Deep Learning

Lecture 4: Training neural networks

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Today

How to optimize parameters efficiently?

- Optimizers
- Initialization
- Normalization

Optimizers

Empirical risk minimization

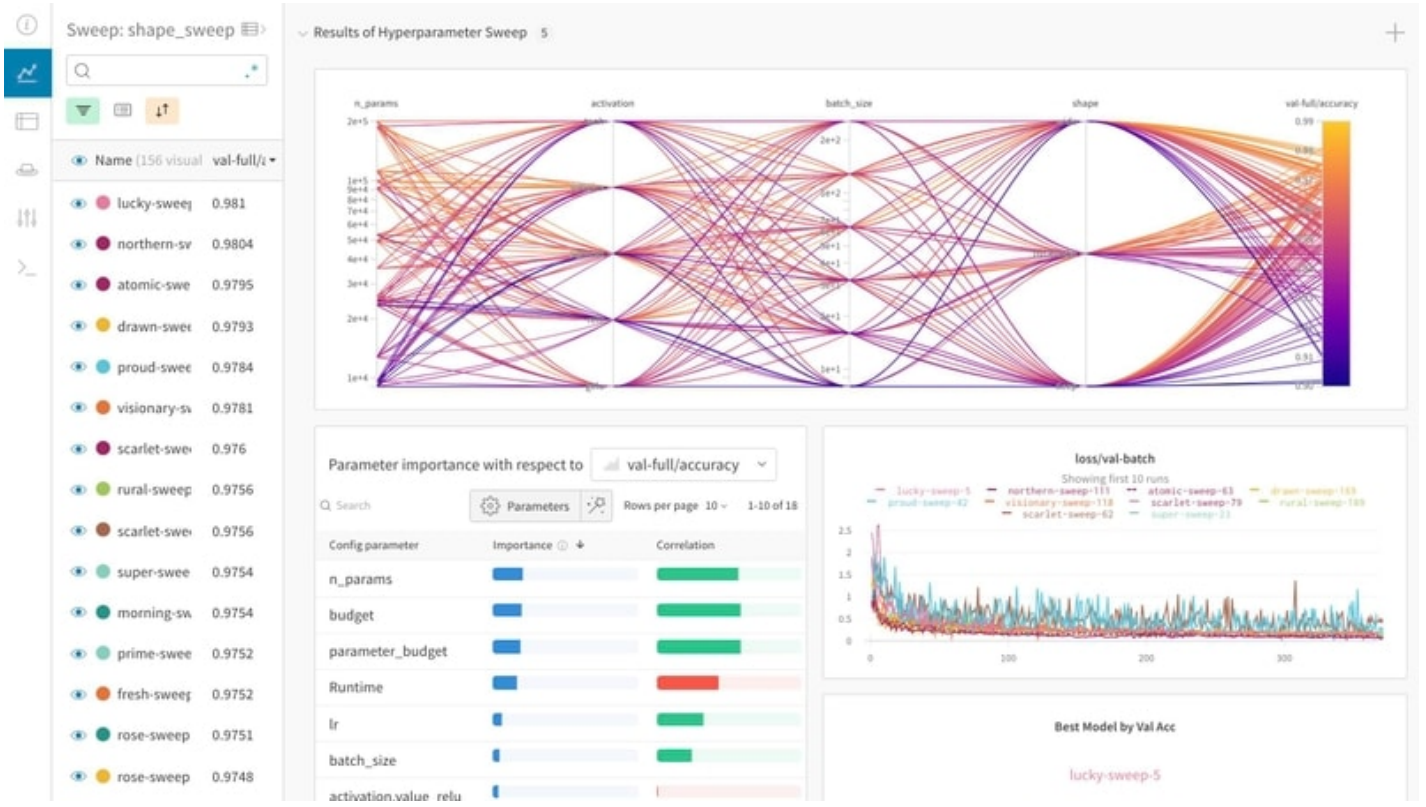
$$\theta_*^{\mathbf{d}} = \arg\min_\theta \mathcal{L}(\theta) = \frac{1}{N}\sum_{n=1}^{N} \ell(y_n, f(\mathbf{x}_n; \theta)).$$

A practical recommendation

Training a massive deep neural network is long, complex and sometimes confusing.

A first step towards understanding, debugging and optimizing neural networks is to make use of visualization tools for

- plotting losses and metrics,
- visualizing computational graphs,
- or showing additional data as the network is being trained.



Weights & Biases (wandb.ai)

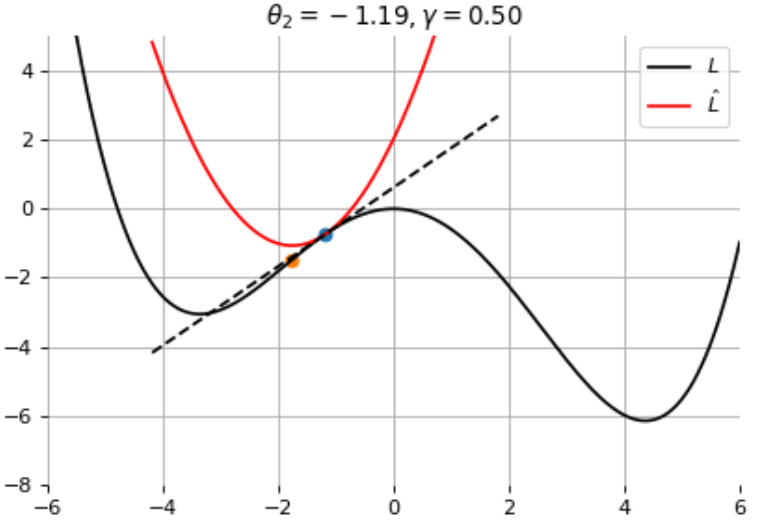
Let me say this once again: **plot your losses**.

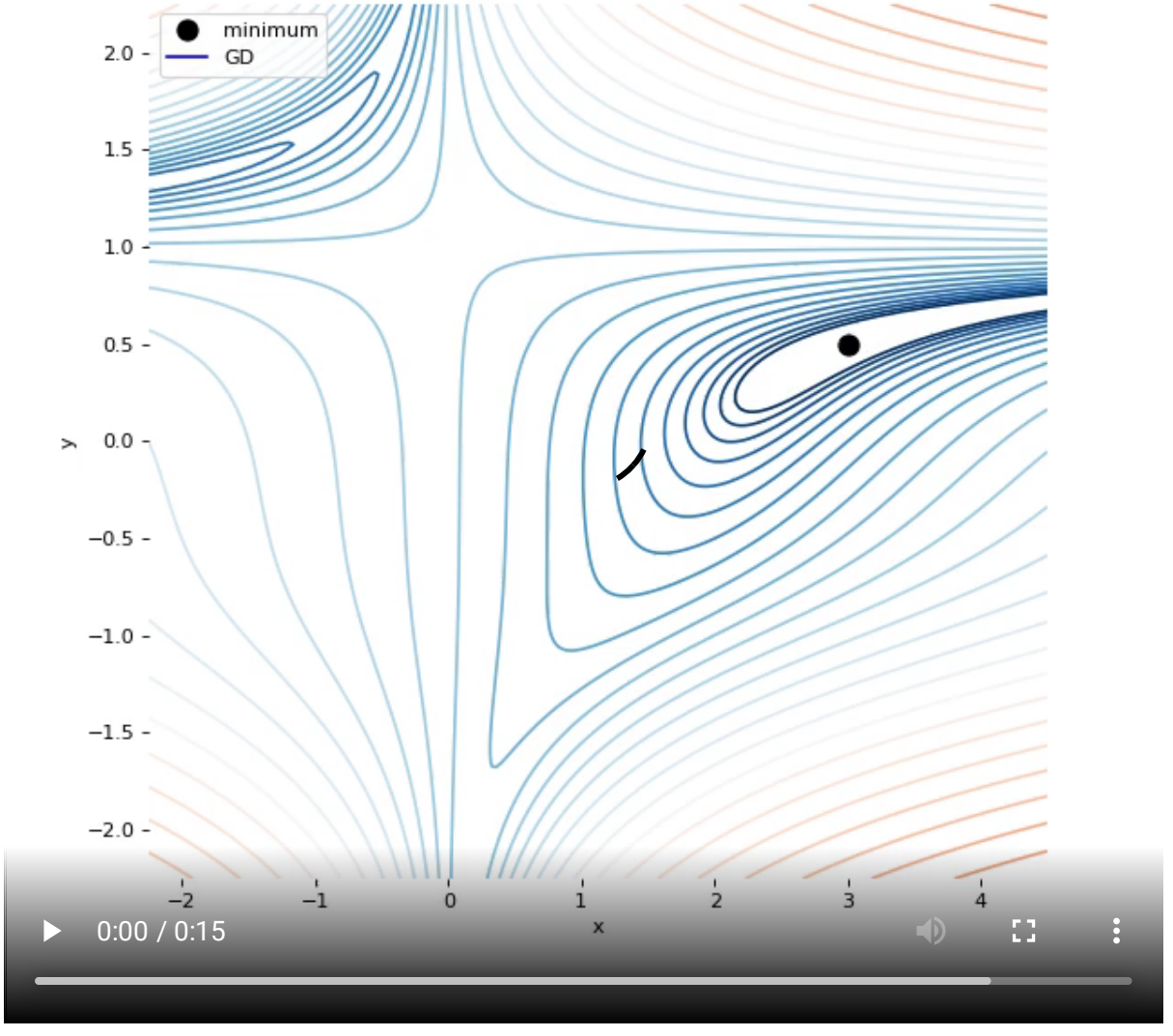
Gradient descent

To minimize $\mathcal{L}(\theta)$, standard batch gradient descent (GD) consists in applying the update rule

$$g_t = \frac{1}{N} \sum_{n=1}^{N} \nabla_\theta \ell(y_n, f(\mathbf{x}_n; \theta_t))$$
$$\theta_{t+1} = \theta_t - \gamma g_t,$$

where γ is the learning rate.

