Scaling ResNets in the large-depth regime

Non-Linear and High Dimensional Inference, IHP, October 3rd 2022

Adeline Fermanian

Joint work with

Gérard Biau
SORBONNE UNIVERSITY

Pierre Marion
SORBONNE UNIVERSITY

Jean-Philippe Vert
OWKIN

Agenda

Learning with ResNets

Scaling deep ResNets

Scaling in the continuous-time setting

Beyond initialization

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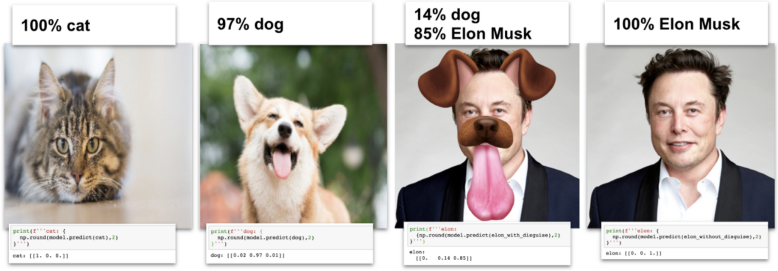
Beyond initialization

How most people see the supervised learning problem

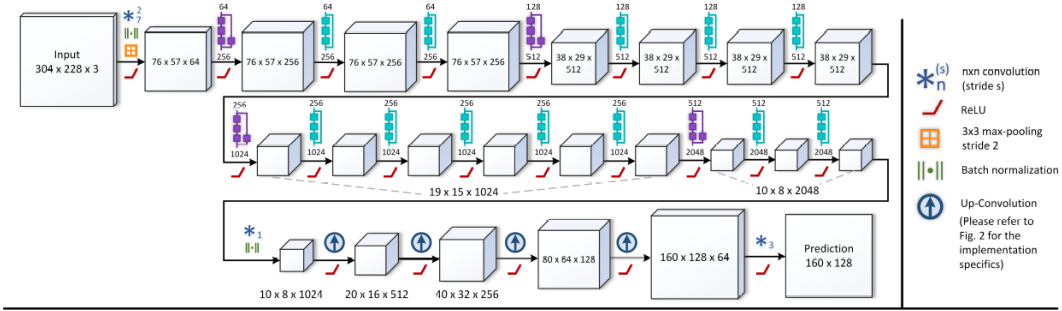
Learn how to build an image-recognizing convolutional neural network with Python and Keras in less than 15minutes!

Fabian Bosler Oct 5, 2019 · 10 min read ★



https://towardsdatascience.com/cat-dog-or-elon-musk-145658489730

How machine learners see the supervised learning problem



https://medium.datadriveninvestor.com/depth-estimation-with-deep-neural-networks-part-2-81ee374888eb

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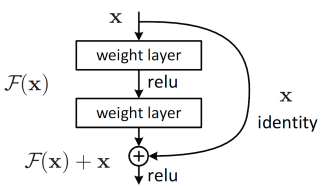
Original Parametric Simple General **ResNet**

$$f(h_k, \theta_{k+1}) = V_{k+1}\,\mathrm{ReLU}(W_{k+1}h_k + b_{k+1})$$

- $\mathrm{ReLU}(x) = \max(x, 0)$ = activation function
- $\theta_k = (W_k, b_k)$ = weight matrice + bias
- $\pi = (A, B, (V_k)_{1 \leqslant k \leqslant L}, (\theta_k)_{1 \leqslant k \leqslant L})$



He et al. (2016)

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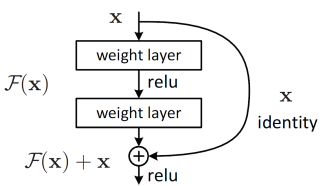

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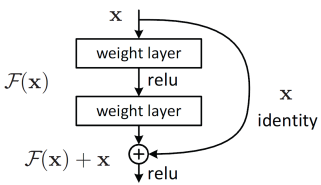

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Original Parametric Simple **General ResNet**

$$f(h_k, \theta_{k+1}) = V_{k+1} g(h_k, \theta_{k+1})$$

- $g : \mathbb{R}^d \times \mathbb{R}^p \to \mathbb{R}^d$
- $\theta_k =$ parameters
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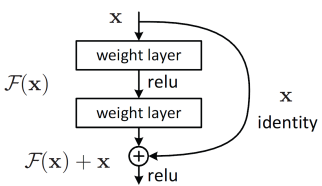

