Optimization for Machine Learning

Lecture 19: Optimization for Neural networks

6.881: MIT

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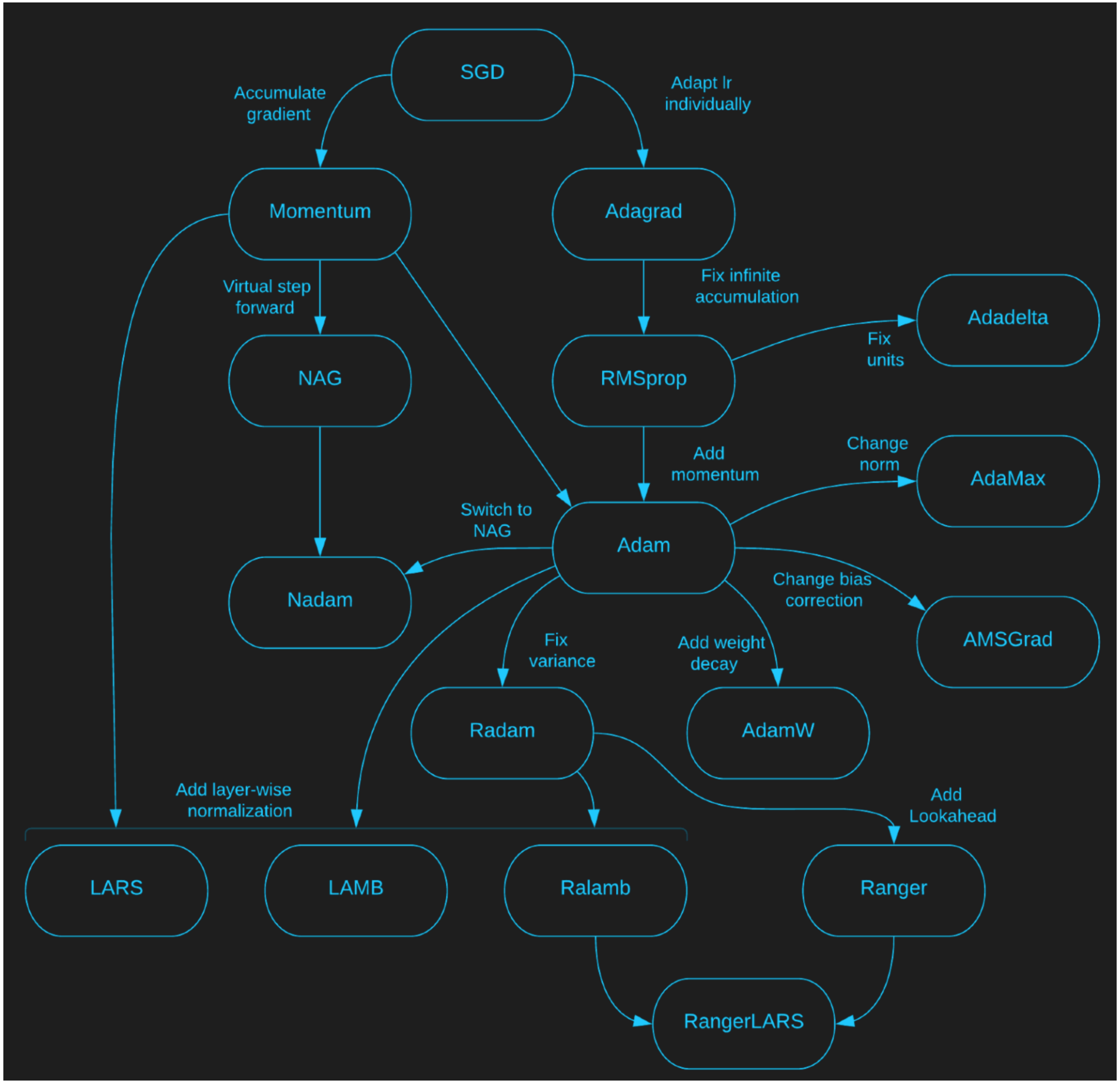
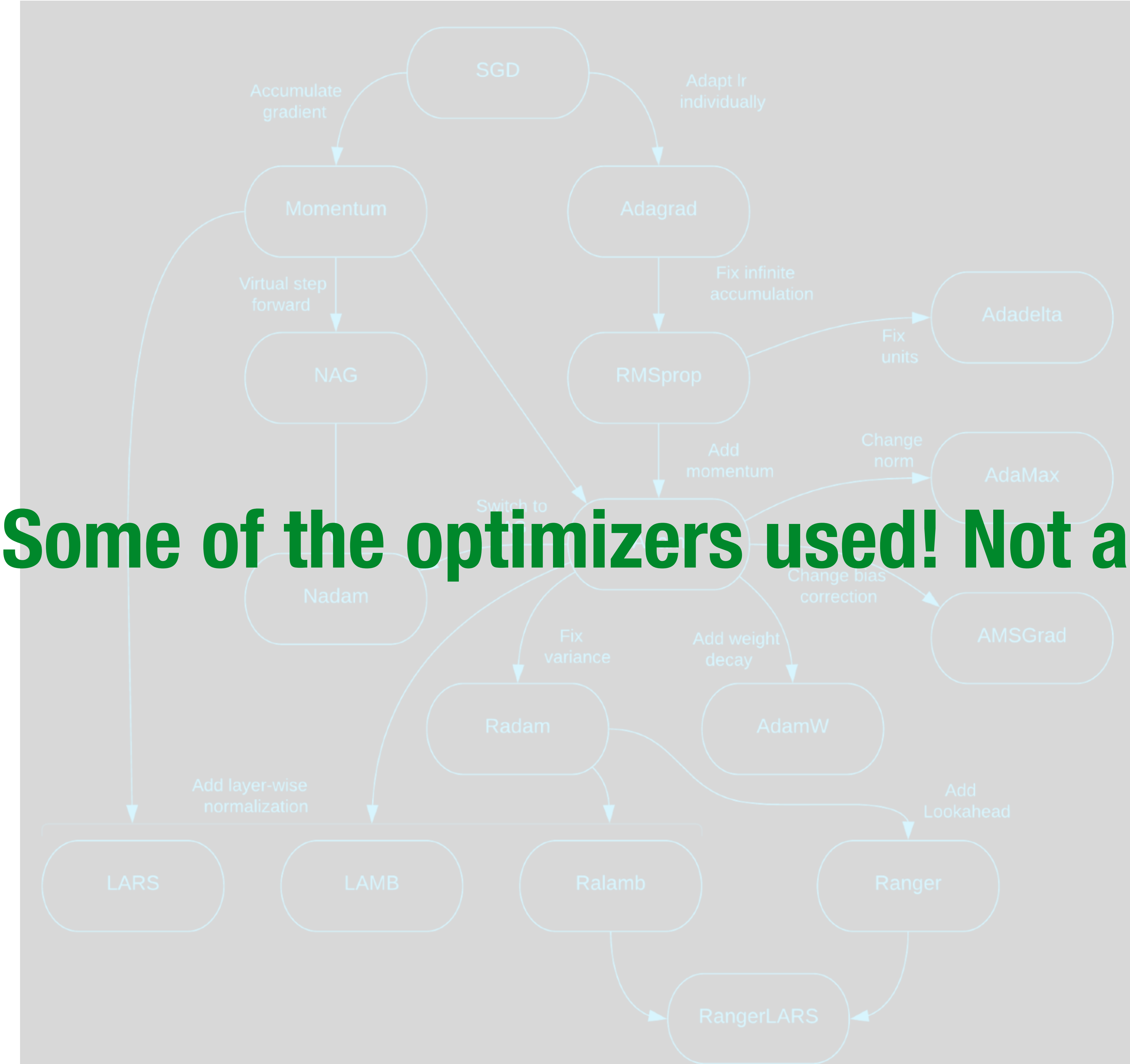
May 04, 2021



https://darel13712.github.io/ml/optimizers.html



Some of the optimizers used! Not all!

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Some Aspects of NN Optimization

- Backprop ➠ SGD
- Mini-batches
- Initialization
- Batchnorm
- Gradient clipping
- Adaptive methods
- Momentum
- Layerwise params
- …and more!

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- …and more!

All while keeping validation / test error performance in mind

SGD: Neural network training

$$\min_{\theta} \; R_N(\theta) := \frac{1}{N}\sum_{i=1}^{N} \ell(y_i, F(x_i;\theta))$$

label

network output

$\ell(y, z) = \max(0, 1 - yz)$

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4 In reality: momentum, clipping, adaptivity, …

1 Iterative method. How to select θ_0?

1. Initialization

Properly initializing a NN important. NN loss is highly nonconvex; optimizing it to attain a "good" solution hard, requires careful tuning.