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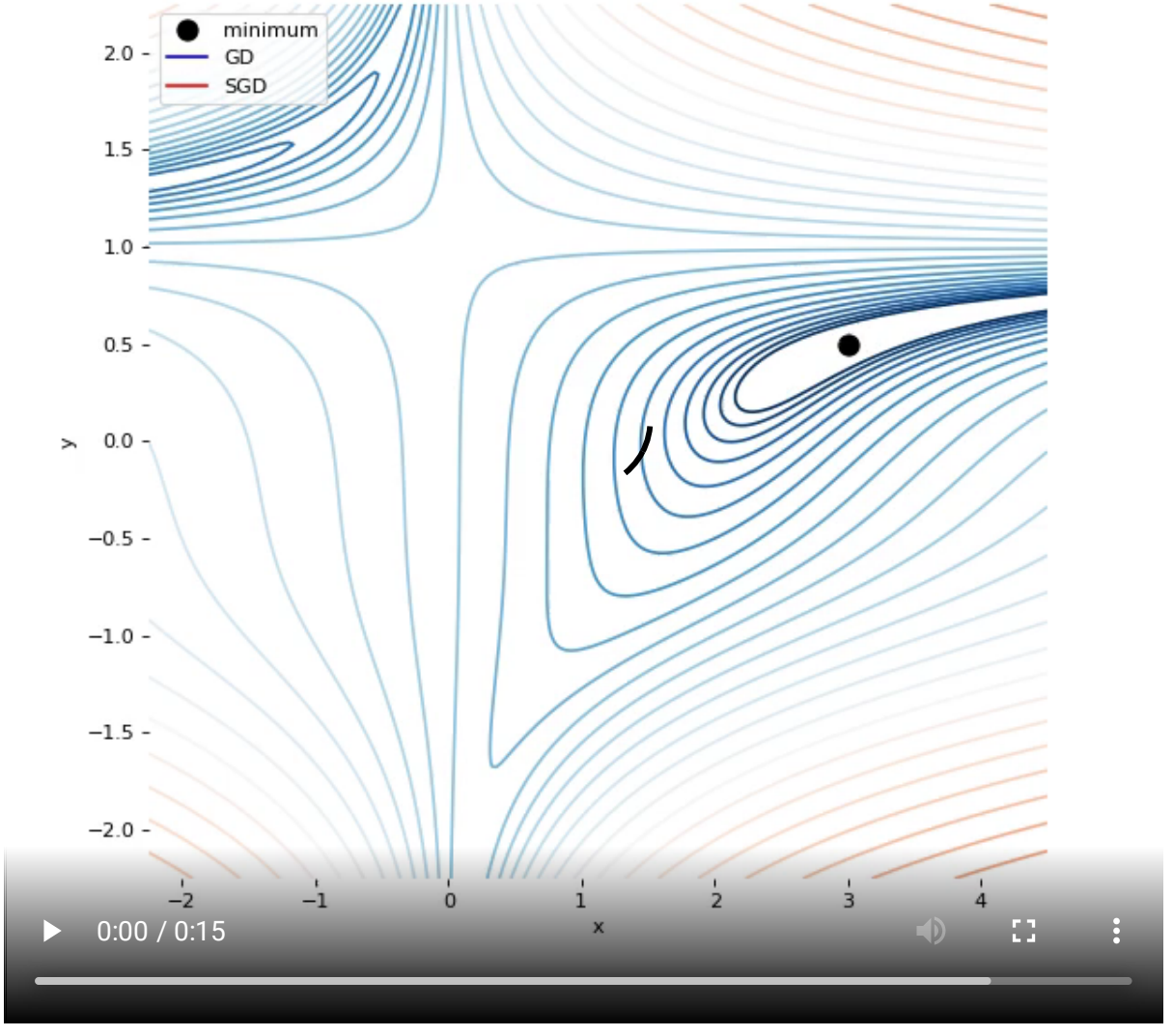
Stochastic gradient descent

While it makes sense to compute the gradient exactly,

- it takes time to compute and becomes inefficient for large N,
- it is an empirical estimation of an hidden quantity (the expected risk), and any partial sum is also an unbiased estimate, although of greater variance.

To reduce the computational complexity, stochastic gradient descent (SGD) consists in updating the parameters after every sample

$$
\begin{aligned}
g_t &= \nabla_\theta \ell(y_{n(t)}, f(\mathbf{x}_{n(t)}; \theta_t)) \\
\theta_{t+1} &= \theta_t - \gamma g_t.
\end{aligned}
$$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While being computationally faster than batch gradient descent,

- gradient estimates used by SGD can be very noisy, which may help escape from local minima;
- but SGD does not benefit from the speed-up of batch-processing.

Mini-batching

Instead, mini-batch SGD consists in visiting the samples in mini-batches and updating the parameters each time

$$g_t = \frac{1}{B} \sum_{b=1}^{B} \nabla_\theta \ell(y_{n(t,b)}, f(\mathbf{x}_{n(t,b)}; \theta_t))$$
$$\theta_{t+1} = \theta_t - \gamma g_t,$$

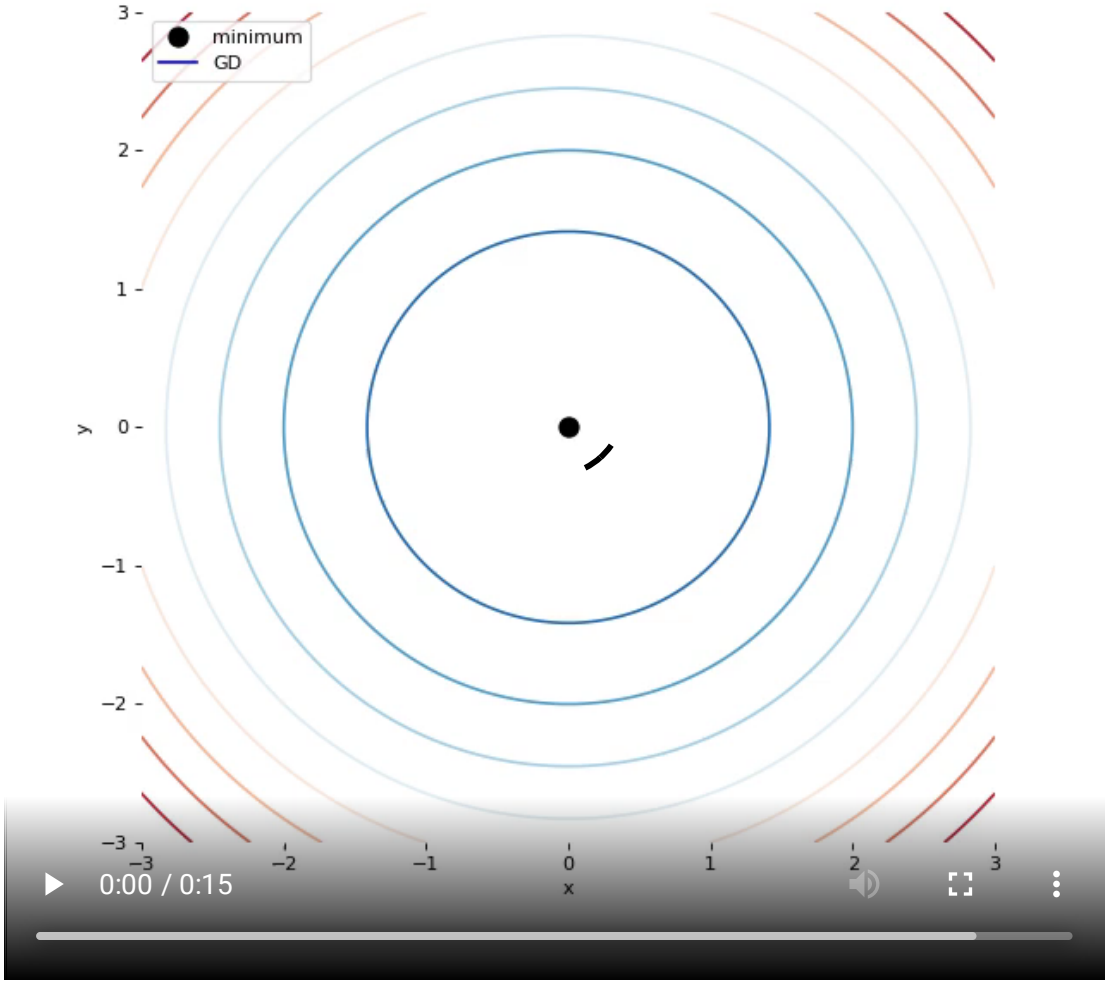
where the order $n(t, b)$ to visit the samples can be either sequential or random.

- Increasing the batch size B reduces the variance of the gradient estimates and enables the speed-up of batch processing.
- The interplay between B and γ is still unclear.