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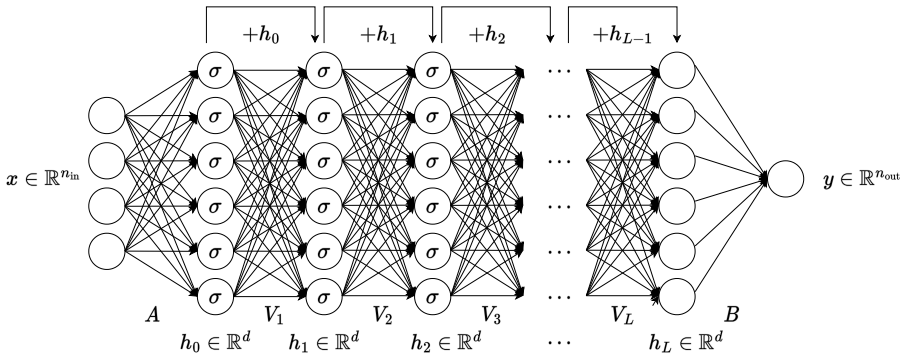
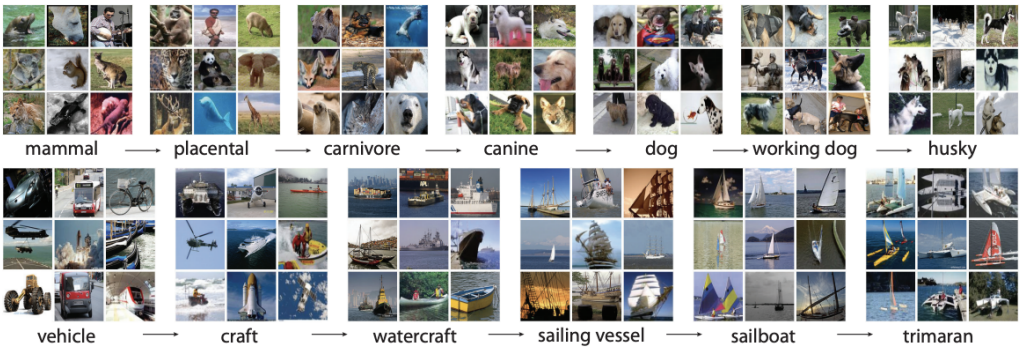


The revolution of ResNets



Examples from the ImageNet dataset

https://blog.roboflow.com/introduction-to-imagenet

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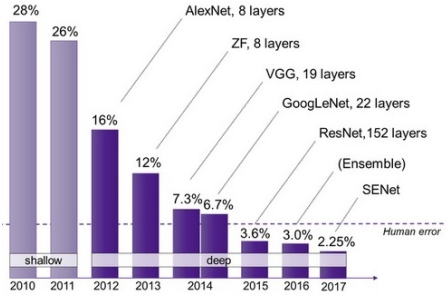

ImageNet performance over time

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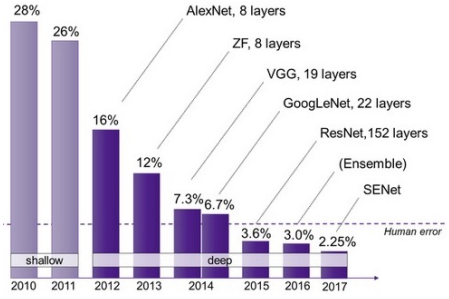

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Deep learning → neural ODE ← ODE

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Deep learning $\rightarrow$ neural ODE $\leftarrow$ ODE

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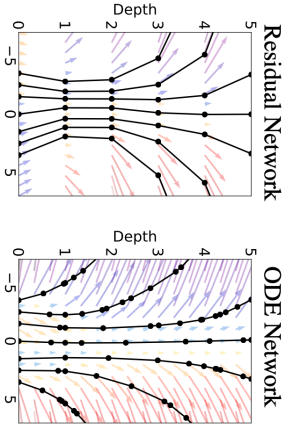
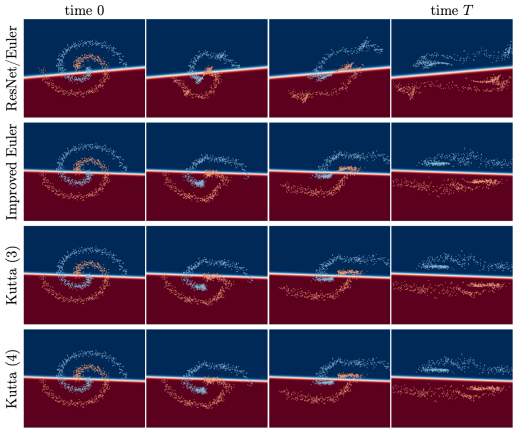
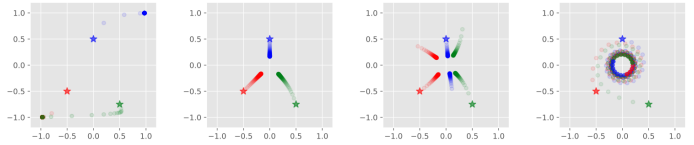


New network architectures: Runge-Kutta networks



Benning et al. (2019)

New network architectures: antisymmetric networks



(a) Vanilla RNN with a random weight matrix.

(b) Vanilla RNN with an identity weight matrix.

(c) Vanilla RNN with a random orthogonal weight matrix (seed = 0).

(d) Vanilla RNN with a random orthogonal weight matrix (seed = 1).

(e) RNN with feedback with positive eigenvalues.

(f) RNN with feedback with negative eigenvalues.

(g) RNN with feedback with imaginary eigenvalues.

(h) RNN with feedback with imaginary eigenvalues and diffusion.