On the importance of initialization and momentum in deep learning

Ilya Sutskever[1] ILYASU@GOOGLE.COM
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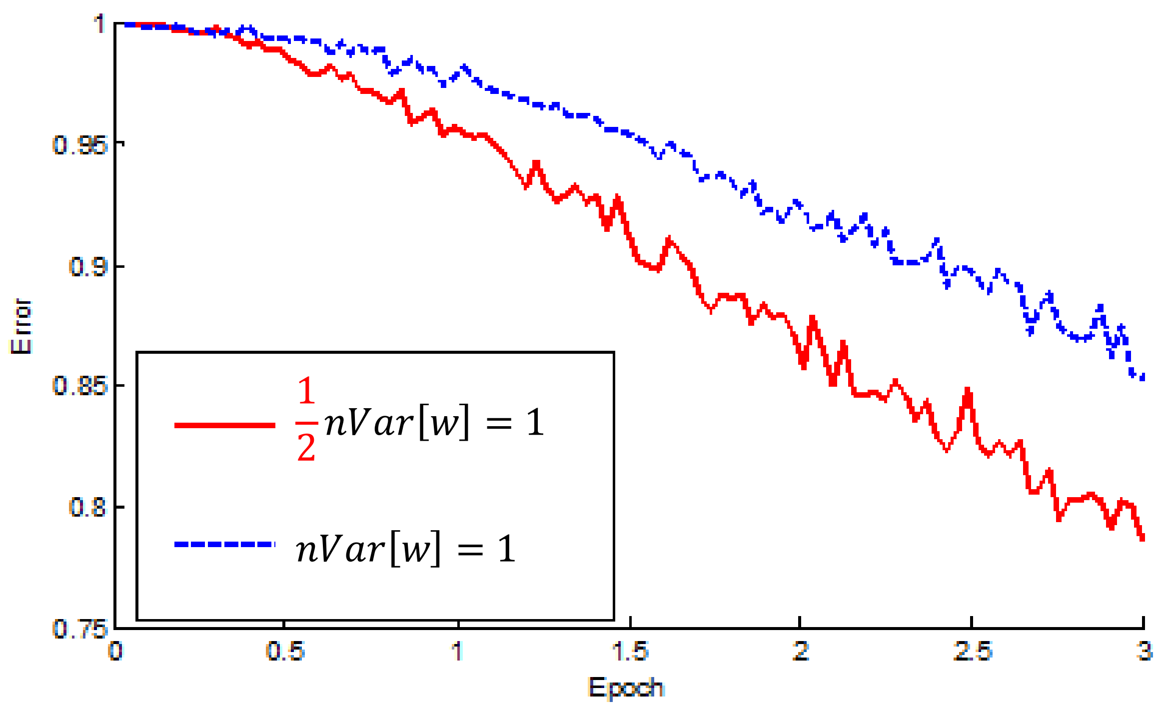
See also: http://cs231n.github.io/neural-networks-2/ for additional practical notes

1. Impact of initialization

22-layer ReLU net:
good init converges faster



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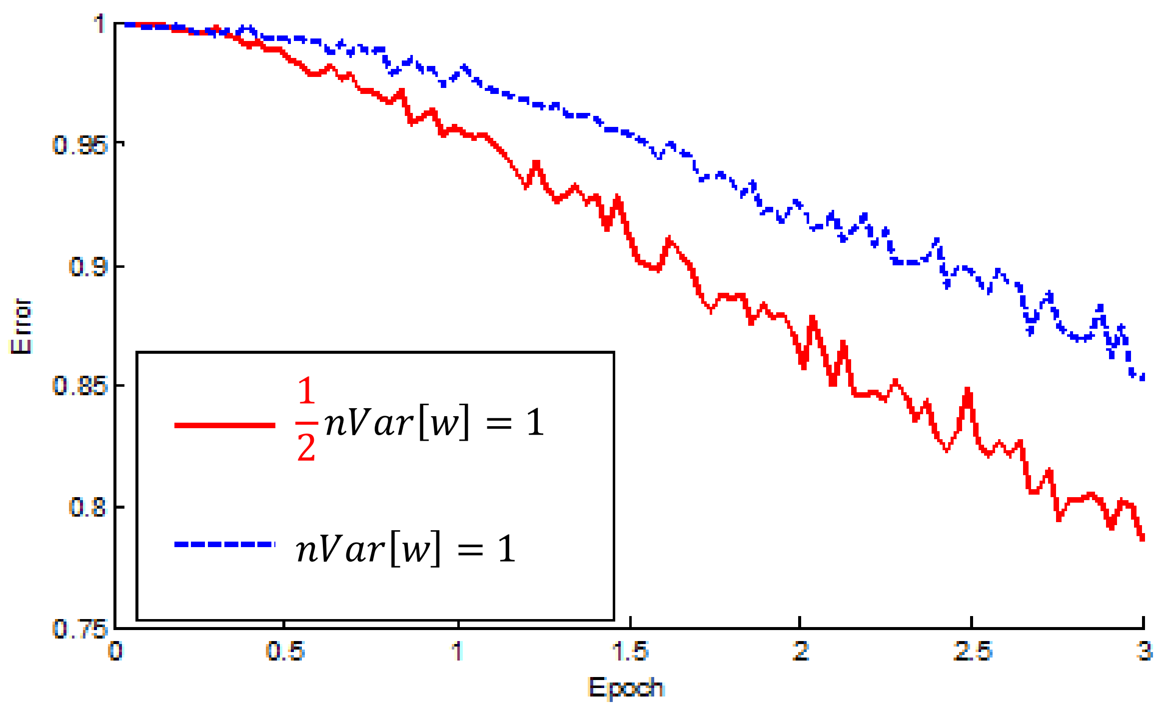

30-layer ReLU net:
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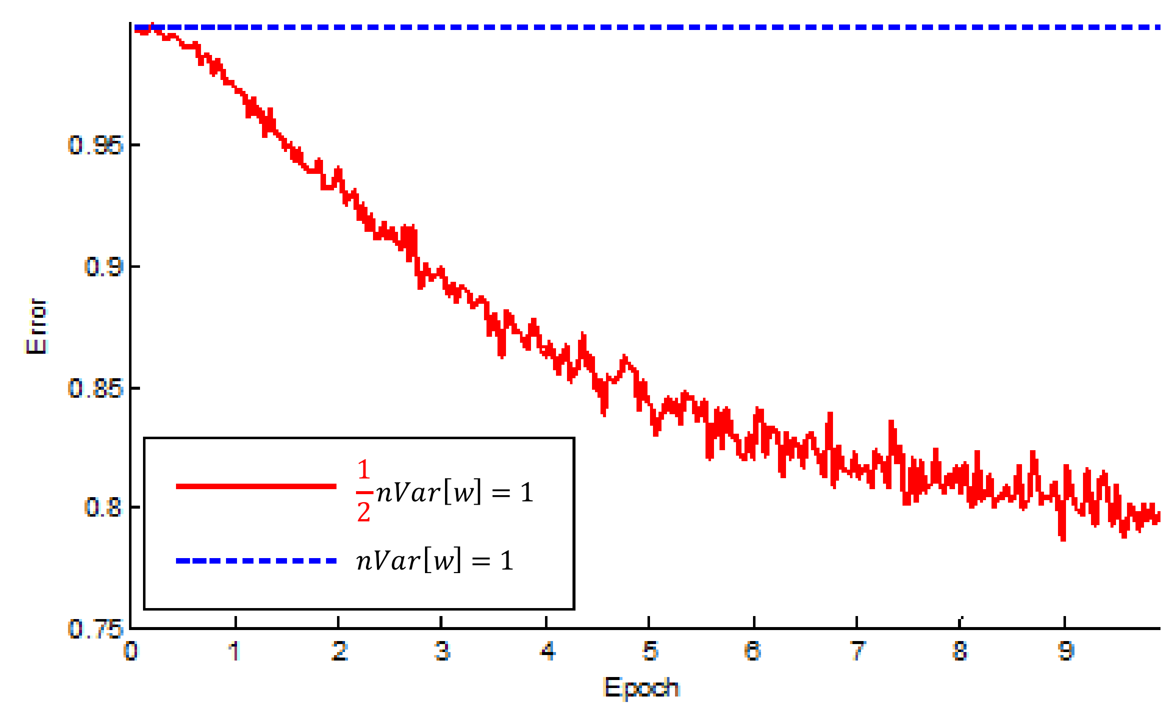

*Figures show the beginning of training

Kaiming He, Xiangyu Zhang, Shaoqing Ren, & Jian Sun. "Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification". ICCV 2015.

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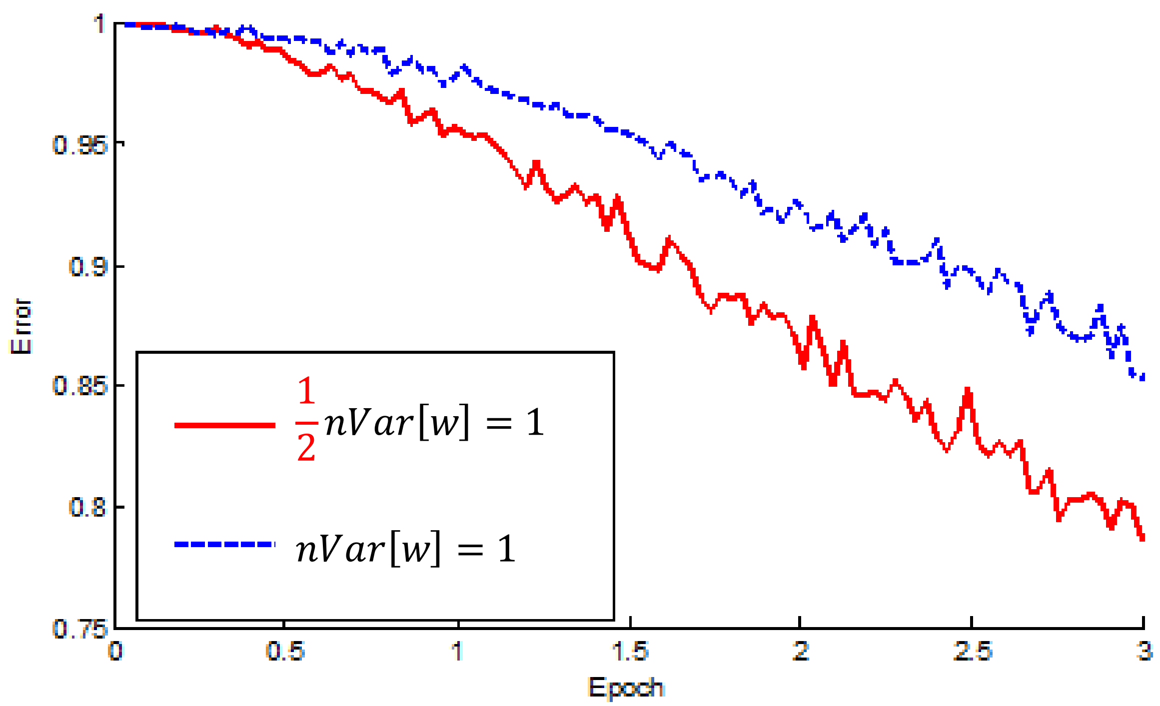