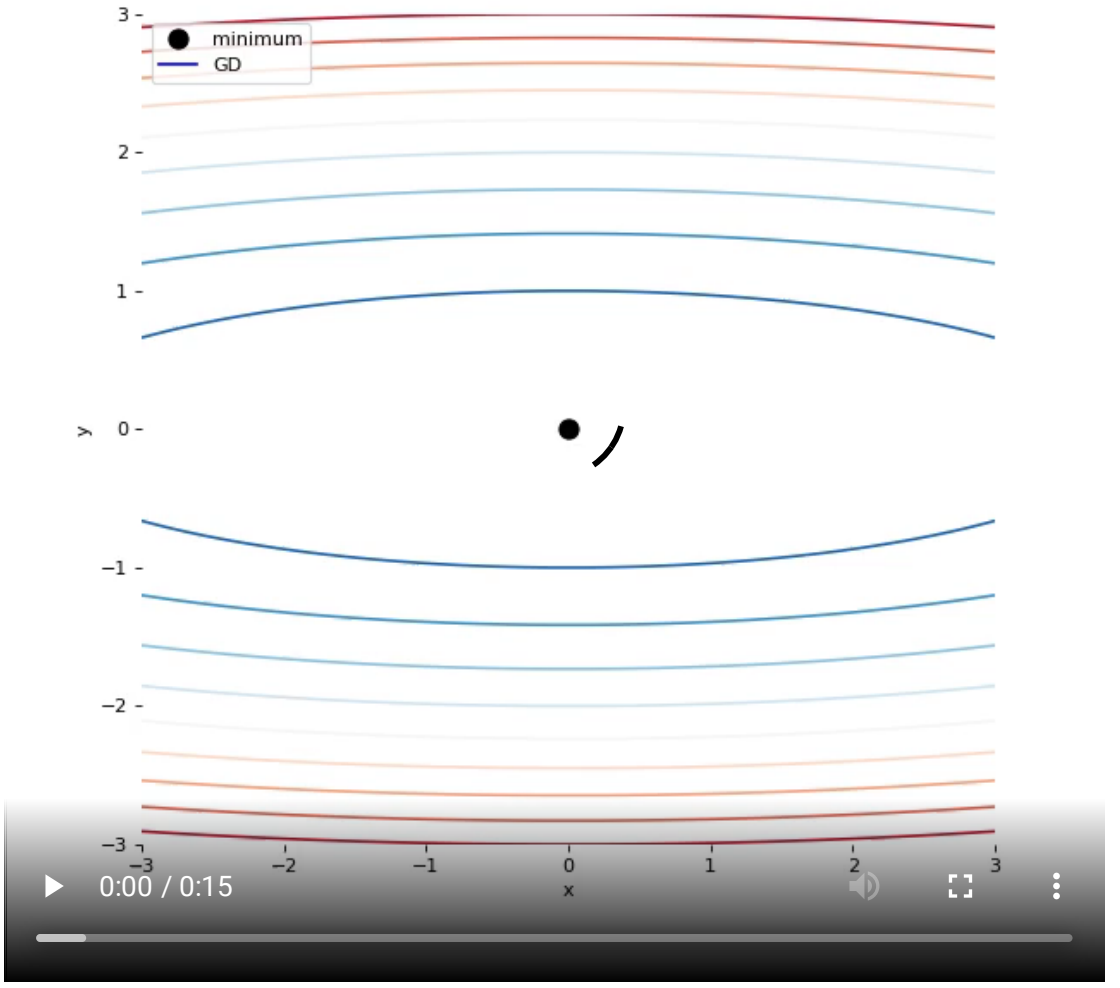
Limitations

The gradient descent method makes strong assumptions about

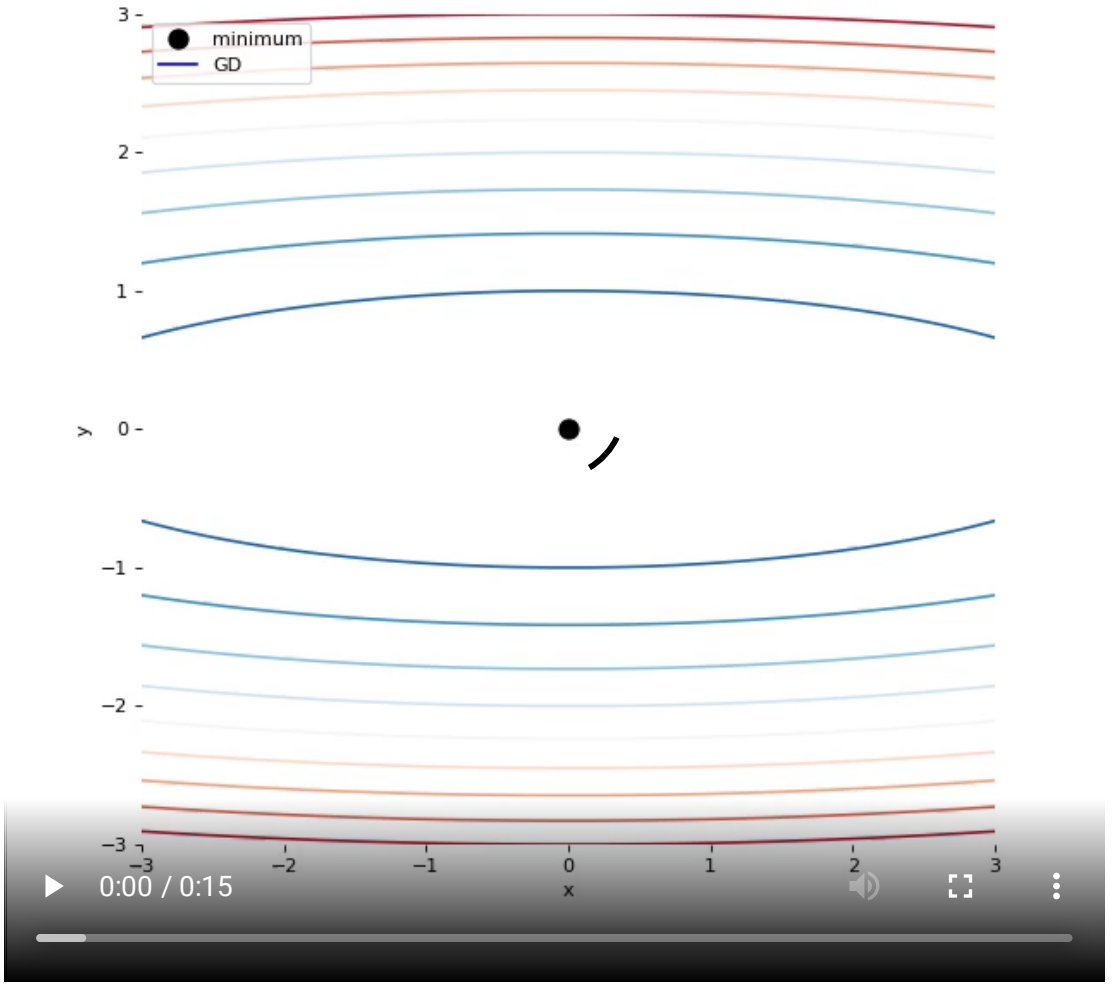
- the magnitude of the local curvature to set the step size,
- the isotropy of the curvature, so that the same step size γ makes sense in all directions.



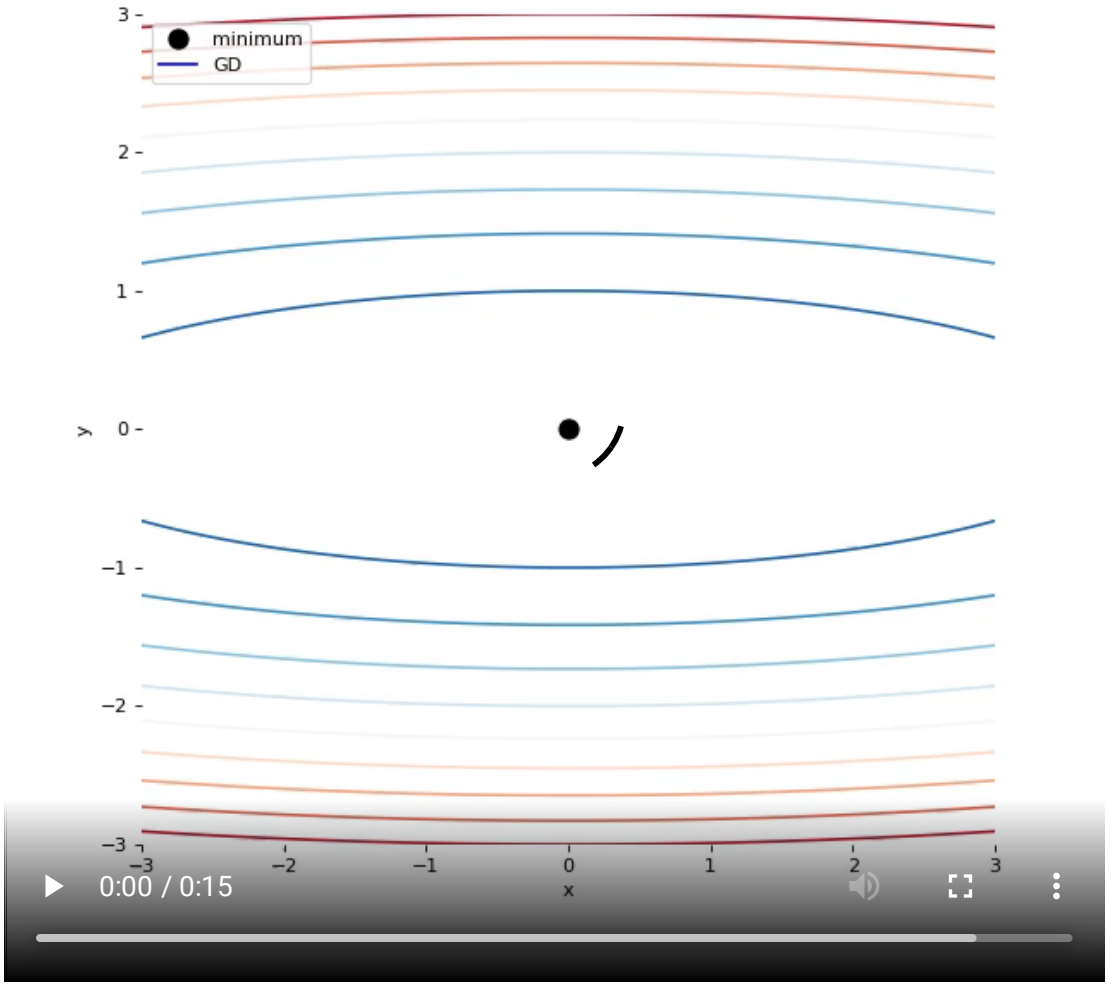
$\gamma = 0.01$



$\gamma = 0.01$



$\gamma = 0.1$



$\gamma = 0.4$

Wolfe conditions could be used to design line search algorithms to automatically determine a step size γ_t, hence ensuring convergence towards a local minima.

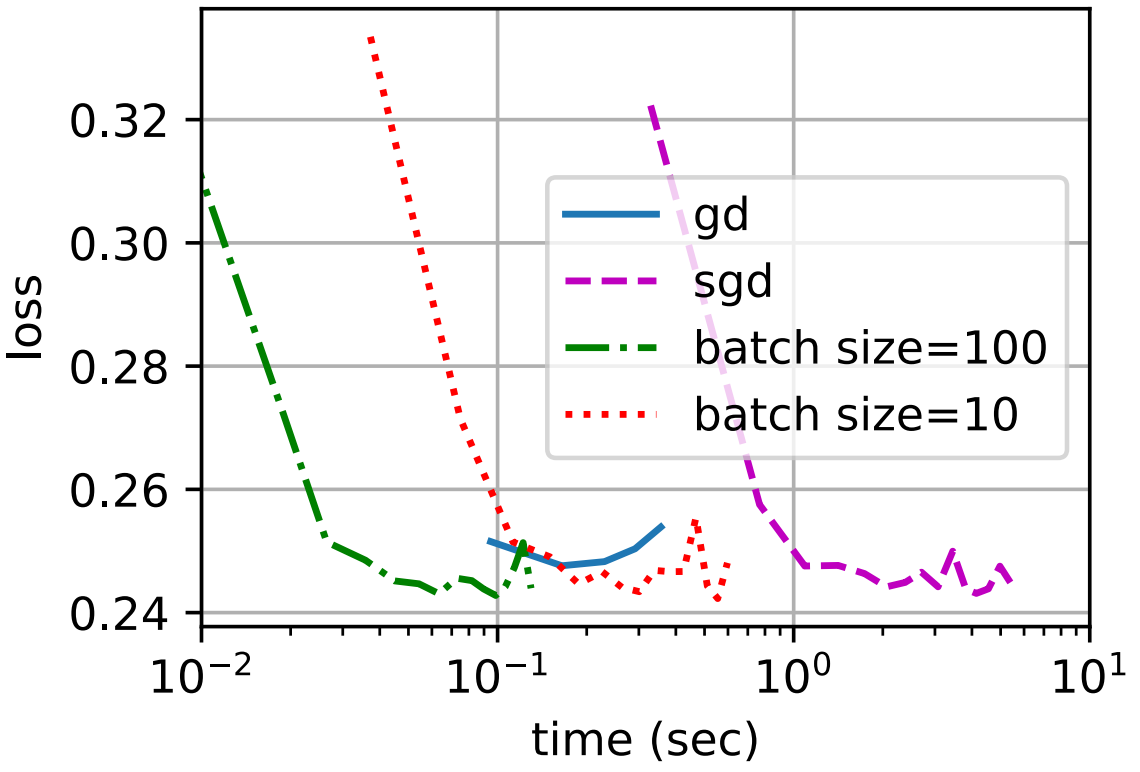
However, in deep learning,

- these algorithms are impractical because of the size of the parameter space and the overhead it would induce,
- they might lead to overfitting when the empirical risk is minimized too well.