Chang et al. (2019)

In summary

ResNet	**Neural ODE**
$h_0 = Ax$	$H_0 = Ax$
$h_{k+1} = h_k + \frac{1}{L} f(h_k, \theta_{k+1})$	$dH_t = f(H_t, \Theta_t)dt$
$F_\pi(x) = Bh_T$	$F_\Pi(x) = BH_1$

$$f(h, \theta) = V\sigma(Wh + b)$$

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Stability at initialization

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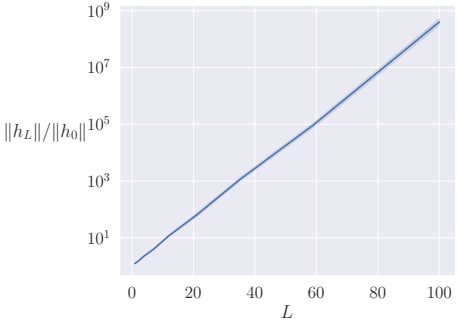

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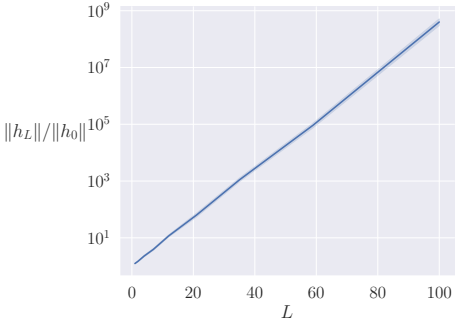

☞ Solution: batch normalization or scaling.

Scaling ResNets

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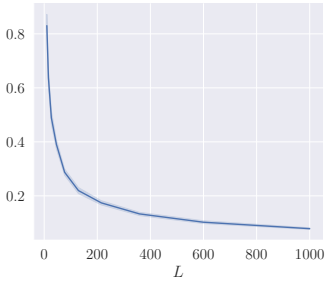
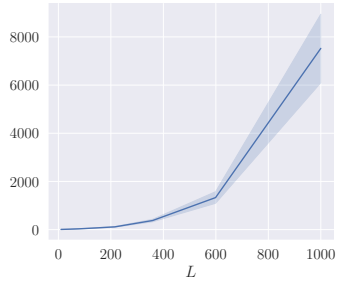
- Our approach: mathematical analysis at initialization.

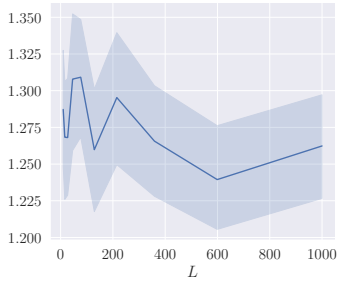
Scaling with standard initialization



(a) $\|h_L - h_0\|/\|h_0\|$, $\beta = 1$

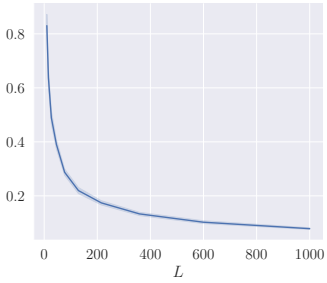


(b) $\|h_L - h_0\|/\|h_0\|$, $\beta = 0.25$



(c) $\|h_L - h_0\|/\|h_0\|$, $\beta = 0.5$

Scaling with standard initialization



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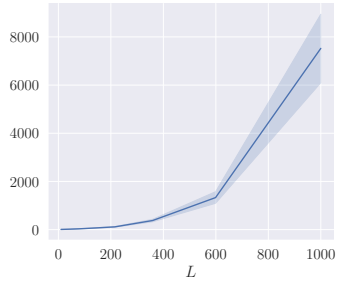

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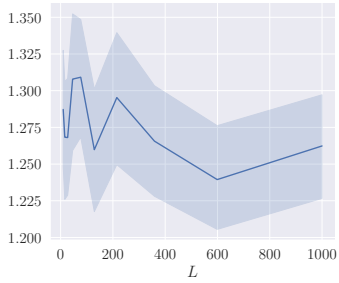

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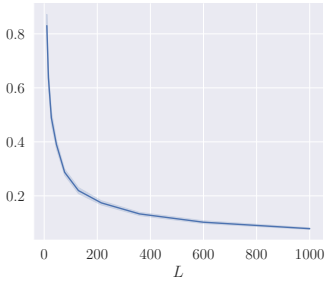

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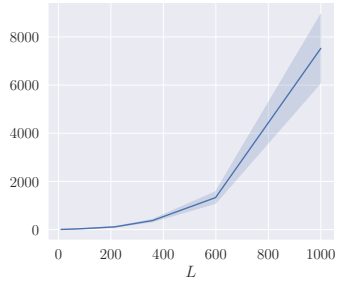

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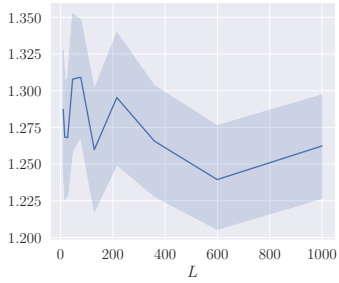

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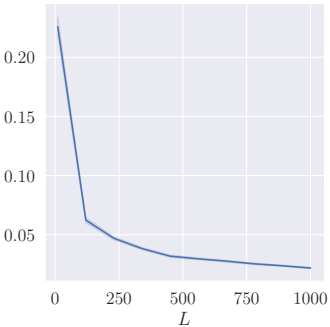
Scaling with standard initialization – Gradients



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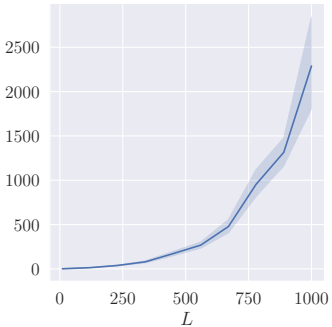