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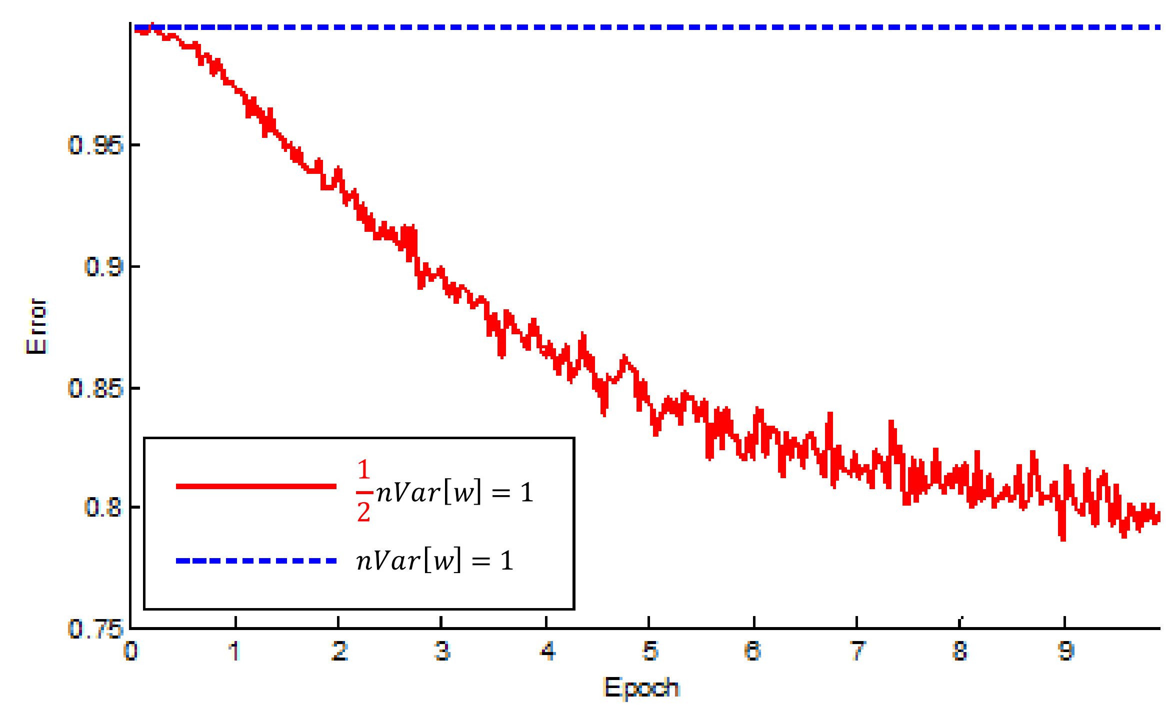

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Ultimately, coming up with good initializations is hard, worthy of deeper investigation

2 What about the step-size η, aka “learning rate”?

2. Step size tuning

Decaying

Adaptive

Architecture Sensitive

Others!

Often the most pesky parameter; tuning well can have big impact

NN toolkits use so-called "step-size Schedulers"

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A Second look at Exponential and Cosine Step Sizes: Simplicity, Convergence, and Performance

Xiaoyu Li, Zhenxun Zhuang, Francesco Orabona

Layerwise Adaptive Rate Scaling: popular for large batch training

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Algorithm 1 LARS

Input: $x_1 \in \mathbb{R}^d$, learning rate $\{\eta_t\}_{t=1}^T$, parameter $0 < \beta_1 < 1$, scaling function ϕ, $\epsilon > 0$

Set $m_0 = 0$

for $t = 1$ **to** T **do**

  Draw b samples S_t from $\mathbb{P}$

  Compute $g_t = \frac{1}{|\mathcal{S}_t|} \sum_{s_t \in \mathcal{S}_t} \nabla \ell(x_t, s_t)$

  $m_t = \beta_1 m_{t-1} + (1 - \beta_1)(g_t + \lambda x_t)$

  $x_{t+1}^{(i)} = x_t^{(i)} - \eta_t \frac{\phi(\|x_t^{(i)}\|)}{\|m_t^{(i)}\|} m_t^{(i)}$ for all $i \in [h]$

end for

Layerwise Adaptive Rate Scaling: popular for large batch training

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3 How to compute a stochastic gradient?

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w_{ij} 1≤ i ≤ m (hidden units)
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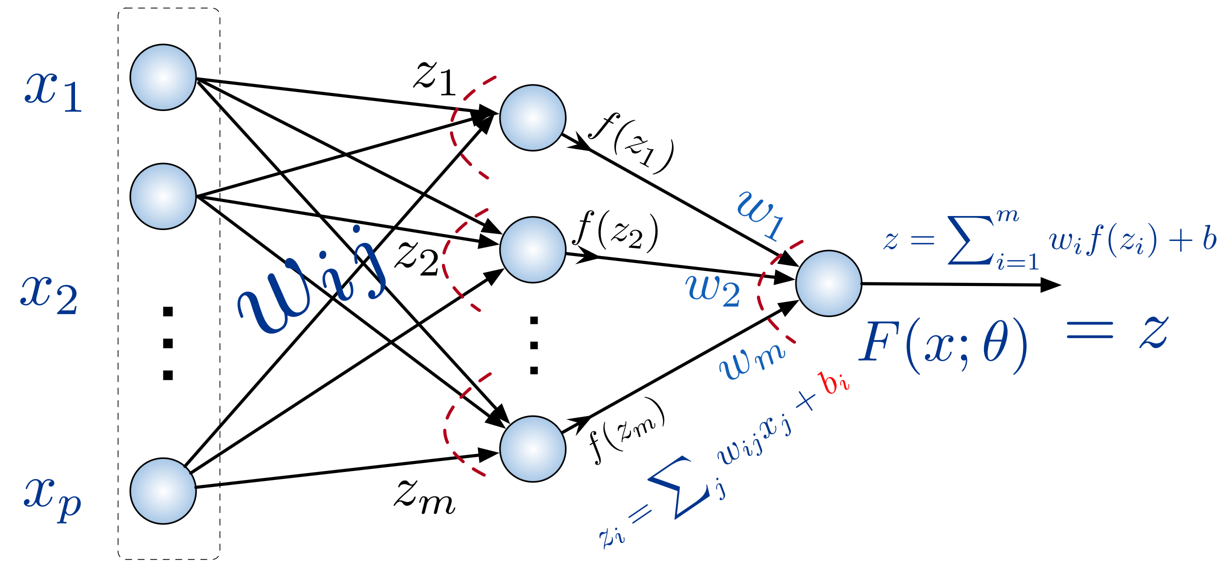

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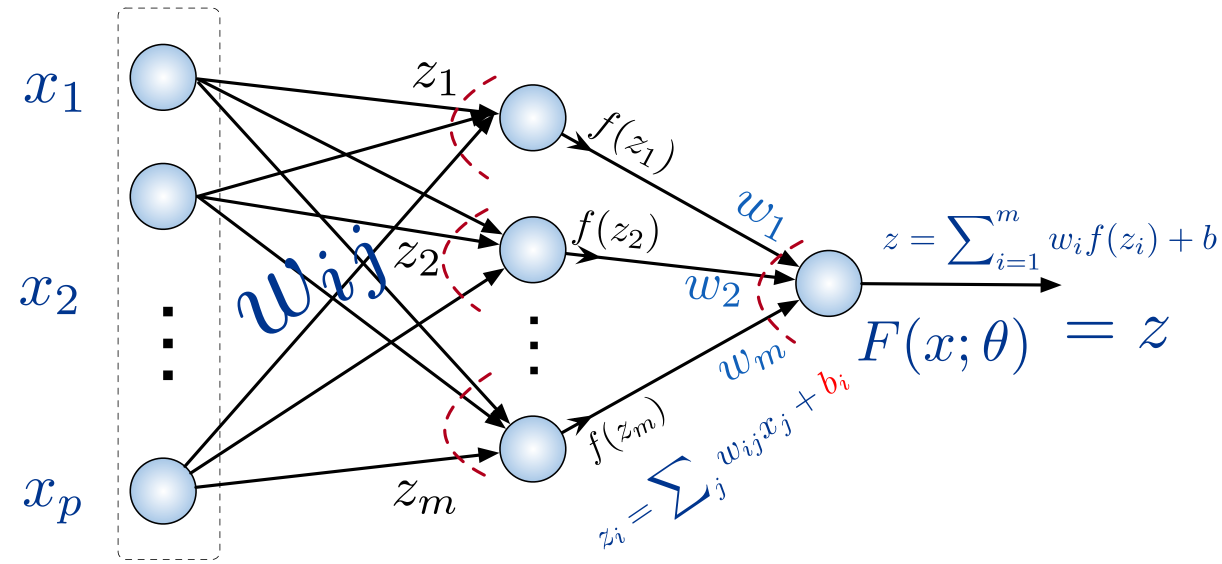

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$$z = \sum_{i=1}^{m} w_i f(z_i) + b$$ input to output unit

$$f(z) = F(x;\theta) = z$$ network output

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Aim: compute $\partial \ell / \partial \theta$

Computing gradients: backpropagation

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Chain-rule of calculus

$$\frac{\partial \ell(y,z)}{\partial w_{ij}} = \left[\frac{\partial z_i}{\partial w_{ij}}\right]\left[\frac{\partial f(z_i)}{\partial z_i}\right]\left[\frac{\partial z}{\partial f(z_i)}\right]\frac{\partial \ell}{\partial z}$$

$$= [x_j][\![z_i > 0]\!][w_i]\begin{bmatrix} -y, & \text{if } \ell(y,z) > 0, \\ 0, & \text{otherwise.} \end{bmatrix}$$

Backpropagation

Challenge: How to apply the chain rule in a deep network?