The tradeoffs of large-scale learning

A fundamental result due to Bottou and Bousquet (2011) states that stochastic optimization algorithms (e.g., SGD) yield the best generalization performance (in terms of excess error) despite being the worst optimization algorithms for minimizing the empirical risk.

That is, **for a fixed computational budget, stochastic optimization algorithms reach a lower test error than more sophisticated algorithms** (2nd order methods, line search algorithms, etc) that would fit the training error too well or would consume too large a part of the computational budget at every step.



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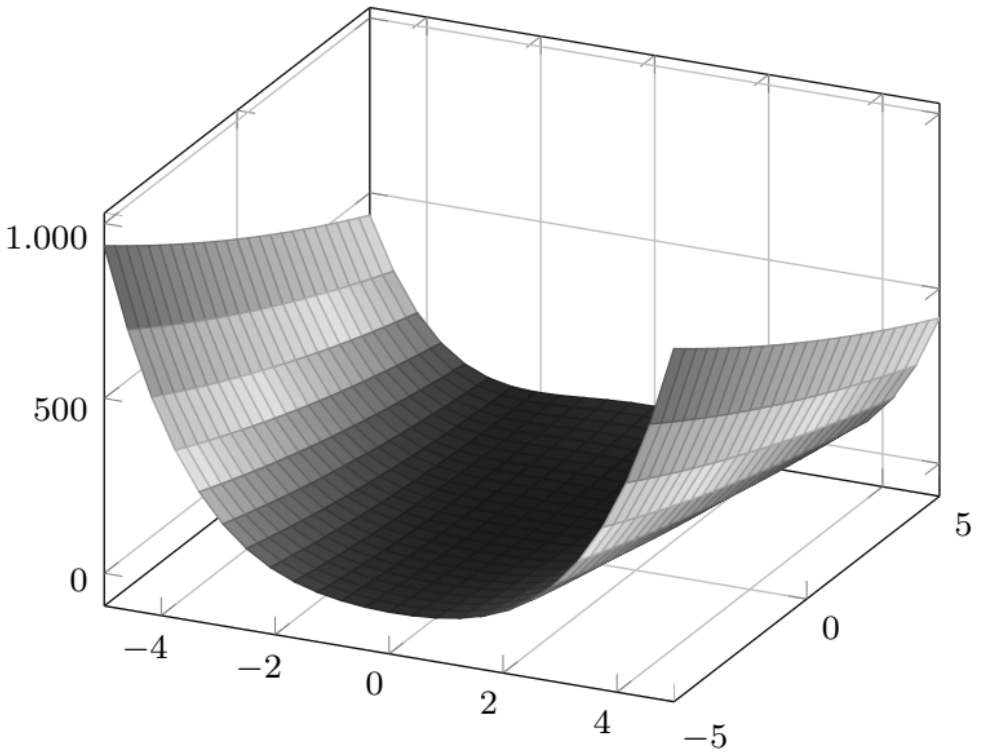
Credits: Dive Into Deep Learning, 2020.

Momentum



In the situation of small but consistent gradients, as through valley floors, gradient descent moves very slowly.

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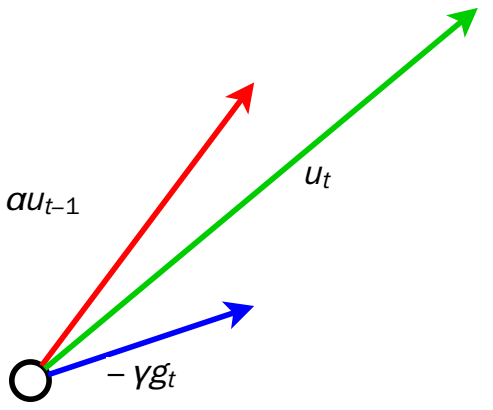
Image credits: Kosta Derpanis, Deep Learning in Computer Vision, 2018

An improvement to gradient descent is to use momentum to add inertia in the choice of the step direction, that is

$$u_t = \alpha u_{t-1} - \gamma g_t$$
$$\theta_{t+1} = \theta_t + u_t.$$

- The new variable u_t is the velocity. It corresponds to the direction and speed by which the parameters move as the learning dynamics progresses, modeled as an exponentially decaying moving average of negative gradients.
- Gradient descent with momentum has three nice properties:
  - it can go through local barriers,
  - it accelerates if the gradient does not change much,
  - it dampens oscillations in narrow valleys.

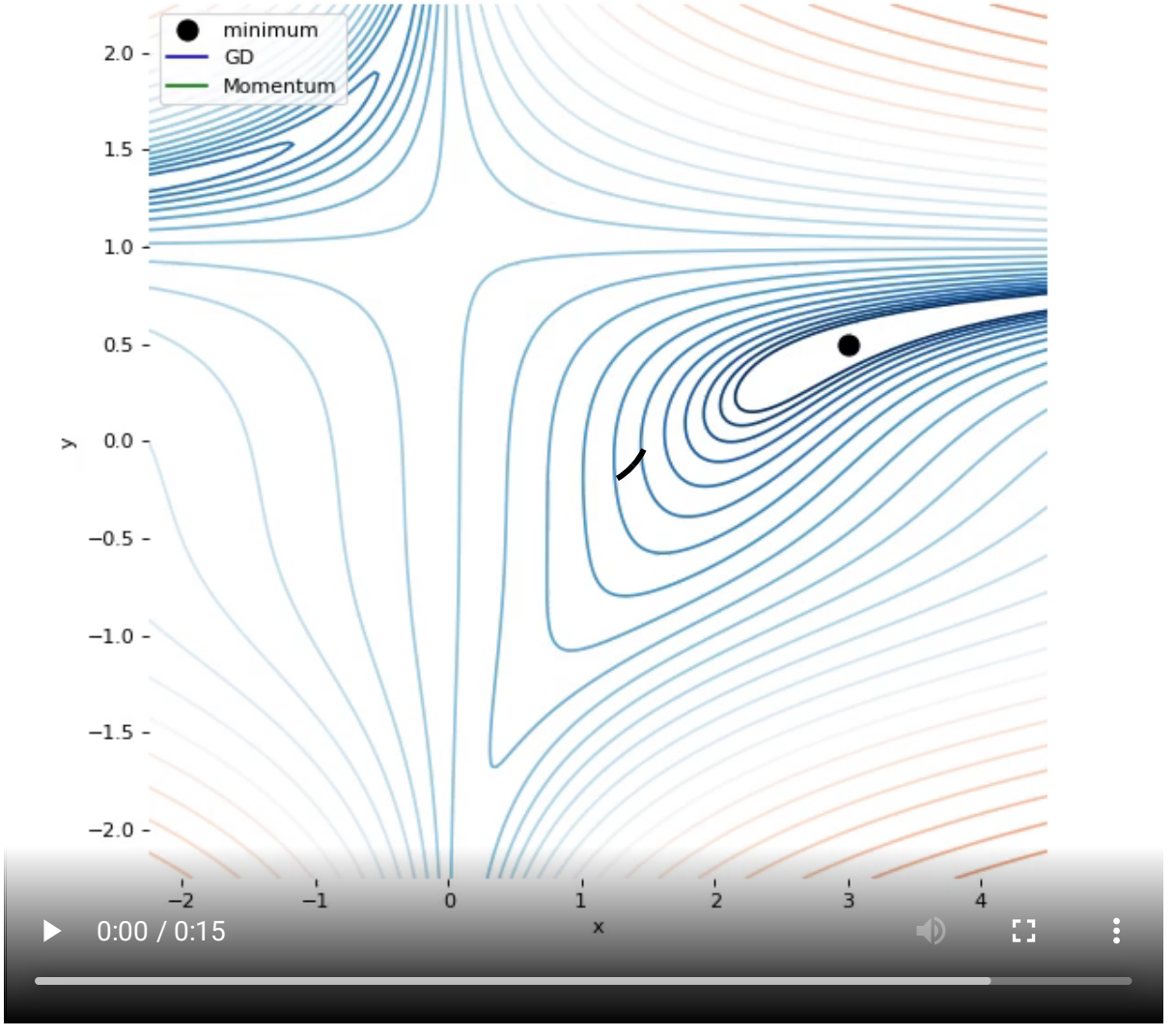


The hyper-parameter α controls how recent gradients affect the current update.