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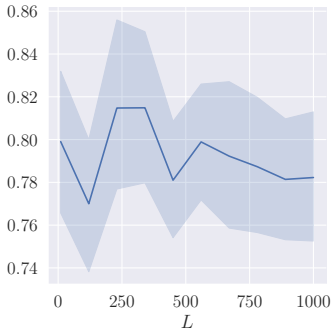

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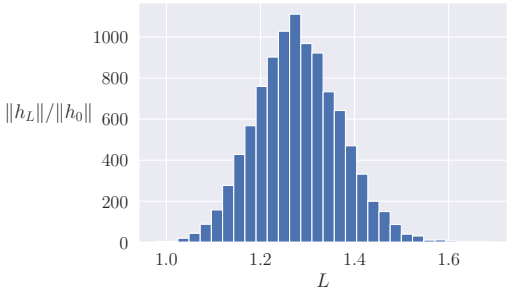
Stability – output/gradients



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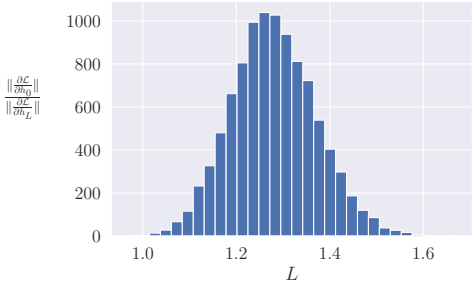

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Then the SDE has a unique solution H and, for any $0 \leqslant k \leqslant L$,

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Key: link between β and the weight distributions.

Agenda

Learning with ResNets

Scaling deep ResNets

Scaling in the continuous-time setting

Beyond initialization

Leaving the i.i.d. world behind

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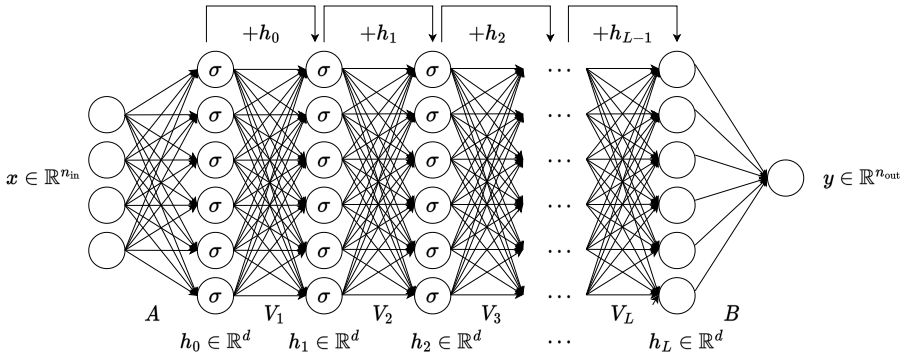
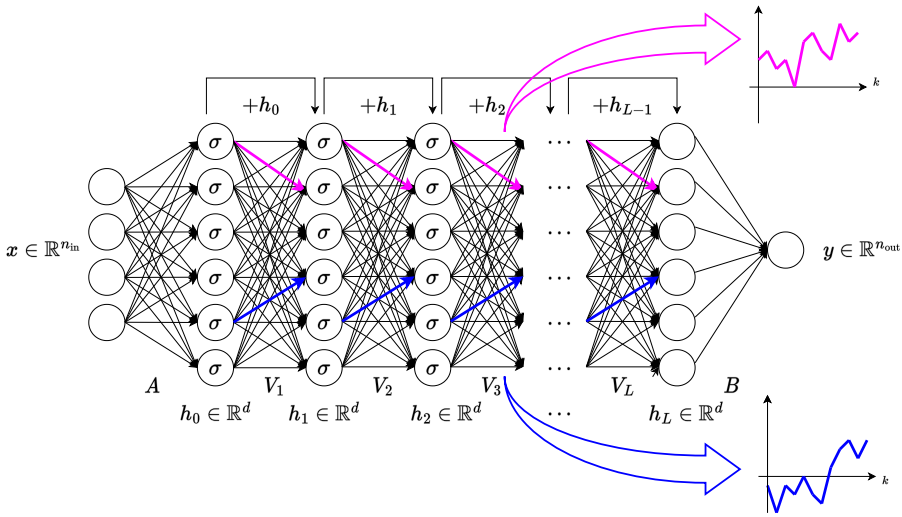
- Example: the entries of $\mathscr{V}$ and Θ are independent Gaussian processes with zero expectation and covariance $K(x,x') = \exp(-\frac{(x-x')^2}{2\ell^2})$.