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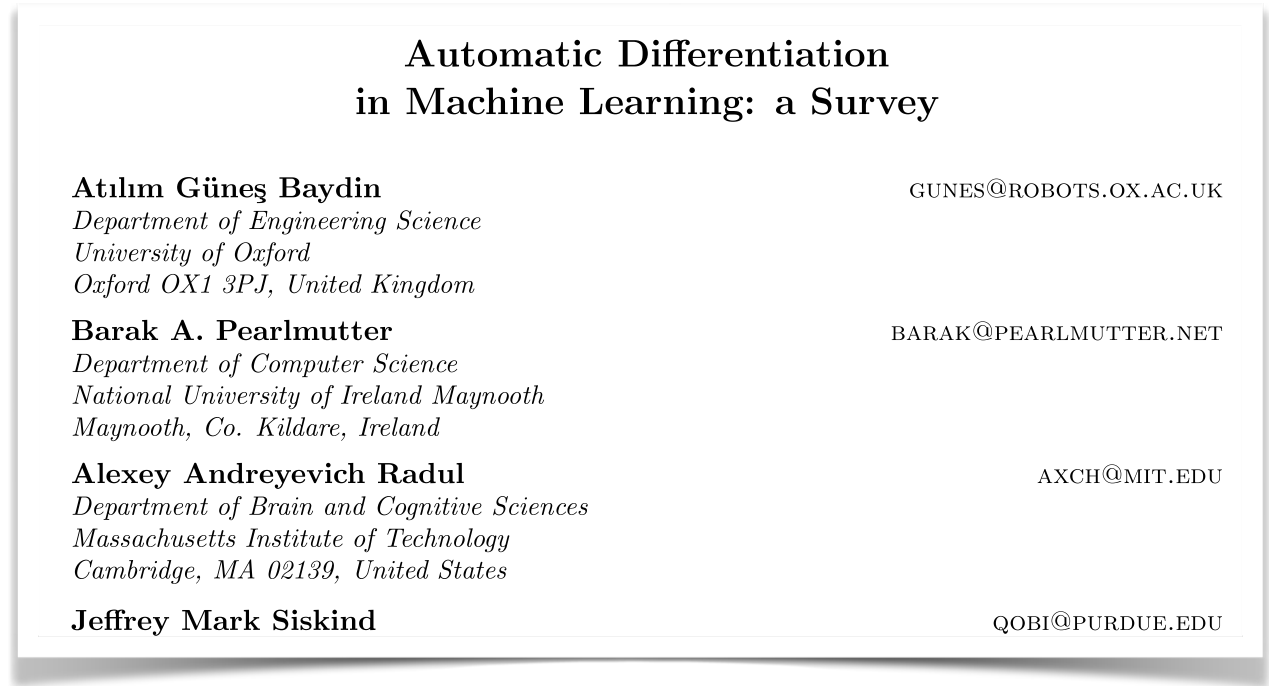
Key insight: Trade space for time (dynamic programming).

Thus, keep track of how a change to the input of one layer impacts its output, and **use extra storage to save this** (*change=derivative*).

Automatic differentiation

Forward mode AD
Backward mode AD
(Backprop a special case)


Automatic Differentiation
in Machine Learning: a Survey

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Department of Brain and Cognitive Sciences
Massachusetts Institute of Technology
Cambridge, MA 02139, United States

Jeffrey Mark Siskind QOBI@PURDUE.EDU

Optimal Jacobian Accumulation: NP-Complete

All NN toolkits use autodiff libraries

AD: Generate algorithm for efficient evaluation of derivatives

Numerous tutorials and notes online; well-developed area in PL and numerics

4 In reality: BN, momentum,clipping,adaptivity and many other ideas!

Key motivation: unstable gradients

$$\delta^l = \frac{\partial \ell}{\partial z^l} = \text{Diag}[f'(z^l)]W^{l+1}\delta^{l+1}.$$

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- Coping with unstable gradients poses several challenges, and must be dealt with to achieve good results.

Partial remedies for unstable gradients

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- Residual Networks (Resnets)

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$$+ \lambda ||\theta||^2$$

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NN folks call this: "*weight decay*," though to be pedantic, some reserve the term "weight decay" for the part subtracted from weights θ when updating them (e.g., ADAMW optimizer)

Regularizing with Dropout

Motivation

- When fitting to the nitty-gritty of the input, including noise hidden units must rely on each other to co-adapt and have complementary coverage of the data space.
- To hinder fitting to noise we must avoid overdoing co-adaptation

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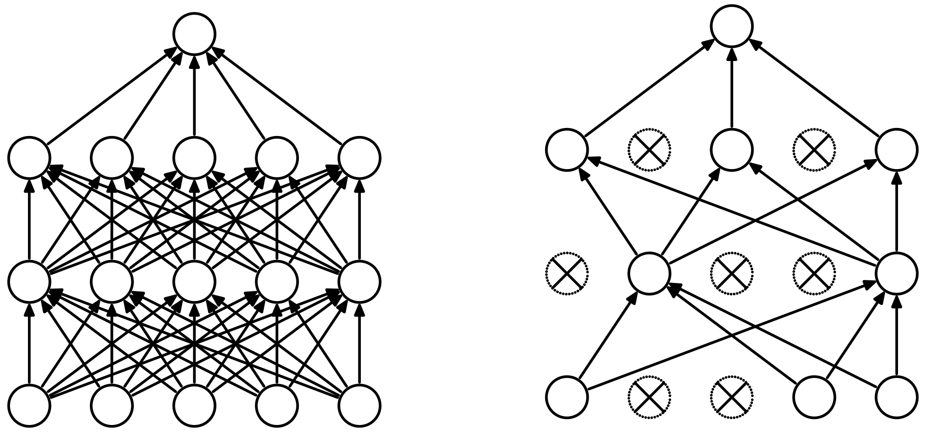
figure from the [dropout] paper



(a) Standard Neural Net

(b) After applying dropout.

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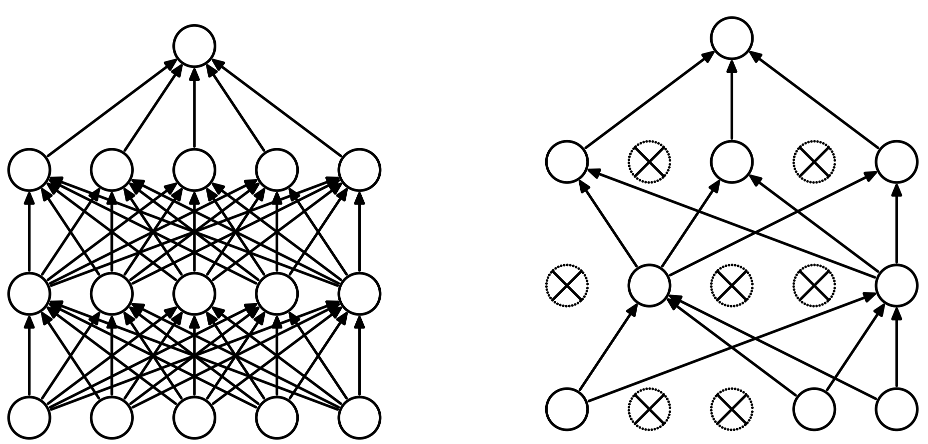

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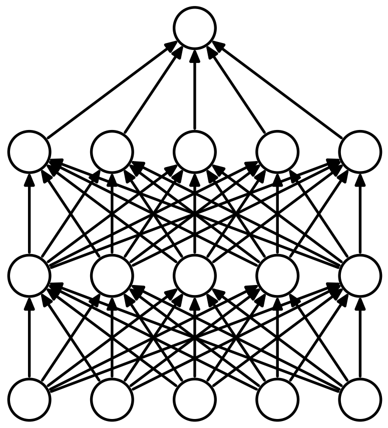
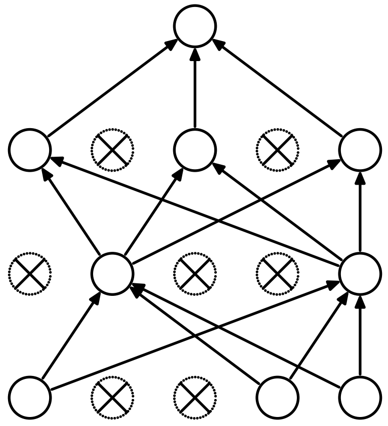


(a) Standard Neural Net



(b) After applying dropout.

Regularizing with Dropout

Motivation

- When fitting to the nitty-gritty of the input, including noise hidden units must rely on each other to co-adapt and have complementary coverage of the data space.
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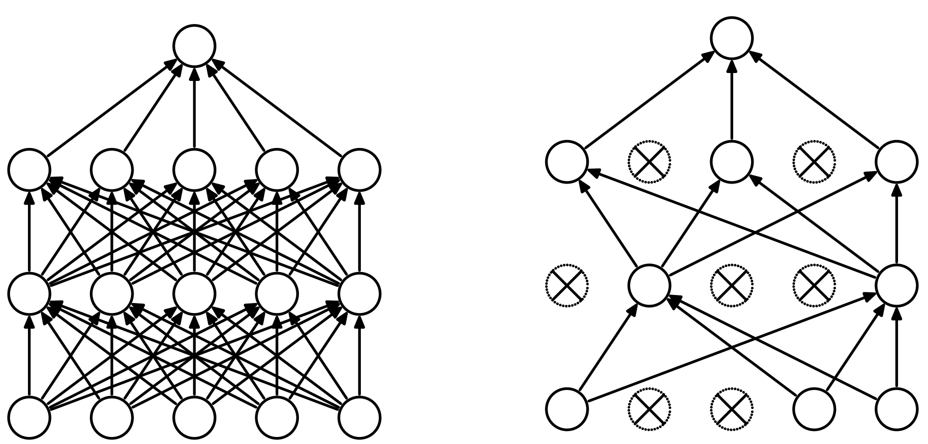

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  - For units turned off for that round, input weights and activations **not** updated; unit effectively dropped out for that particular training sample. This additional stochasticity helps in regularization. **Explore:** other ways of adding stochasticity to NN training