- Usually, $\alpha = 0.9$, with $\alpha > \gamma$.
- If at each update we observed g, the step would (eventually) be

$$u = -\frac{\gamma}{1-\alpha} g.$$

- Therefore, for $\alpha = 0.9$, it is like multiplying the maximum speed by 10 relative to the current direction.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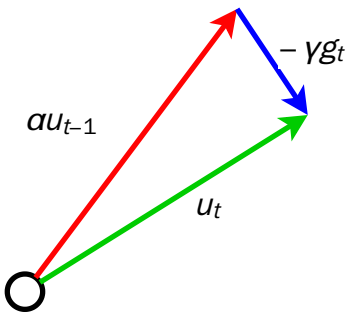
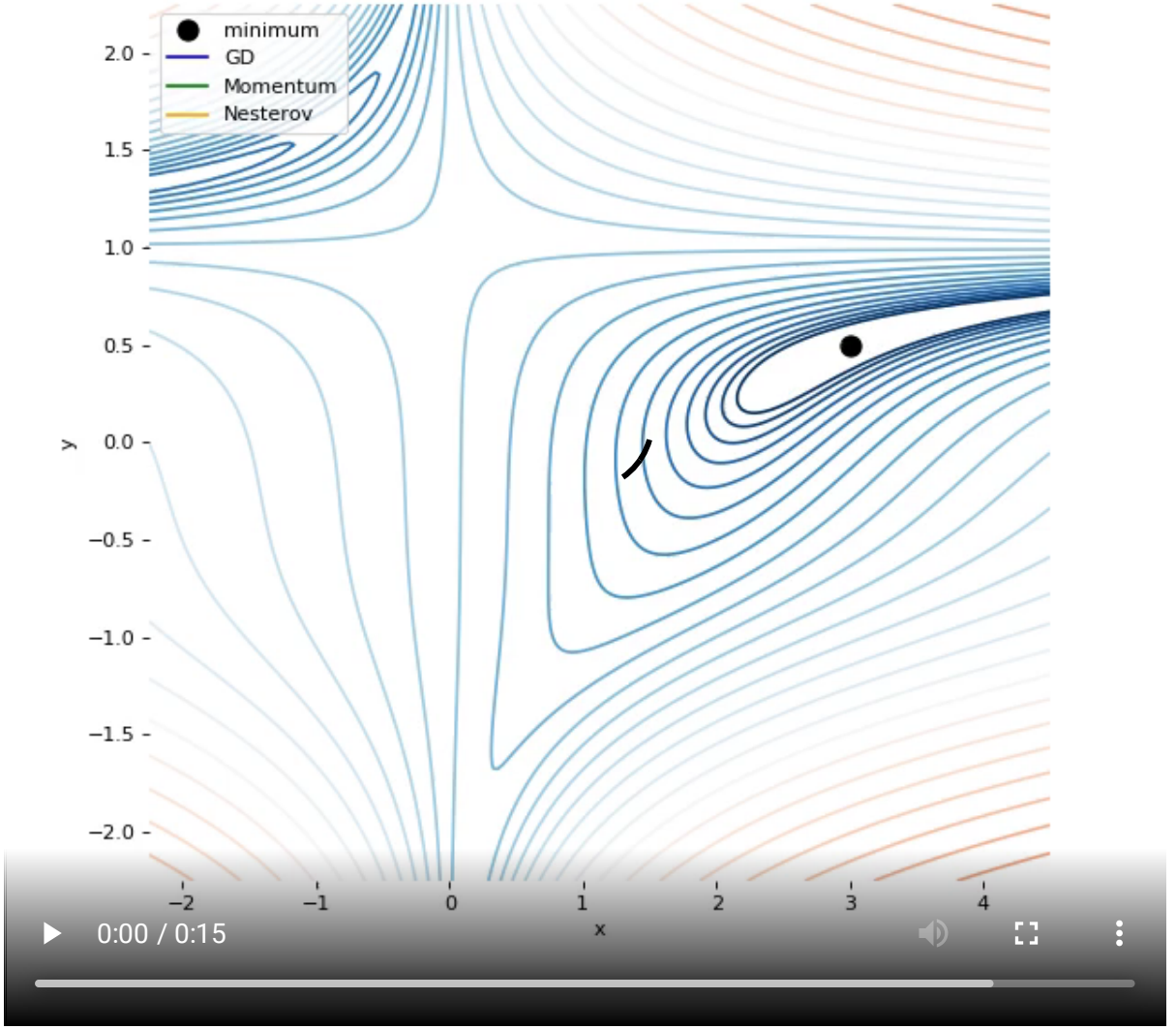
Nesterov momentum

An alternative consists in simulating a step in the direction of the velocity, then calculate the gradient and make a correction.

$$g_t = \frac{1}{N} \sum_{n=1}^{N} \nabla_\theta \ell(y_n, f(\mathbf{x}_n; \theta_t + \alpha u_{t-1}))$$
$$u_t = \alpha u_{t-1} - \gamma g_t$$
$$\theta_{t+1} = \theta_t + u_t$$

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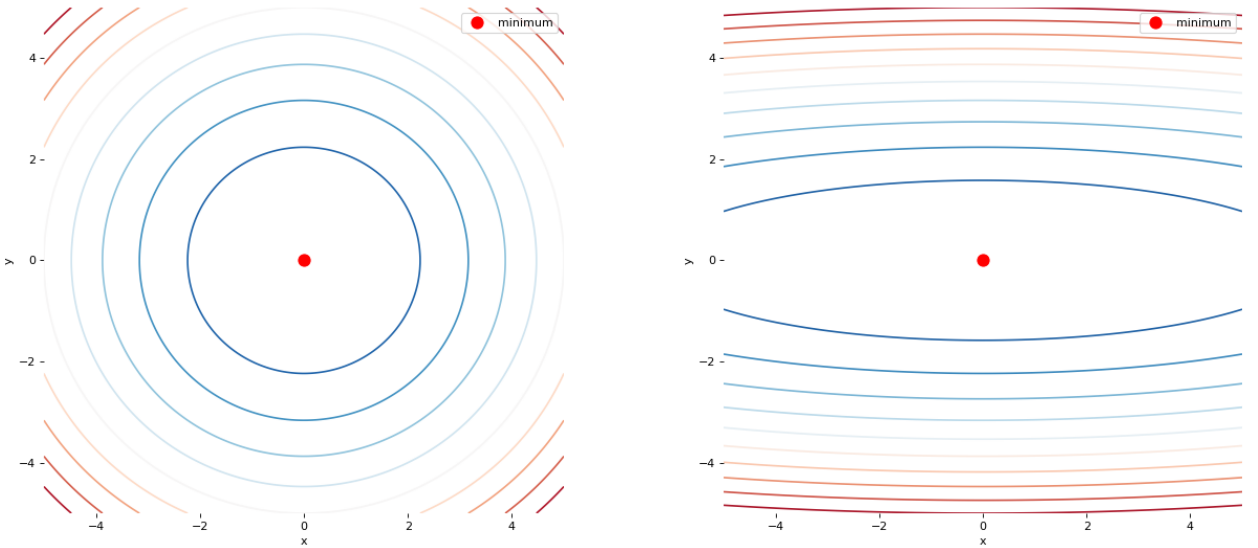
Adaptive learning rate

Vanilla gradient descent assumes the isotropy of the curvature, so that the same step size γ applies to all parameters.



Isotropic vs. Anistropic

AdaGrad

Per-parameter downscale by square-root of sum of squares of all its historical values.

$$r_t = r_{t-1} + g_t \odot g_t$$
$$\theta_{t+1} = \theta_t - \frac{\gamma}{\delta + \sqrt{r_t}} \odot g_t.$$

- AdaGrad eliminates the need to manually tune the learning rate. Most implementation use $\gamma = 0.01$ as default.
- It is good when the objective is convex.
- r_t grows unboundedly during training, which may cause the step size to shrink and eventually become infinitesimally small.

RMSProp

Same as AdaGrad but accumulate an exponentially decaying average of the gradient.

$$r_t = \rho r_{t-1} + (1-\rho) g_t \odot g_t$$
$$\theta_{t+1} = \theta_t - \frac{\gamma}{\delta + \sqrt{r_t}} \odot g_t.$$

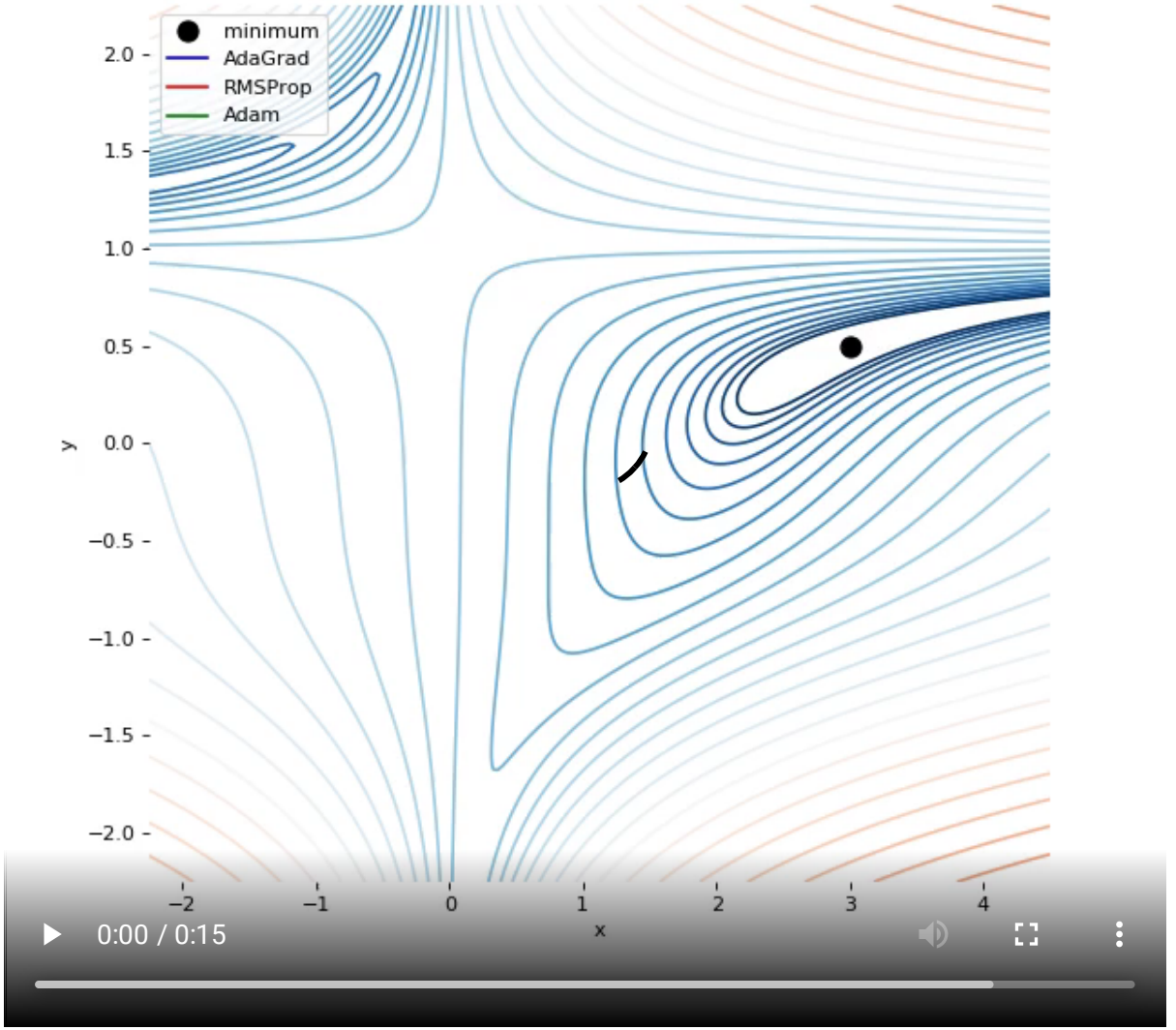
- Perform better in non-convex settings.
- Does not grow unboundedly.