$+h_0$
$+h_1$
$+h_2$
$+h_{L-1}$
σ
$\cdots$
$x \in \mathbb{R}^{n_{\text{in}}}$
$y \in \mathbb{R}^{n_{\text{out}}}$
A
V_1
V_2
V_3
V_L
B
$h_0 \in \mathbb{R}^d$
$h_1 \in \mathbb{R}^d$
$h_2 \in \mathbb{R}^d$
$h_L \in \mathbb{R}^d$


$+h_0$
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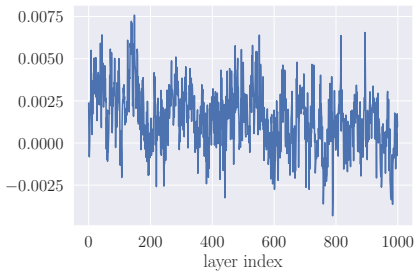
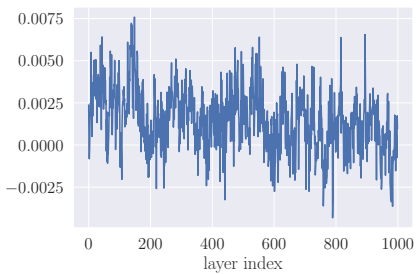
$h_1 \in \mathbb{R}^d$
$h_2 \in \mathbb{R}^d$
$h_L \in \mathbb{R}^d$
k
k

Scaling and weight regularity

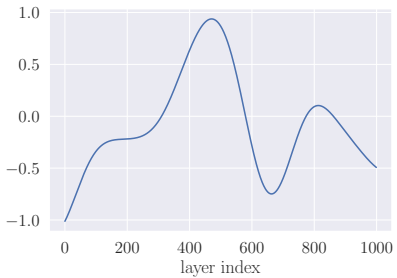


(a) I.i.d.

Scaling and weight regularity



(a) I.i.d.



(b) Smooth

ODE regime

ResNet	**Neural ODE**
$h_0 = Ax$	$H_0 = Ax$
$h_{k+1} = h_k + \frac{1}{L} V_{k+1} g(h_k, \theta_{k+1})$	$dH_t = \mathscr{V}_t g(H_t, \Theta_t) dt$
$F_\pi(x) = B h_L$	$F_\Pi(x) = B H_1$

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Proposition

Assumption: the function g is Lipschitz continuous on compact sets.

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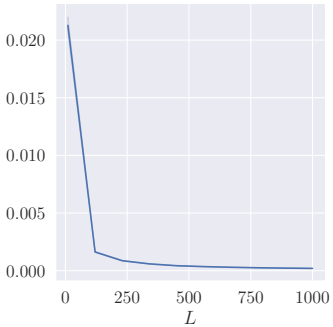
Proposition

Assumption: the function g is Lipschitz continuous on compact sets.

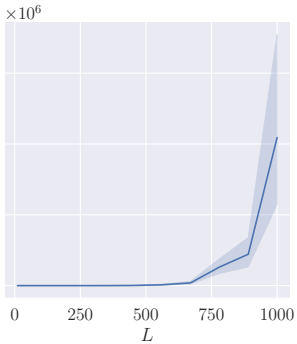
Then the ODE has a unique solution H and, a.s., for any $0 \leqslant k \leqslant L$,

$$\|H_{k/L} - h_k\| \leqslant \frac{c}{L}.$$

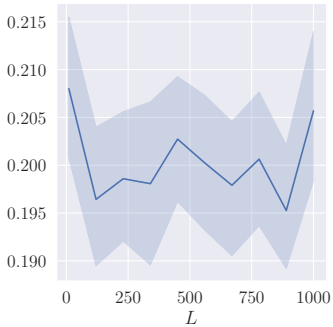
Scaling with a smooth initialization



(a) $\|h_L - h_0\|/\|h_0\|$, $\beta = 2$

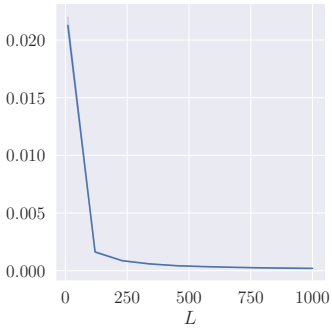


(b) $\|h_L - h_0\|/\|h_0\|$, $\beta = 0.5$

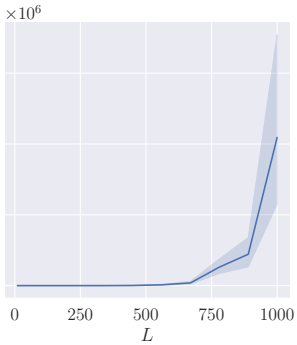


(c) $\|h_L - h_0\|/\|h_0\|$, $\beta = 1$

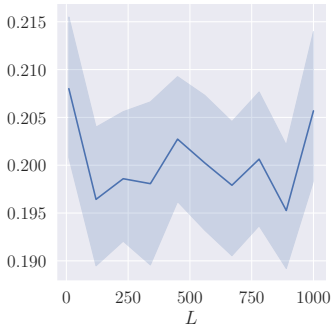
Scaling with a smooth initialization



(a) $\|h_L - h_0\|/\|h_0\|$, $\beta = 2$



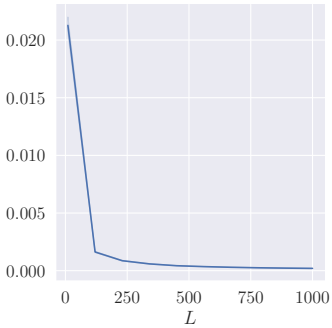
(b) $\|h_L - h_0\|/\|h_0\|$, $\beta = 0.5$



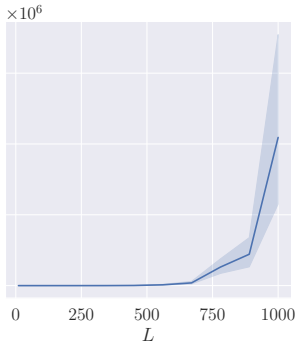
(c) $\|h_L - h_0\|/\|h_0\|$, $\beta = 1$

- Again 3 cases: identity/explosion/stability.

