Momentum in Stochastic Gradient Descent and Neural Architecture Design

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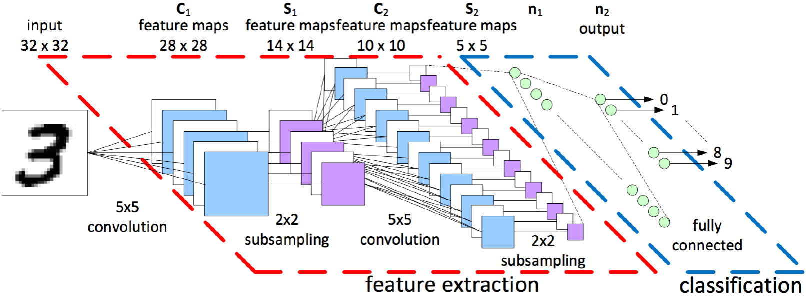
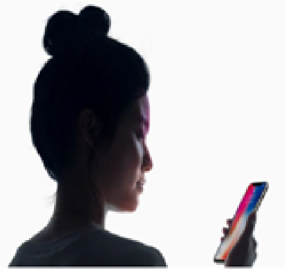
Deep Learning (DL)



DL = Big Data + Deep Nets + SGD + HPC

Deep Learning: Revolution in Technology

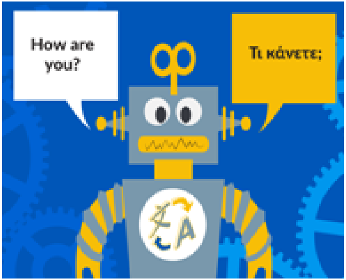
Face ID



Autonomous Cars

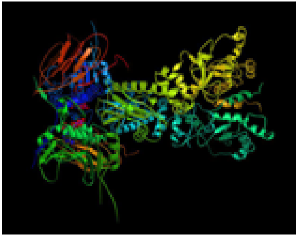
Alpha Go

Machine Translation

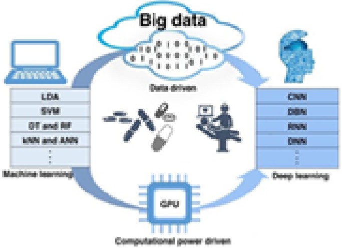


Deep Learning: Revolution in Science

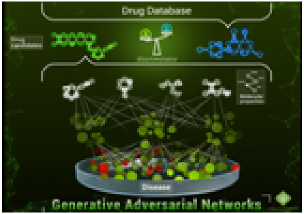
Protein Structure Prediction



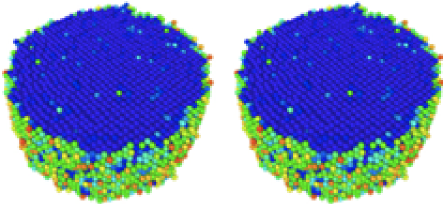
Drug Discovery



Molecular Generation



Material Design



Momentum in SGD

Accelerate convergence

Better generalizable models

Momentum in Deep Nets Design

Principled approach

Easier to train & Better generalizability

Momentum in Optimization

Machine Learning – Empirical Risk Minimization (ERM)

Consider training a machine learning model:

$$y = g(\mathbf{x}, \mathbf{w}), \mathbf{w} \in \mathbb{R}^d,$$

which is parameterized by $\mathbf{w}$, $(\mathbf{x}, y)$ is an input data-predicted label pair.

$\mathbf{w}$ is usually learned by solving the following ERM problem:

$$\min_{\mathbf{w}} f(\mathbf{w}) := \frac{1}{N}\sum_{i=1}^{N} f_i(\mathbf{w}) := \frac{1}{N}\sum_{i=1}^{N} \mathcal{L}(g(\mathbf{x}_i, \mathbf{w}), y_i),$$

where $\mathcal{L}$ is the loss between the predicted label $\hat{y}_i$ and the ground-truth label y_i.

For classification, typically we have:

$$\mathcal{L}(\hat{y}_i, y_i) = -\sum_{j=1}^{M} y_i^j \log(p_i^j),$$

where p_i^j is the predicted probability that y_i is belong to y_i^j's class.

$f(\mathbf{w})$ can be highly nonconvex, and $d \sim 10^{10}$, $N \sim 10^9$.

Convex Optimization – Gradient Descent

Suppose $f(\mathbf{w})$ is convex and L-smooth. Start from $\mathbf{w_0}$, and perform:

$$\mathbf{w}_k = \mathbf{w}_{k-1} - s\nabla f(\mathbf{w}_{k-1}), \text{ and } s = 1/L.$$

Gradient descent has a convergence rate $O(1/k)$ for convex smooth functions.