Adam

Similar to RMSProp with momentum, but with bias correction terms for the first and second moments.

$$
\begin{aligned}
\boldsymbol{s}_t &= \rho_1 \boldsymbol{s}_{t-1} + (1 - \rho_1) \boldsymbol{g}_t \\
\hat{\boldsymbol{s}}_t &= \frac{\boldsymbol{s}_t}{1 - \rho_1^t} \\
\boldsymbol{r}_t &= \rho_2 \boldsymbol{r}_{t-1} + (1 - \rho_2) \boldsymbol{g}_t \odot \boldsymbol{g}_t \\
\hat{\boldsymbol{r}}_t &= \frac{\boldsymbol{r}_t}{1 - \rho_2^t} \\
\boldsymbol{\theta}_{t+1} &= \boldsymbol{\theta}_t - \gamma \frac{\hat{\boldsymbol{s}}_t}{\delta + \sqrt{\hat{\boldsymbol{r}}_t}}
\end{aligned}
$$

- Good defaults are $\rho_1 = 0.9$ and $\rho_2 = 0.999$.
- Adam is one of the default optimizers in deep learning, along with SGD with momentum.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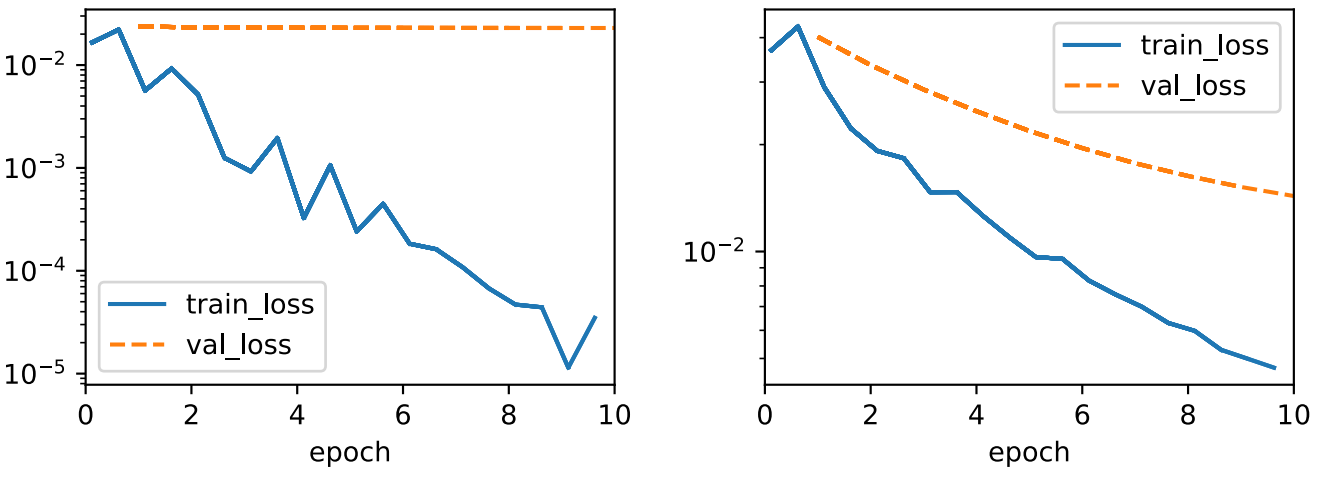
Weight decay

- Weight decay is a regularization technique that penalizes large weights.
- For vanilla SGD, it is equivalent to adding a penalty term to the loss function

$$\ell_\theta + \frac{\lambda}{2}||\theta||^2.$$

- For more complex optimizers, it is equivalent to adding a penalty term to the update rule

$$\theta_{t+1} = \theta_t - \gamma \left(g_t + \lambda\theta\right).$$



Training without (left) and with (right) weight decay.

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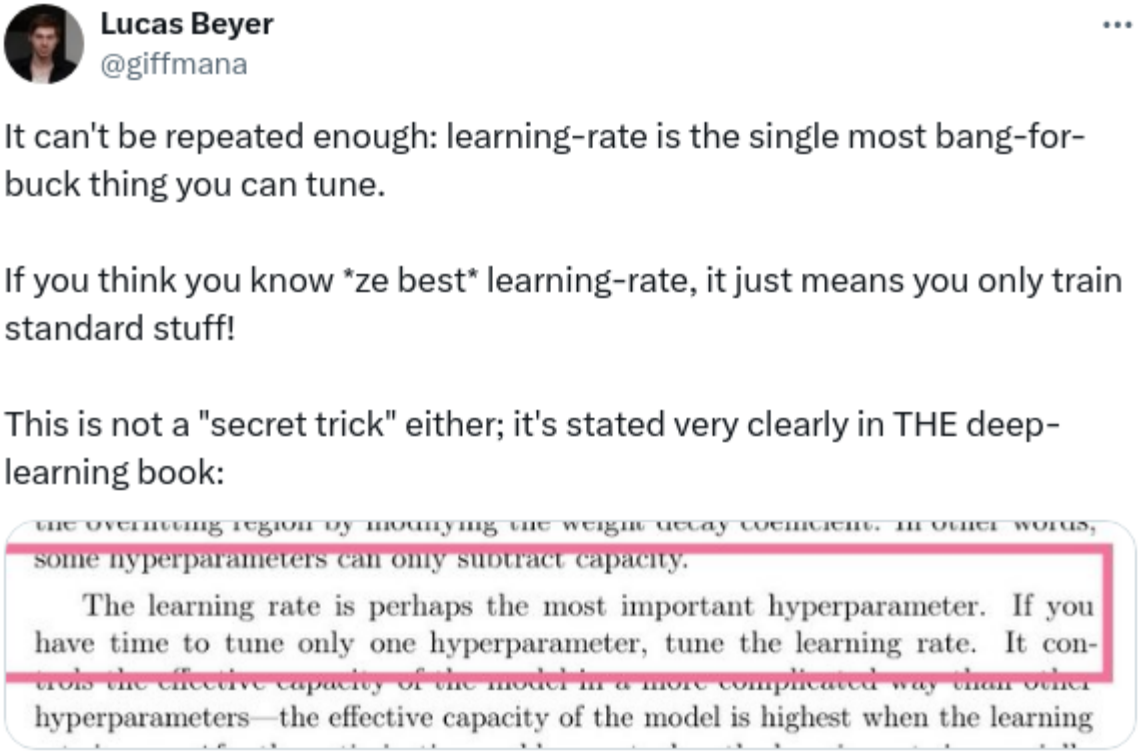
Learning rate



Lucas Beyer
@giffmana

It can't be repeated enough: learning-rate is the single most bang-for-buck thing you can tune.

If you think you know *ze best* learning-rate, it just means you only train standard stuff!

This is not a "secret trick" either; it's stated very clearly in THE deep-learning book:

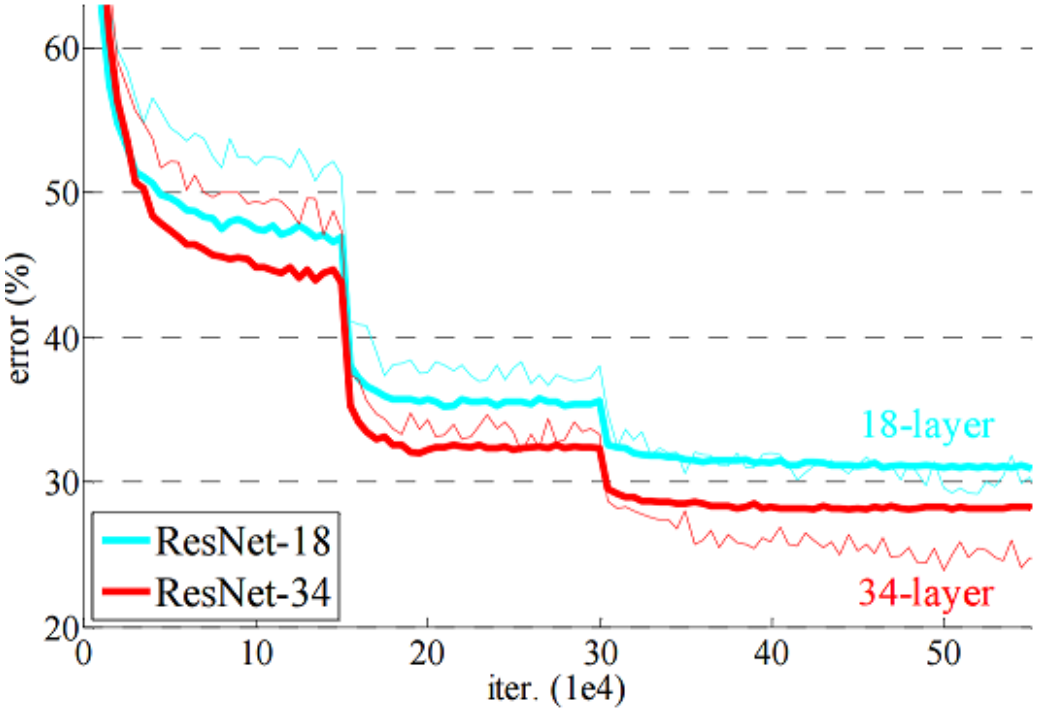
some hyperparameters can only subtract capacity.