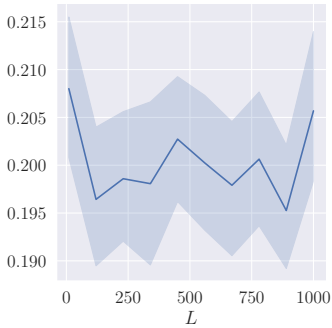
Scaling with a smooth initialization



(a) $\|h_L - h_0\|/\|h_0\|$, $\beta = 2$



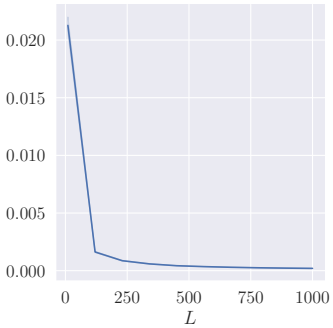
(b) $\|h_L - h_0\|/\|h_0\|$, $\beta = 0.5$



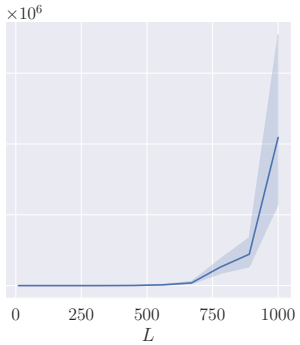
(c) $\|h_L - h_0\|/\|h_0\|$, $\beta = 1$

- Again 3 cases: identity/explosion/stability.
- With a smooth initialization, the critical scaling is $\beta = 1$.

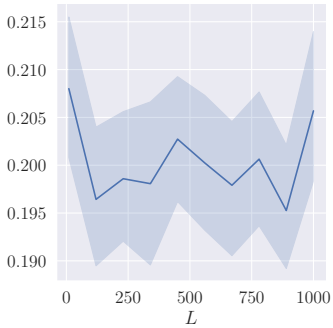
Scaling with a smooth initialization



(a) $\|h_L - h_0\|/\|h_0\|$, $\beta = 2$



(b) $\|h_L - h_0\|/\|h_0\|$, $\beta = 0.5$



(c) $\|h_L - h_0\|/\|h_0\|$, $\beta = 1$

- Again 3 cases: identity/explosion/stability.
- With a smooth initialization, the critical scaling is $\beta = 1$.
- It is the scaling that corresponds in the deep limit to an ODE.

Scaling with with a smooth initialization

Theorem

Assumption: $\mathscr{V}$ and Θ are a.s. Lipschitz continuous and bounded.

Scaling with with a smooth initialization

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1. If $\beta > 1$
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Scaling with with a smooth initialization

Theorem

Assumption: $\mathscr{V}$ and Θ are a.s. Lipschitz continuous and bounded.

1. If $\beta > 1$ then, a.s., $\|h_L - h_0\|/\|h_0\| \xrightarrow{L\to\infty} 0$.
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Scaling with with a smooth initialization

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2. If $\beta = 1$ then, a.s., $\|h_L - h_0\|/\|h_0\| \leqslant c$.
3. If $\beta < 1$

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Scaling with with a smooth initialization

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3. If $\beta < 1$ + assumptions, then $\max_k \dfrac{\|h_k - h_0\|}{\|h_0\|} \xrightarrow{L\to\infty} \infty$.

Scaling with with a smooth initialization

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1. If $\beta > 1$ then, a.s., $\|h_L - h_0\|/\|h_0\| \xrightarrow{L\to\infty} 0$. $\to$ identity
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3. If $\beta < 1$ + assumptions, then $\max_k \dfrac{\|h_k - h_0\|}{\|h_0\|} \xrightarrow{L\to\infty} \infty$. $\to$ explosion

Intermediate regimes

- Challenge: describe the transition between the i.i.d. and smooth cases.

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- We initialize the weights as increments of a fractional Brownian motion $(B_t^H)_{t\in[0,1]}$.

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- Recall: B^H is Gaussian, starts at zero, has zero expectation, and covariance function

$$\mathbb{E}(B_s^H B_t^H) = \frac{1}{2}(|s|^{2H} + |t|^{2H} - |t-s|^{2H}), \quad 0 \leqslant s, t \leqslant 1.$$

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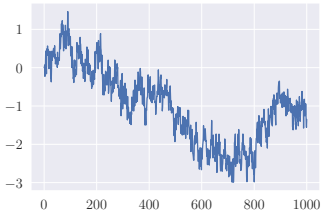
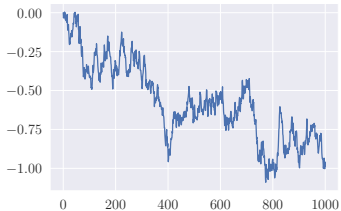
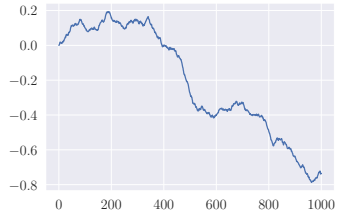
- The Hurst index $H \in (0,1)$ describes the raggedness of the process.



