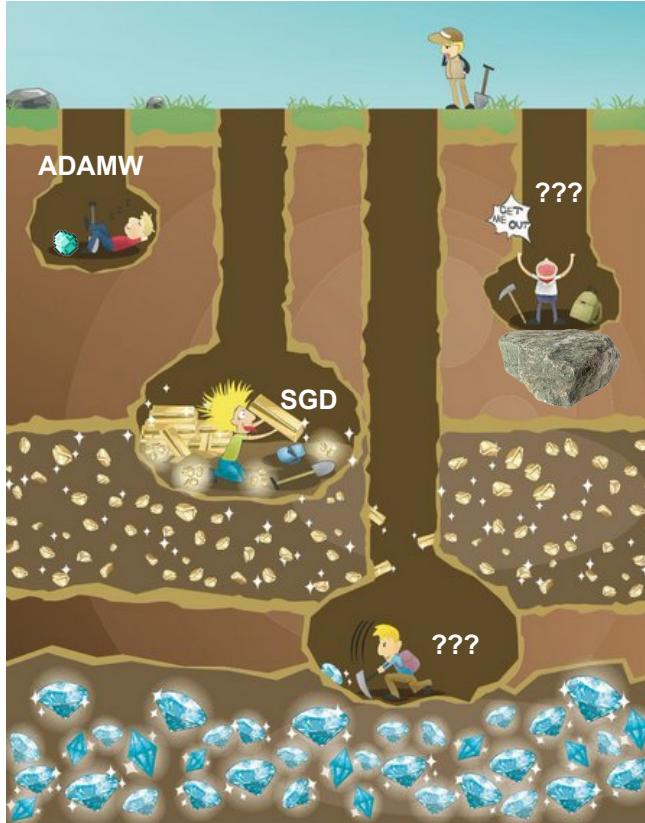


Table 2: List of optimizers considered for our benchmark. This is only a subset of all existing methods for deep learning.

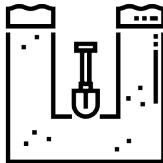
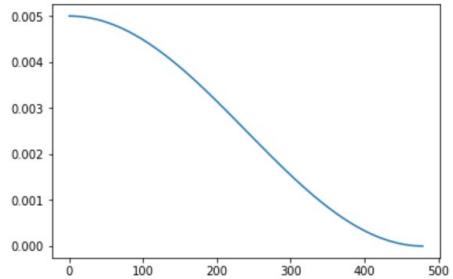
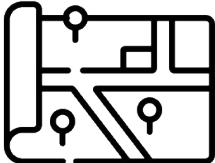


Schmidt, Robin M., Frank Schneider, and Philipp Hennig. "Descending through a crowded valley-benchmarking deep learning optimizers." *International Conference on Machine Learning*. PMLR, 2021.

LION : un nouvel optimiseur

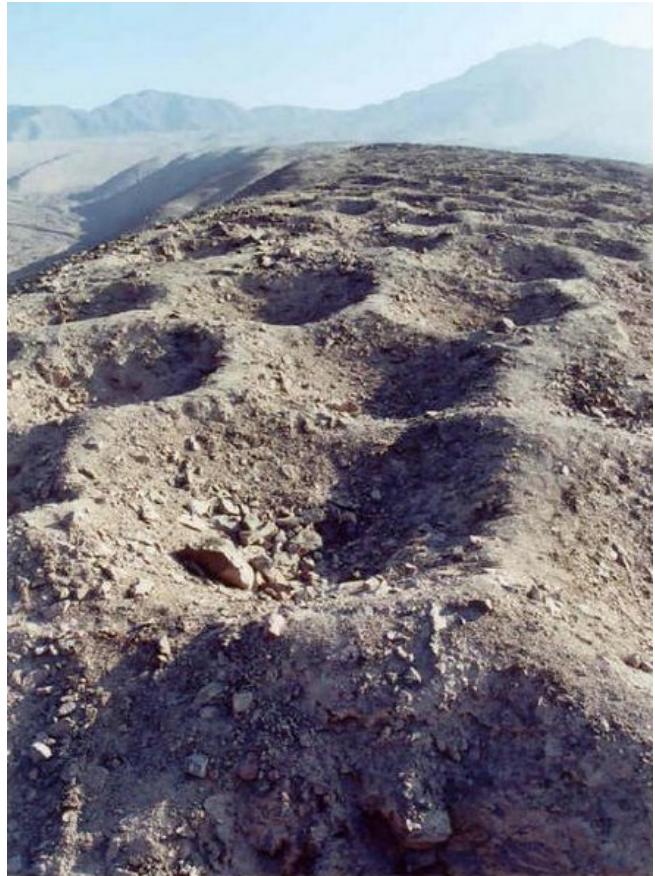
Algorithm 1 AdamW Optimizer

```
given  $\beta_1, \beta_2, \epsilon, \lambda, \eta, f$ 
initialize  $\theta_0, m_0 \leftarrow 0, v_0 \leftarrow 0, t \leftarrow 0$ 
while  $\theta_t$  not converged do
     $t \leftarrow t + 1$ 
     $g_t \leftarrow \nabla_{\theta} f(\theta_{t-1})$ 
    update EMA of  $g_t$  and  $g_t^2$ 
     $m_t \leftarrow \beta_1 m_{t-1} + (1 - \beta_1) g_t$ 
     $v_t \leftarrow \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$ 
    bias correction
     $\hat{m}_t \leftarrow m_t / (1 - \beta_1^t)$ 
     $\hat{v}_t \leftarrow v_t / (1 - \beta_2^t)$ 
    update model parameters
     $\theta_t \leftarrow \theta_{t-1} - \eta_t (\hat{m}_t / (\sqrt{\hat{v}_t} + \epsilon) + \lambda \theta_{t-1})$ 
end while
return  $\theta_t$ 
```



Algorithm 2 Lion Optimizer (ours)

```
given  $\beta_1, \beta_2, \lambda, \eta, f$ 
initialize  $\theta_0, m_0 \leftarrow 0$ 
while  $\theta_t$  not converged do
     $g_t \leftarrow \nabla_{\theta} f(\theta_{t-1})$ 
    update model parameters
     $c_t \leftarrow \beta_1 m_{t-1} + (1 - \beta_1) g_t$ 
     $\theta_t \leftarrow \theta_{t-1} - \eta_t (\text{sign}(c_t) + \lambda \theta_{t-1})$ 
    update EMA of  $g_t$ 
     $m_t \leftarrow \beta_2 m_{t-1} + (1 - \beta_2) g_t$ 
end while
return  $\theta_t$ 
```

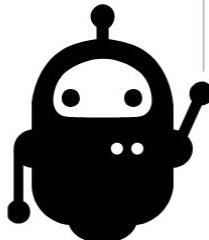


TP : Learning rate + Optimiseurs



Objectifs :

- Modifier le learning rate scheduler
- Modifier l'optimiseur
- Faire des entraînements avec des large batches



Depuis JupyterHub :

- Lancer une instance SLURM CPU
- Allez dans le dossier tp_optimiseurs
- Ouvrez le notebook DLO-JZ_Optimiseurs