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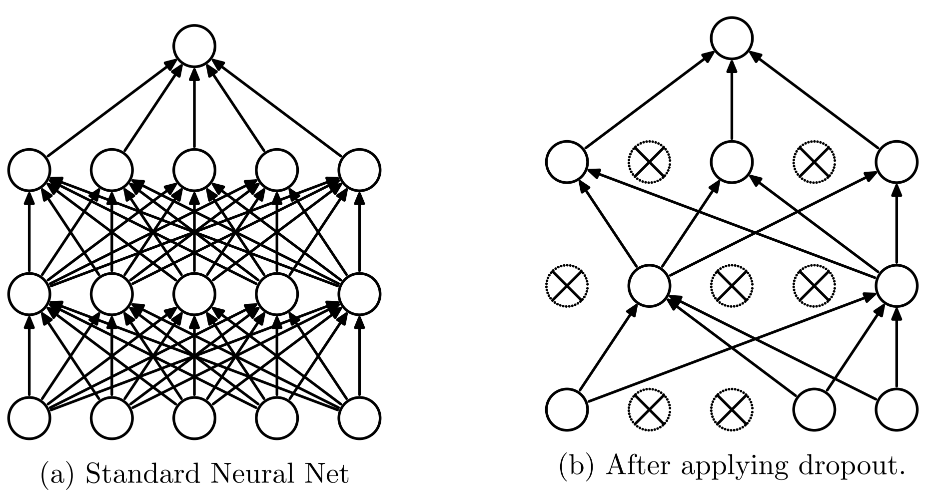

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BN transform applied to activation *x* over a mini-batch

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1\ldots m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

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figure: [Ioffe, Szegedy, 2015]

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Exercise: Derive backprop rules to figure out how to update scale γ and shift β

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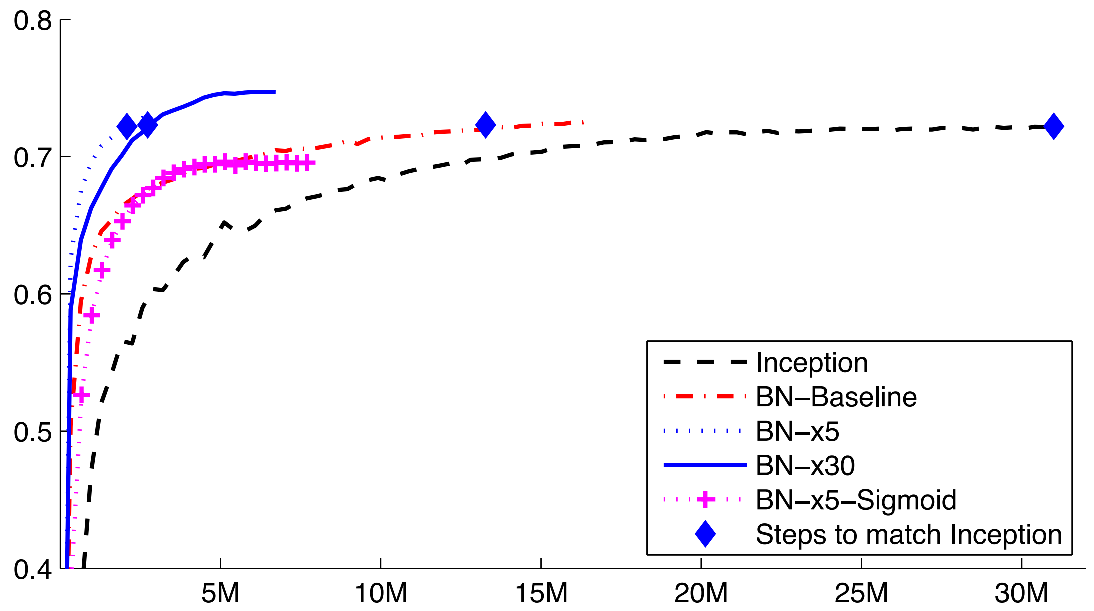

Figure 2: *Single crop validation accuracy of Inception and its batch-normalized variants, vs. the number of training steps.*

(several other speedups enabled, and used for this plot)

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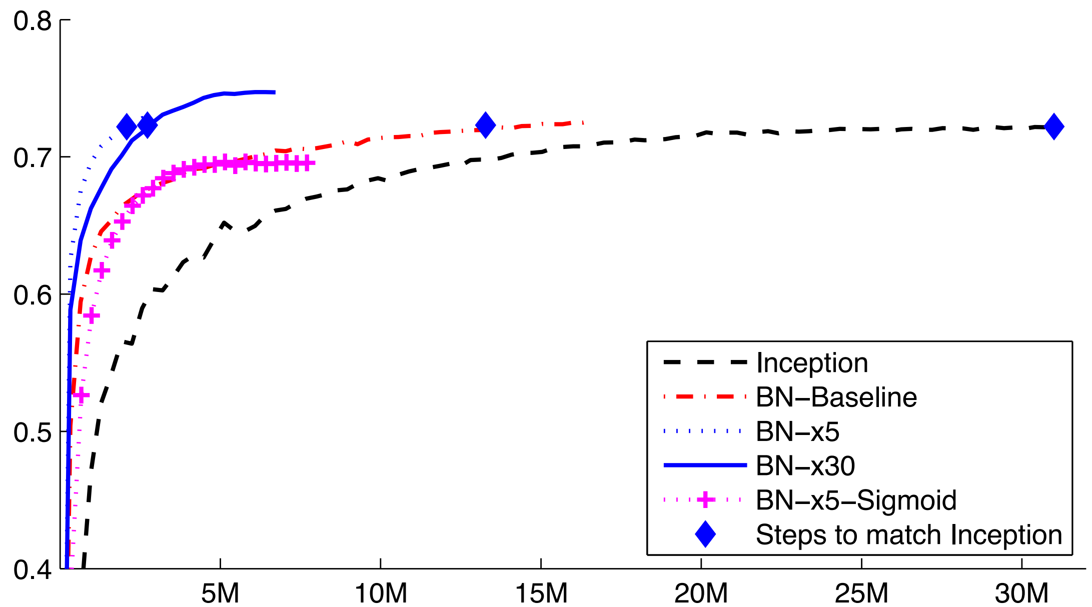
Batch Normalization

- ✓ BN layer can be added to many networks (e.g., CNNs, Resnets, etc.)
  - ➡ *Current Challenge*: BN for RNNs; also, is BN truly necessary?
- ✓ BN enables higher learning rates: backprop through a BN layer is unaffected by the scale of its parameters, BN(Wx)=BN((aW)x)
- ✓ BN has a regularizing effect (Dropout can even be dropped out)
- ✓ **Challenge:** Formally understand and explain BN



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Residual Networks (Resnets)

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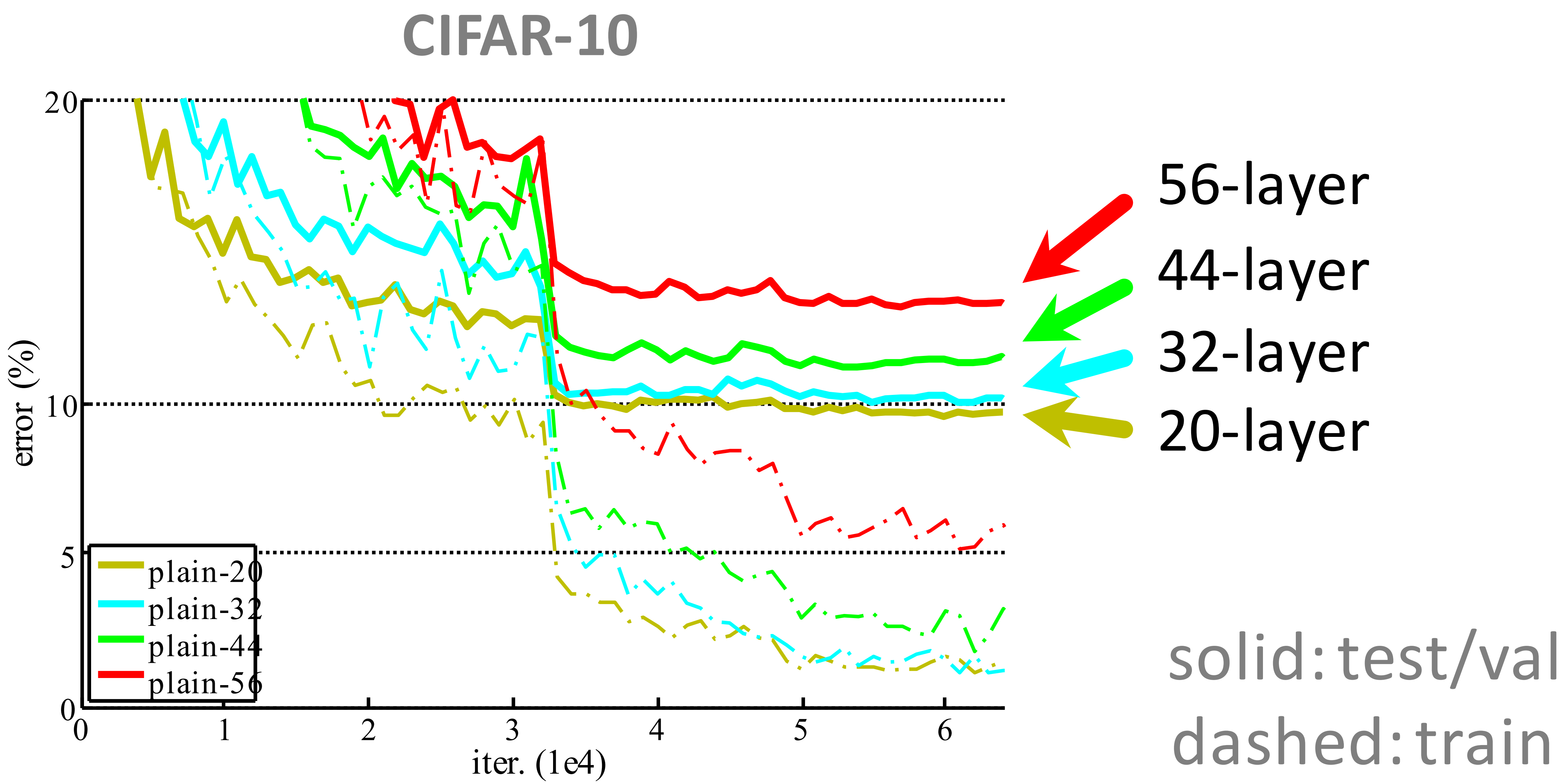
$$x \mapsto h_L \circ h_{L-1} \circ \cdots \circ h_1(x)$$

$$h_i(z) := z + \sigma(W_i z + b_i)$$

Id + σ(.)