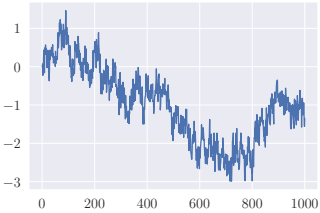
(a) $H = 0.2$



(b) $H = 0.5$



(c) $H = 0.8$



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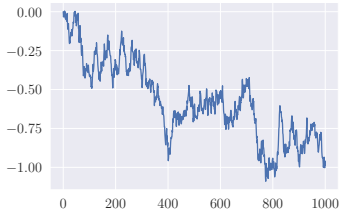
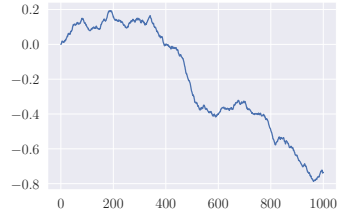
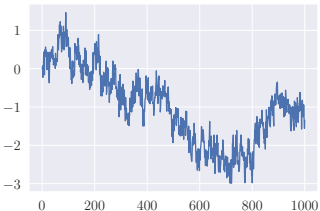


(b) $H = 0.5$

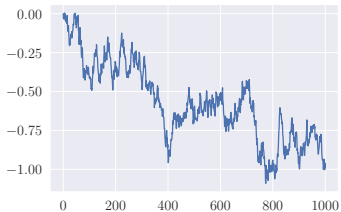


(c) $H = 0.8$

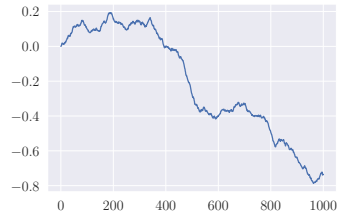
- $H = 1/2$: standard Brownian motion (SDE regime).



(a) $H = 0.2$

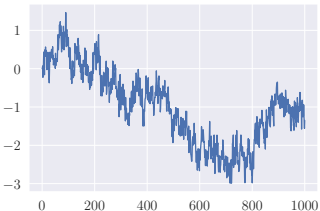


(b) $H = 0.5$



(c) $H = 0.8$

- $H = 1/2$: standard Brownian motion (SDE regime).
- $H < 1/2$: the increments are negatively correlated.
- $H > 1/2$: the increments are positively correlated.



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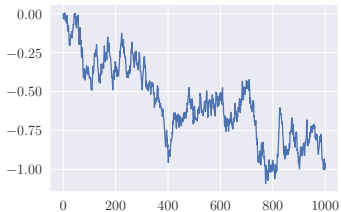

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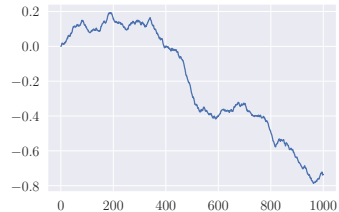
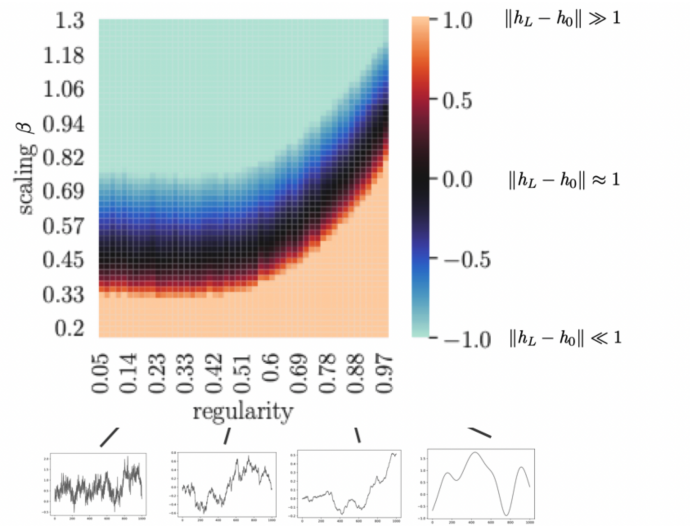


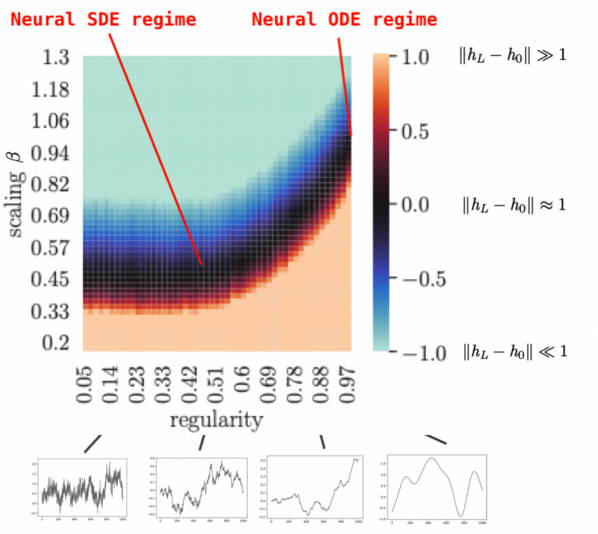
(c) $H = 0.8$

- $H = 1/2$: standard Brownian motion (SDE regime).
- $H < 1/2$: the increments are negatively correlated.
- $H > 1/2$: the increments are positively correlated.
- When $H \to 1$: the trajectories converge to linear functions (ODE regime).