The learning rate is perhaps the most important hyperparameter. If you have time to tune only one hyperparameter, tune the learning rate. It controls the effective capacity of the model in a more complicated way than other hyperparameters—the effective capacity of the model is highest when the learning

Scheduling

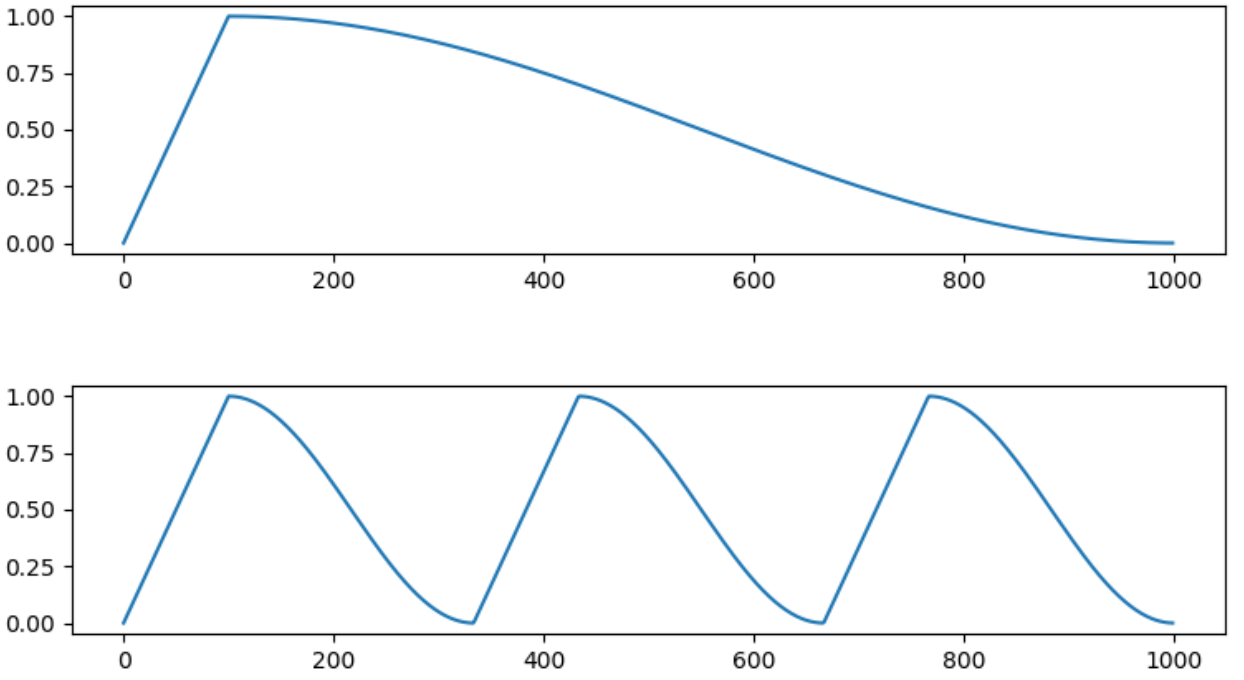
Despite per-parameter adaptive learning rate methods, it is usually helpful to anneal the learning rate γ over time.

- Step decay: reduce the learning rate by some factor every few epochs (e.g, by half every 10 epochs).
- Exponential decay: $\gamma_t = \gamma_0 \exp(-kt)$ where γ_0 and k are hyper-parameters.
- $1/t$ decay: $\gamma_t = \gamma_0/(1 + kt)$ where γ_0 and k are hyper-parameters.



Step decay scheduling for training ResNets.

Warmup and cyclical schedules



Initialization

In convex problems, provided a good learning rate γ, convergence is guaranteed regardless of the initial parameter values.

In the non-convex regime, initialization is much more important! Little is known on the mathematics of initialization strategies of neural networks.

- What is known: initialization should break symmetry.
- What is known: the scale of weights is important.

(demo)

Controlling for the variance in the forward pass

A first strategy is to initialize the network parameters such that activations preserve the same variance across layers.

Intuitively, this ensures that the information keeps flowing during the forward pass, without reducing or magnifying the magnitude of input signals exponentially.

Let us assume that

- we are in a linear regime at initialization (e.g., the positive part of a ReLU or the middle of a sigmoid),
- weights w_{ij}^l are initialized i.i.d,
- biases b_l are initialized to be 0,
- input features are i.i.d, with a variance denoted as $\mathbb{V}[x]$.

Then, the variance of the activation h_i^l of unit i in layer l is

$$\begin{aligned}\mathbb{V}\left[h_i^l\right] &= \mathbb{V}\left[\sum_{j=0}^{q_{l-1}-1} w_{ij}^l h_j^{l-1}\right] \\ &= \sum_{j=0}^{q_{l-1}-1} \mathbb{V}\left[w_{ij}^l\right] \mathbb{V}\left[h_j^{l-1}\right]\end{aligned}$$

where q_l is the width of layer l and $h_j^0 = x_j$ for all $j = 0, ..., p-1$.

Since the weights w_{ij}^l at layer l share the same variance $\mathbb{V}\left[w^l\right]$ and the variance of the activations in the previous layer are the same, we can drop the indices and write

$$\mathbb{V}\left[h^l\right] = q_{l-1}\mathbb{V}\left[w^l\right]\mathbb{V}\left[h^{l-1}\right].$$

Therefore, the variance of the activations is preserved across layers when

$$\mathbb{V}\left[w^l\right] = \frac{1}{q_{l-1}} \quad \forall l.$$

This condition is enforced in LeCun's uniform initialization, which is defined as

$$w_{ij}^l \sim \mathcal{U}\left[-\sqrt{\frac{3}{q_{l-1}}}, \sqrt{\frac{3}{q_{l-1}}}\right].$$

Controlling for the variance in the backward pass

A similar idea can be applied to ensure that the gradients flow in the backward pass (without vanishing nor exploding), by maintaining the variance of the gradient with respect to the activations fixed across layers.

Under the same assumptions as before,

$$
\begin{aligned}
\mathbb{V}\left[\frac{\mathrm{d}\hat{y}}{\mathrm{d}h_i^l}\right] &= \mathbb{V}\left[\sum_{j=0}^{q_{l+1}-1} \frac{\mathrm{d}\hat{y}}{\mathrm{d}h_j^{l+1}} \frac{\partial h_j^{l+1}}{\partial h_i^l}\right] \\
&= \mathbb{V}\left[\sum_{j=0}^{q_{l+1}-1} \frac{\mathrm{d}\hat{y}}{\mathrm{d}h_j^{l+1}} w_{j,i}^{l+1}\right] \\
&= \sum_{j=0}^{q_{l+1}-1} \mathbb{V}\left[\frac{\mathrm{d}\hat{y}}{\mathrm{d}h_j^{l+1}}\right] \mathbb{V}\left[w_{ji}^{l+1}\right]
\end{aligned}
$$

If we further assume that

- the gradients of the activations at layer l share the same variance
- the weights at layer $l+1$ share the same variance $\mathbb{V}\left[w^{l+1}\right]$,

then we can drop the indices and write

$$\mathbb{V}\left[\frac{\mathrm{d}\hat{y}}{\mathrm{d}h^{l}}\right] = q_{l+1}\mathbb{V}\left[\frac{\mathrm{d}\hat{y}}{\mathrm{d}h^{l+1}}\right]\mathbb{V}\left[w^{l+1}\right].$$

Therefore, the variance of the gradients with respect to the activations is preserved across layers when

$$\mathbb{V}\left[w^{l}\right] = \frac{1}{q_{l}} \quad \forall l.$$

Xavier initialization

We have derived two different conditions on the variance of w^l,

- $\mathbb{V}\left[w^l\right] = \frac{1}{q_{l-1}}$
- $\mathbb{V}\left[w^l\right] = \frac{1}{q_l}$.

A compromise is the Xavier initialization, which initializes w^l randomly from a distribution with variance

$$\mathbb{V}\left[w^l\right] = \frac{1}{\frac{q_{l-1}+q_l}{2}} = \frac{2}{q_{l-1}+q_l}.$$

For example, normalized initialization is defined as

$$w_{ij}^l \sim \mathcal{U}\left[-\sqrt{\frac{6}{q_{l-1}+q_l}}, \sqrt{\frac{6}{q_{l-1}+q_l}}\right].$$

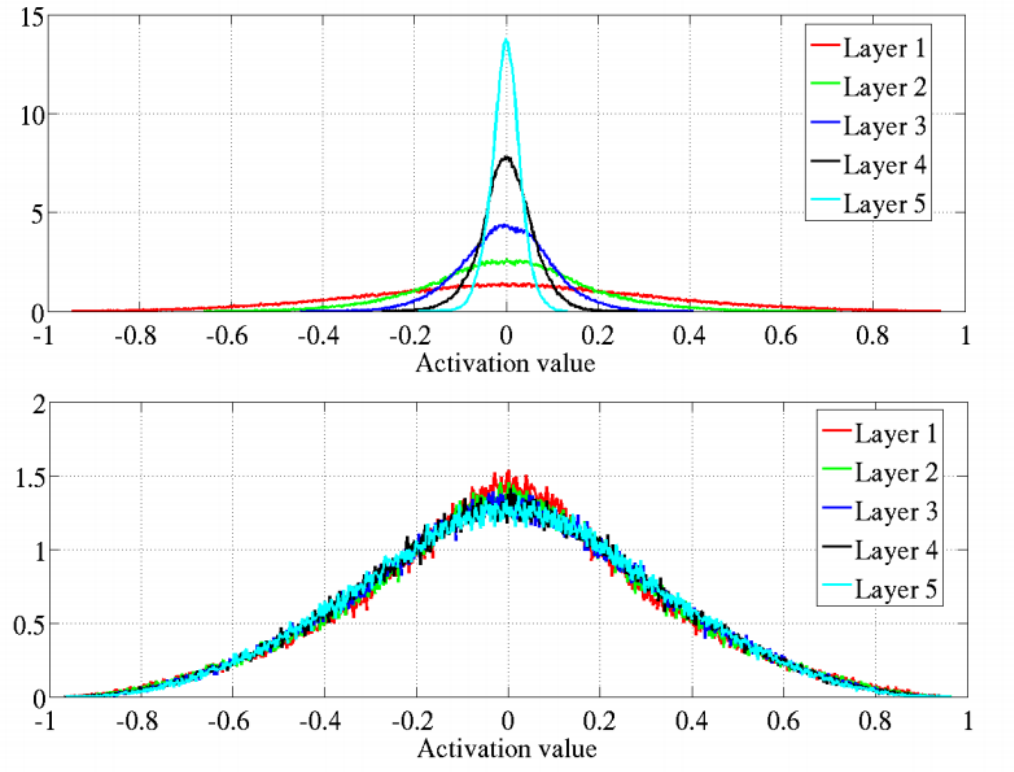


Figure 6: *Activation values normalized histograms with hyperbolic tangent activation, with standard (top) vs normalized initialization (bottom). Top: 0-peak increases for higher layers.*

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Credits: Glorot and Bengio, Understanding the difficulty of training deep feedforward neural networks, 2010.