Note: Without the Identity map (Id), we are back to the usual model

Why resnets?



CIFAR-10
20
10
5
0
error (%)
0
1
2
3
4
5
6
iter. (1e4)
plain-20
plain-32
plain-44
plain-56
56-layer
44-layer
32-layer
20-layer
solid: test/val
dashed: train

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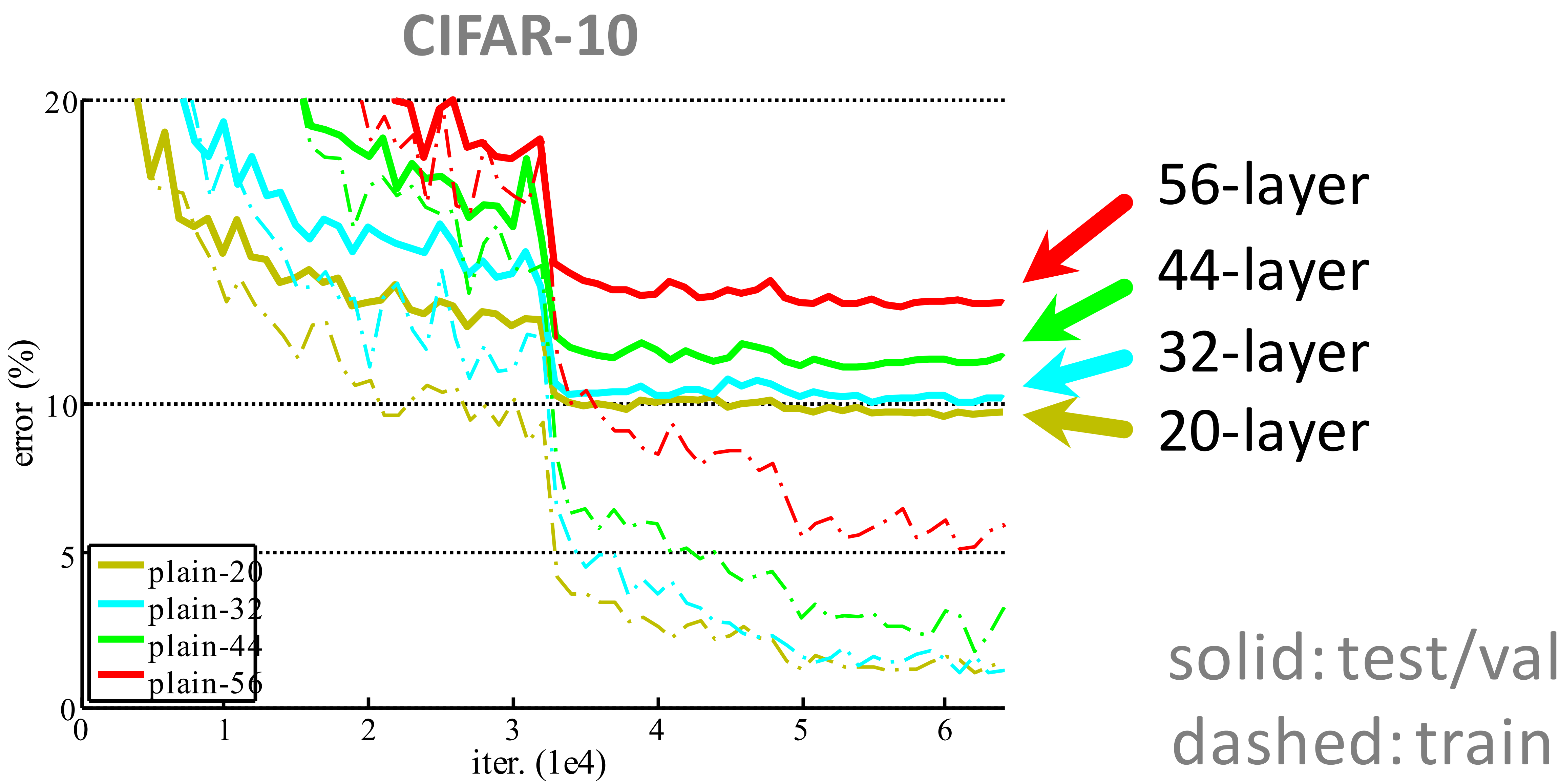
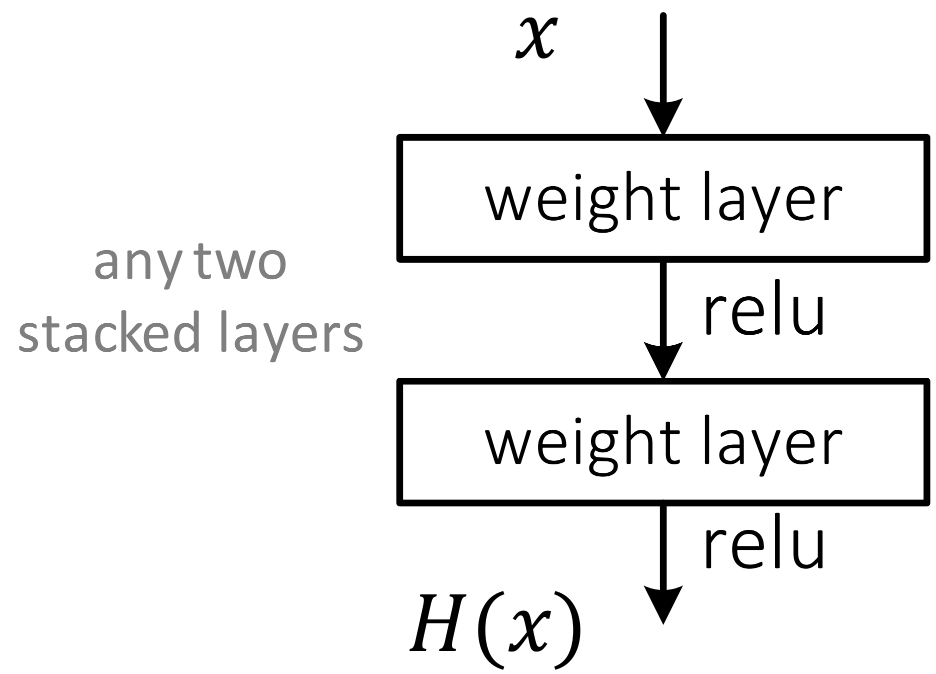


Making network deeper does not necessarily work better

Limits on what initialization and batch normalization give us

Key idea: Identity maps



Aim: Learn map H(x).
Approach: Hope the deep net fits H(x)

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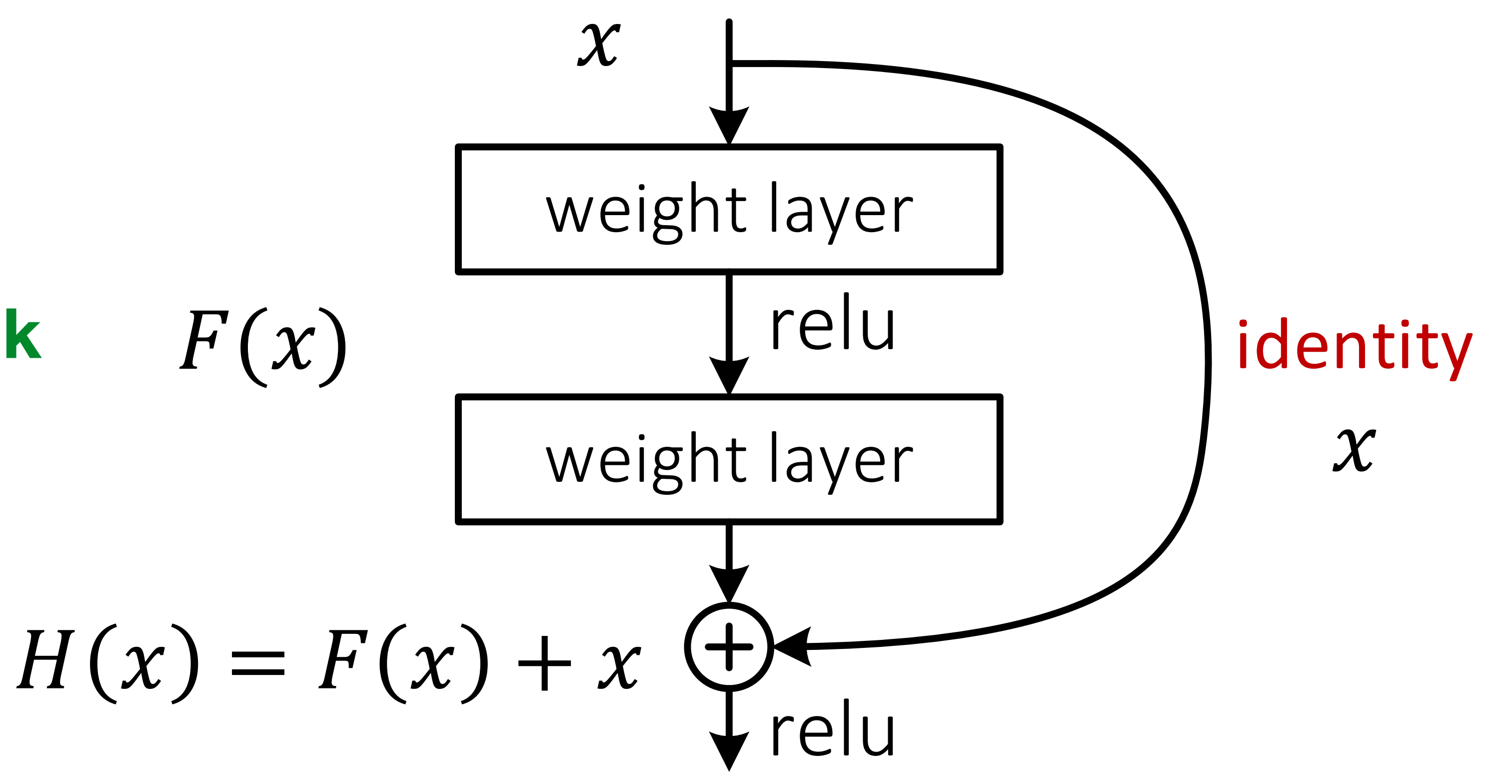
A residual block