A continuum of intermediate regularities



A continuum of intermediate regularities



Agenda

Learning with ResNets

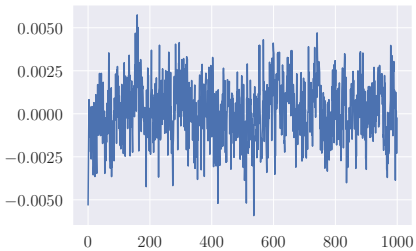
Scaling deep ResNets

Scaling in the continuous-time setting

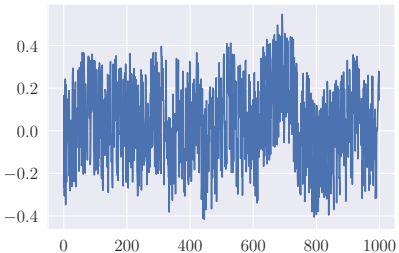
Beyond initialization

Training

Before training



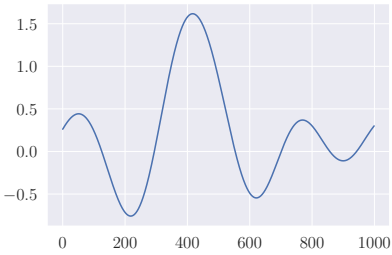
After training



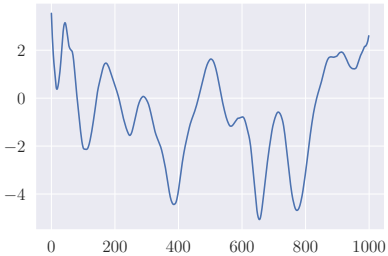
l.i.d. initialization, $\beta = 1/2$

Training

Before training



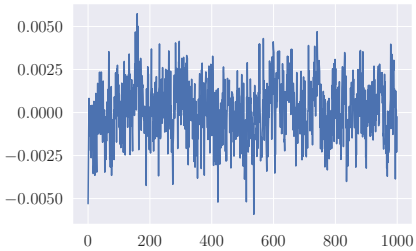
After training



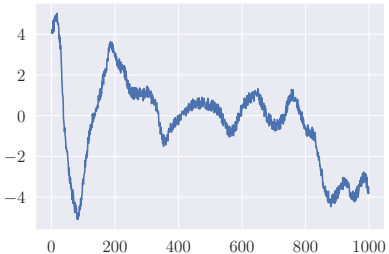
Smooth initialization, $\beta = 1$

Training

Before training



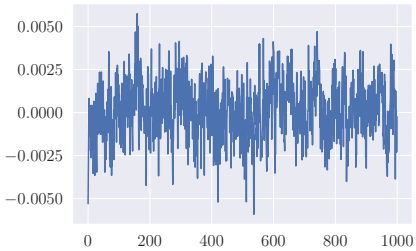
After training



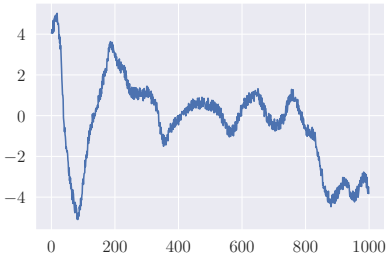
l.i.d. initialization, $\beta = 1$

Training

Before training



After training



i.i.d. initialization, $\beta = 1$

- The weights after training still exhibit a strong structure as functions of the layer.

Training

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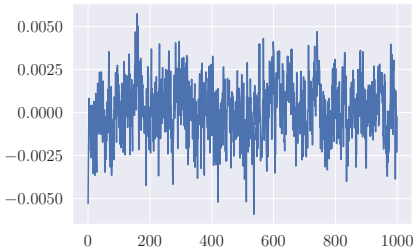
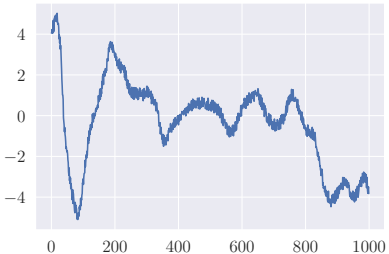


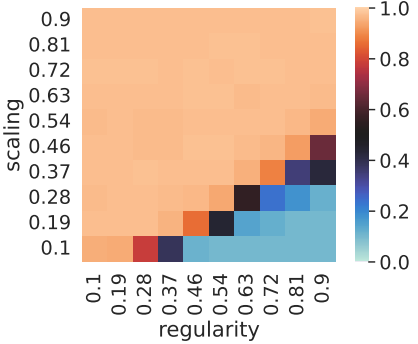
After training



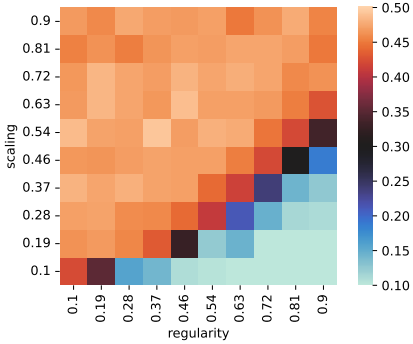
l.i.d. initialization, $\beta = 1$

- The weights after training still exhibit a strong structure as functions of the layer.
- Their regularity is influenced by both the initialization and the choice of β.

Performance after training



(a) On MNIST



(b) On CIFAR-10

Conclusion

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- Perspectives: what about training? how should we choose the regularity for a given problem?
- To know more: arXiv:2206.06929.

Thank you!

adeline.fermanian@mines-paristech.fr

https://afermanian.github.io