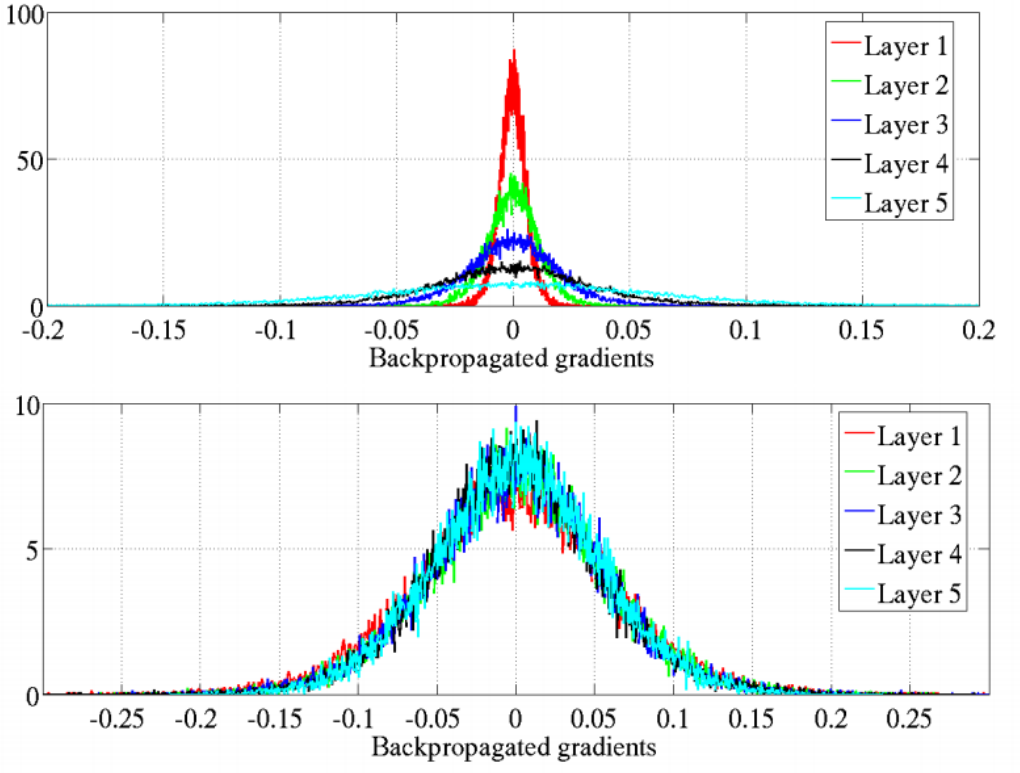

Figure 7: *Back-propagated gradients normalized histograms with hyperbolic tangent activation, with standard (top) vs normalized (bottom) initialization. Top: 0-peak decreases for higher layers.*

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Credits: Glorot and Bengio, Understanding the difficulty of training deep feedforward neural networks, 2010.

He initialization

Because $\mathrm{ReLU}(x) = \max(0, x)$, the mean of the activations at layer l is typically not 0. Therefore, our zero-mean assumption is wrong. Accounting for this shift, He et al (2015) derive a forward initialization scheme that initializes w^l from a distribution with variance

$$\mathbb{V}\left[w^l\right] = \frac{2}{q_{l-1}}.$$

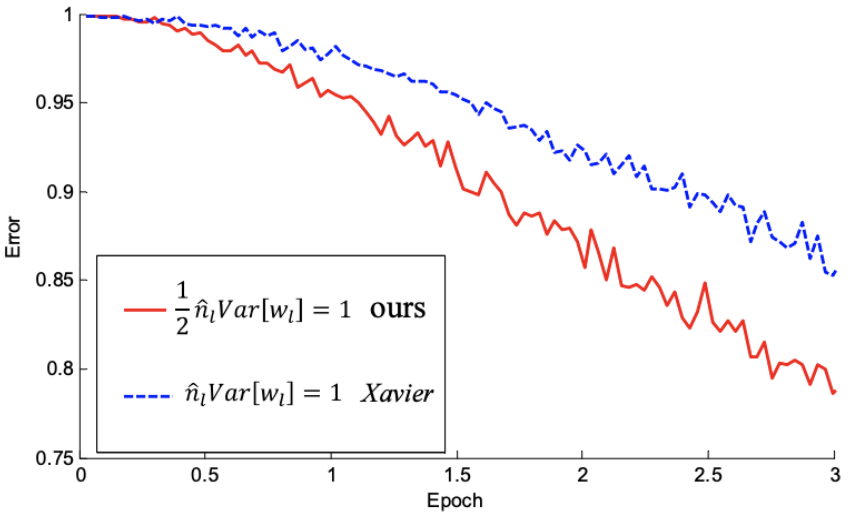


Figure 2. The convergence of a **22-layer** large model (B in Table 3). The x-axis is the number of training epochs. The y-axis is the top-1 error of 3,000 random val samples, evaluated on the center crop. We use ReLU as the activation for both cases. Both our initialization (red) and "*Xavier*" (blue) [7] lead to convergence, but ours starts reducing error earlier.

(Back to demo)

Normalization

Data normalization

Previous weight initialization strategies rely on preserving the activation variance constant across layers, under the assumption that the input feature variances are the same. That is,

$$\mathbb{V}\left[x_i\right] = \mathbb{V}\left[x_j\right] \triangleq \mathbb{V}\left[x\right]$$

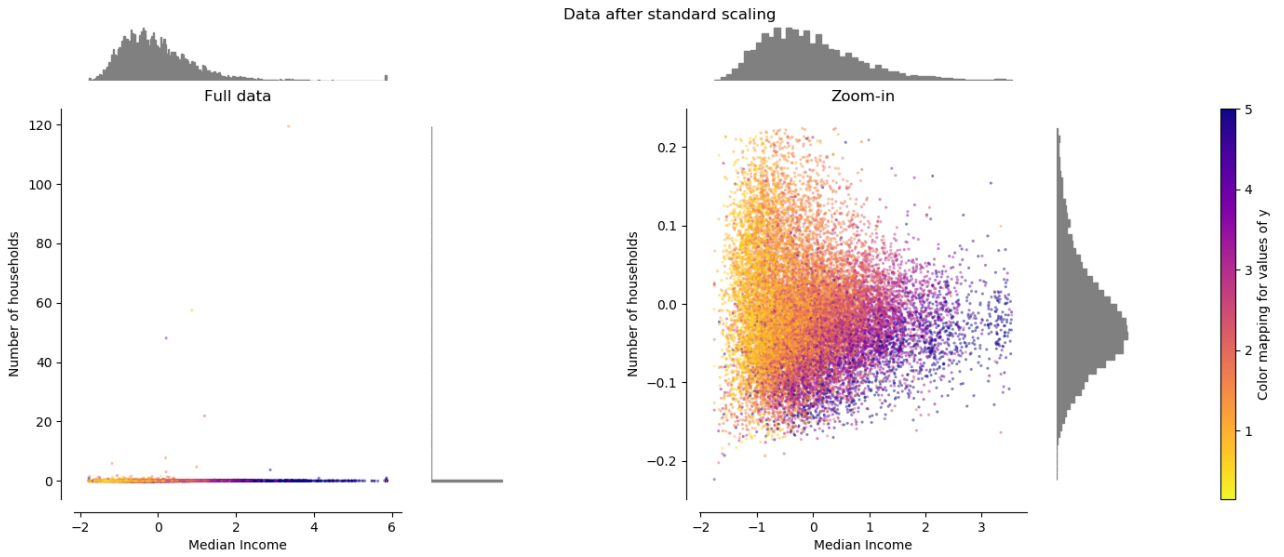
for all pairs of features i, j.

In general, this constraint is not satisfied but can be enforced by standardizing the input data feature-wise,

$$\mathbf{x}' = (\mathbf{x} - \hat{\mu}) \odot \frac{1}{\hat{\sigma}},$$

where

$$\hat{\mu} = \frac{1}{N} \sum_{\mathbf{x} \in \mathbf{d}} \mathbf{x} \qquad \hat{\sigma}^2 = \frac{1}{N} \sum_{\mathbf{x} \in \mathbf{d}} (\mathbf{x} - \hat{\mu})^2.$$



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Credits: Scikit-Learn, Compare the effect of different scalers on data with outliers.

Batch normalization

Maintaining proper statistics of the activations and derivatives is critical for training neural networks.

This constraint can be enforced explicitly during the forward pass by re-normalizing them. Batch normalization was the first method introducing this idea.

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Credits: Francois Fleuret, EE559 Deep Learning, EPFL; Ioffe and Szegedy, Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift, 2015.

Let us consider a minibatch of samples at training, for which $\mathbf{u}_b \in \mathbb{R}^q$, $b = 1, \ldots, B$, are intermediate values computed at some location in the computational graph.

In batch normalization following the node $\mathbf{u}$, the per-component mean and variance are first computed on the batch

$$\hat{\mu}_{\text{batch}} = \frac{1}{B}\sum_{b=1}^{B} \mathbf{u}_b \qquad \hat{\sigma}^2_{\text{batch}} = \frac{1}{B}\sum_{b=1}^{B} (\mathbf{u}_b - \hat{\mu}_{\text{batch}})^2,$$

from which the standardized $\mathbf{u}'_b \in \mathbb{R}^q$ are computed such that

$$\mathbf{u}'_b = \gamma \odot (\mathbf{u}_b - \hat{\mu}_{\text{batch}}) \odot \frac{1}{\hat{\sigma}_{\text{batch}} + \epsilon} + \beta$$

where $\gamma, \beta \in \mathbb{R}^q$ are parameters to optimize.

During testing, the mean and variance computed on the entire training set and used to standardize the activations.

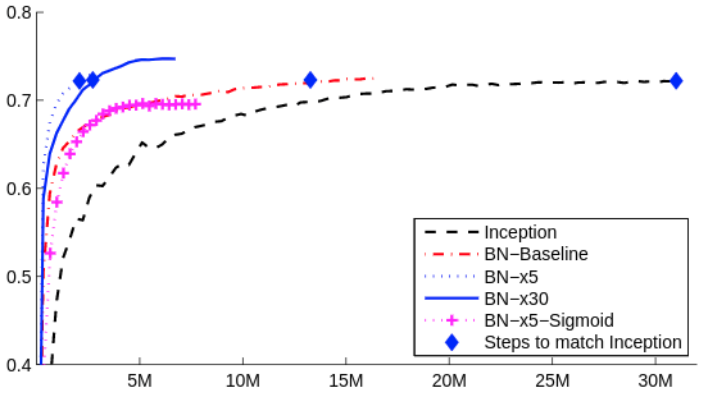

Figure 2: *Single crop validation accuracy of Inception and its batch-normalized variants, vs. the number of training steps.*

Model	Steps to 72.2%	Max accuracy
Inception	$31.0 \cdot 10^6$	72.2%
BN-Baseline	$13.3 \cdot 10^6$	72.7%
BN-x5	$2.1 \cdot 10^6$	73.0%
BN-x30	$2.7 \cdot 10^6$	74.8%
BN-x5-Sigmoid		69.8%

Figure 3: *For Inception and the batch-normalized variants, the number of training steps required to reach the maximum accuracy of Inception (72.2%), and the maximum accuracy achieved by the network.*

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Credits: Ioffe and Szegedy, Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift, 2015.

Layer normalization

Layer normalization is a variant of batch normalization that normalizes the activations across the features of each sample, rather than across the samples of each feature:

$$\mathbf{u}' = \gamma \odot (\mathbf{u} - \hat{\mu}_{\text{layer}}) \odot \frac{1}{\hat{\sigma}_{\text{layer}} + \epsilon} + \beta.$$

The end.