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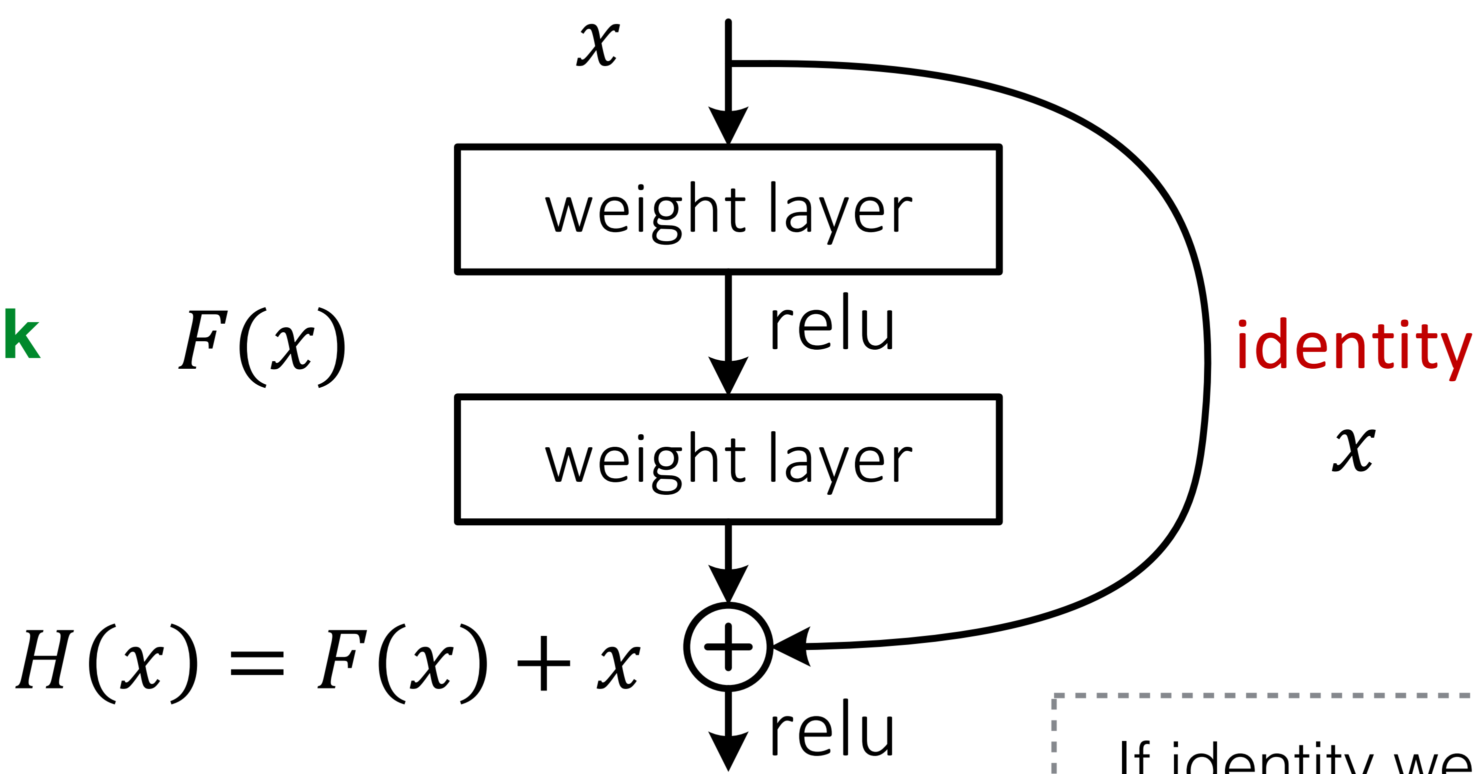

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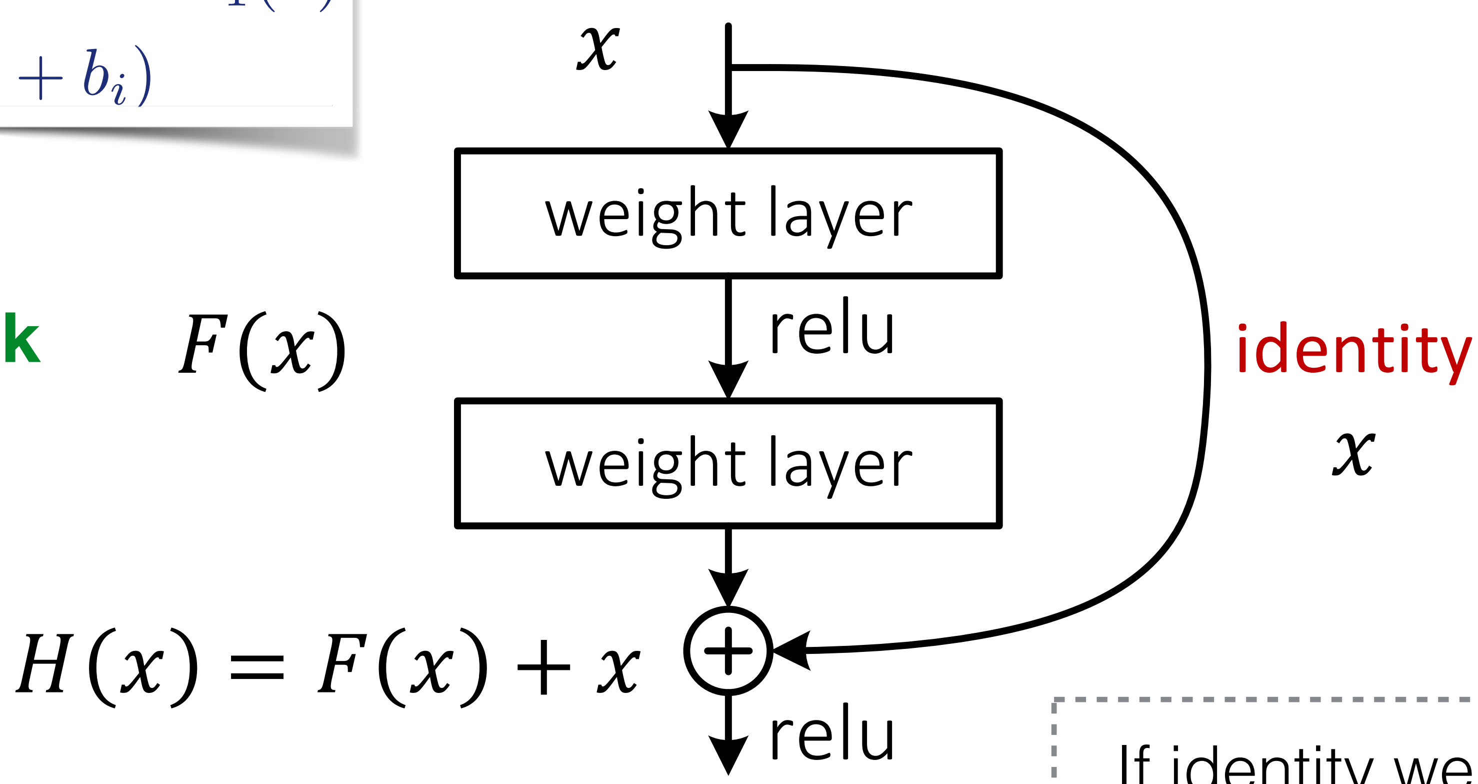

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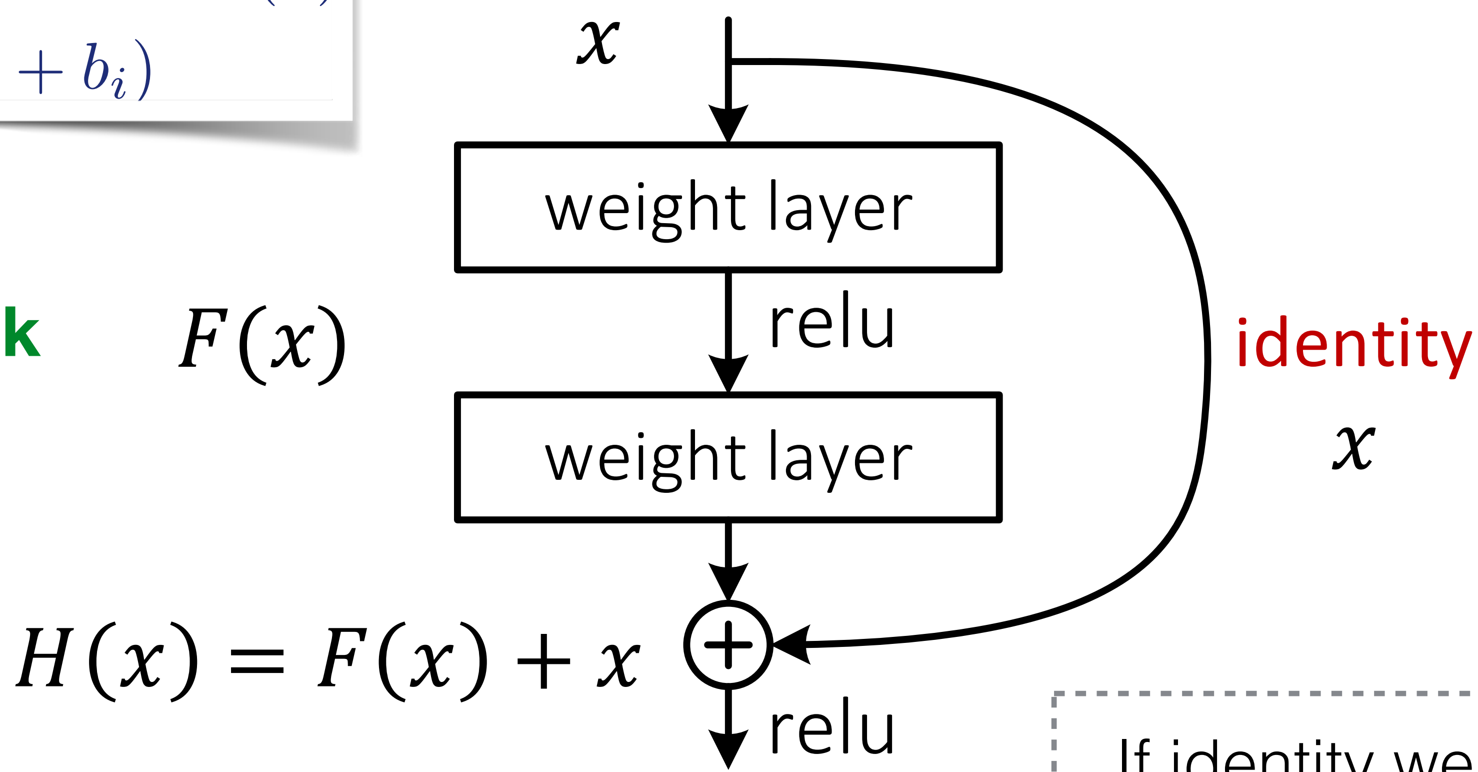

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Explore: Try residual wrt other distinguished (i.e., not Id) mappings

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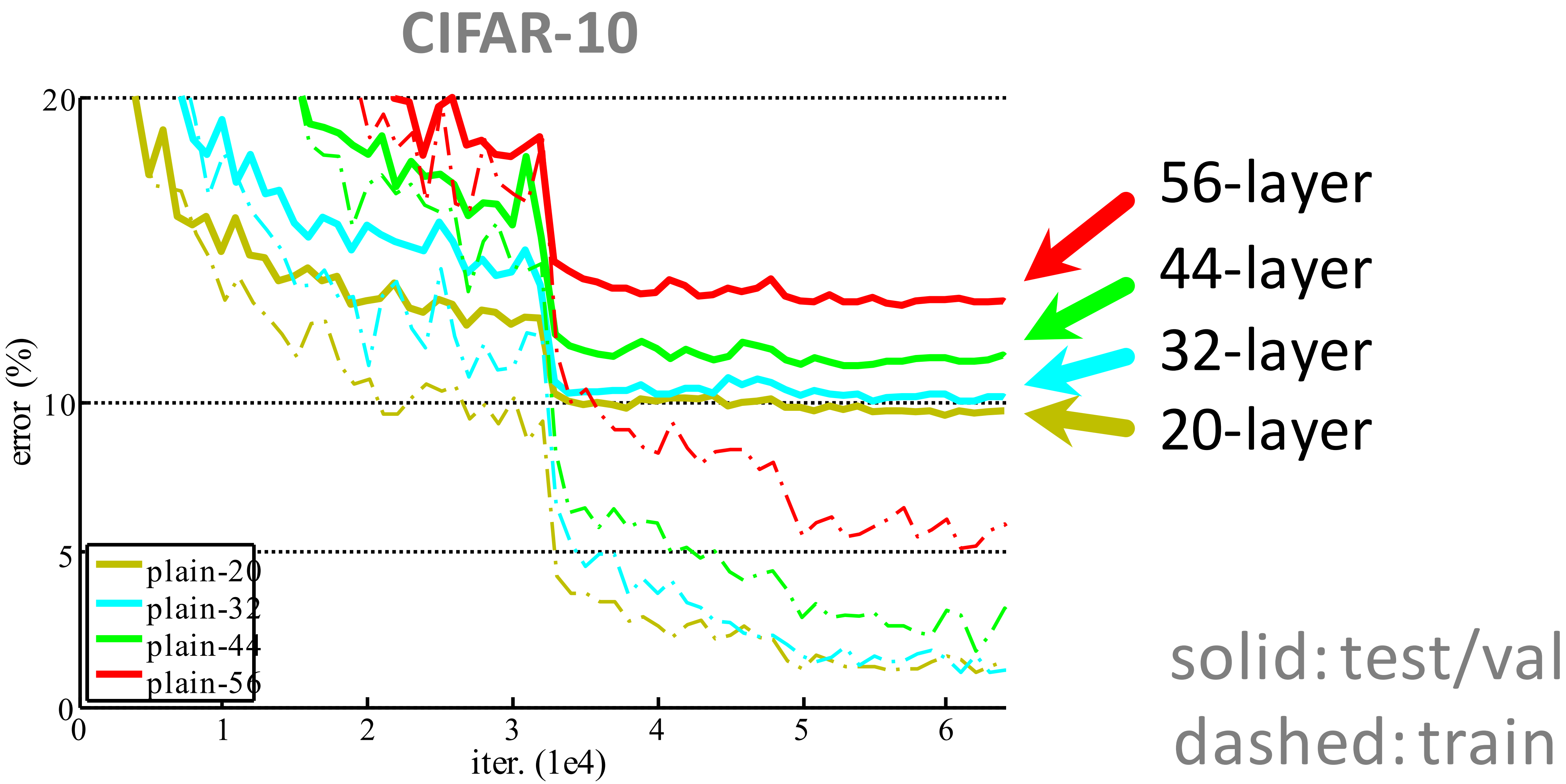

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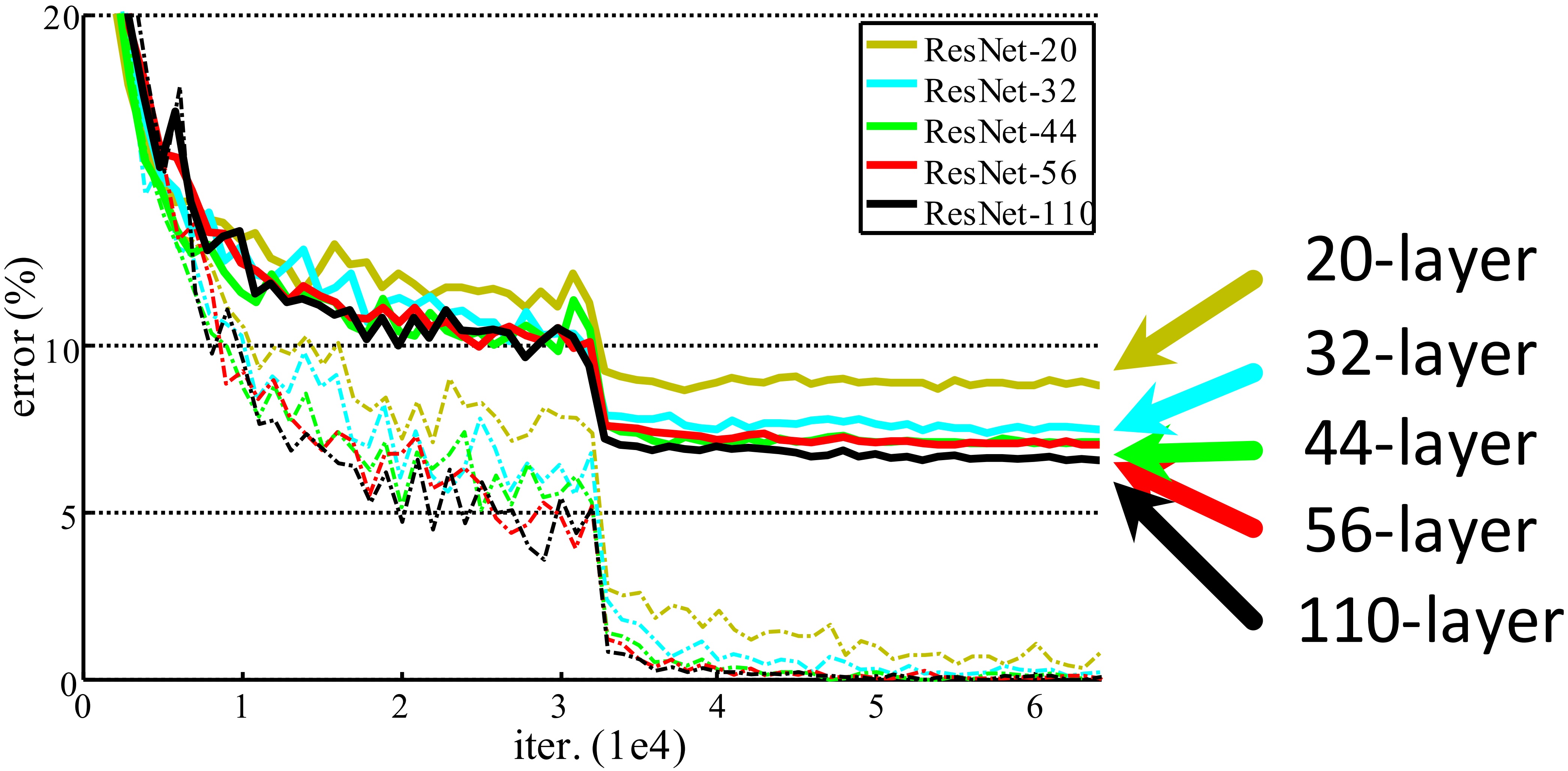
CIFAR-10 ResNets



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- *Allen-Zhu, Li, 2019*. "What can ResNet learn efficiently, Going beyond Kernels?"