Consider

$$\min_{\mathbf{w}} f(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T\mathbf{L}\mathbf{w} - \mathbf{w}^T\mathbf{b},$$

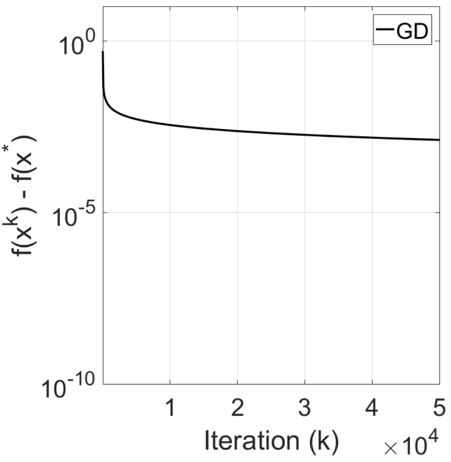
where

$$\mathbf{L} = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & 0 & \cdots & 0 & -1 & 2 \end{pmatrix}_{1000\times 1000},$$

and $\mathbf{b}$ is a 1000-dim vector whose first entry is 1 and all the other entries are 0.

A. Cauchy, 1847

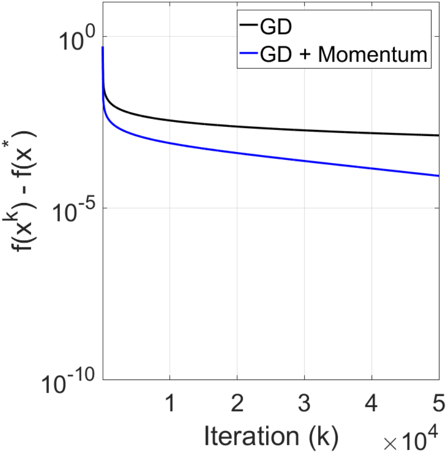
Convex Optimization – Gradient Descent



Convex Optimization – Gradient Descent + Momentum

$$\mathbf{v}_k = \mathbf{w}_{k-1} - s\nabla f(\mathbf{w}_{k-1}),$$
$$\mathbf{w}_k = \mathbf{v}_k + \mu(\mathbf{v}_k - \mathbf{v}_{k-1}).$$

$O(1/k)$ convergence rate!



Heavy Ball

$$\mathbf{w}_k = \mathbf{w}_{k-1} - s\nabla f(\mathbf{w}_{k-1}) + \mu(\mathbf{w}_{k-1} - \mathbf{w}_{k-2}),$$

$O(1/k)$ convergence rate!

B. Polyak, 1964

Why momentum works

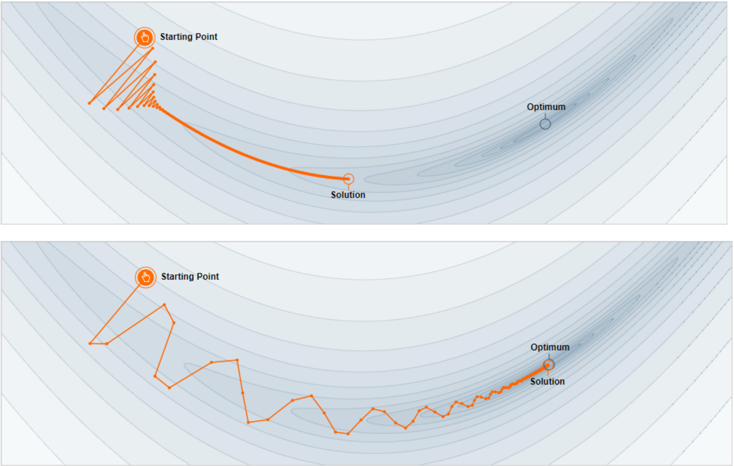


Figure: Top: no momentum; Bottom: with momentum.

G. Goh, Why momentum really works. Distill, 2017

Other Variants (Look-ahead)

Let $\mathbf{u}_k := \mathbf{v}_k - \mathbf{v}_{k-1}$ and $\mathbf{g}_k := \nabla f(\mathbf{v}_{k-1} + s\mathbf{u}_{k-1})$.

Sutskever et al. 2013

$$\begin{cases} \mathbf{v}_k = \mu \mathbf{v}_{k-1} + s\mathbf{g}_k, \\ \mathbf{w}_k = \mathbf{w}_{k-1} - \mathbf{v}_k. \end{cases}$$

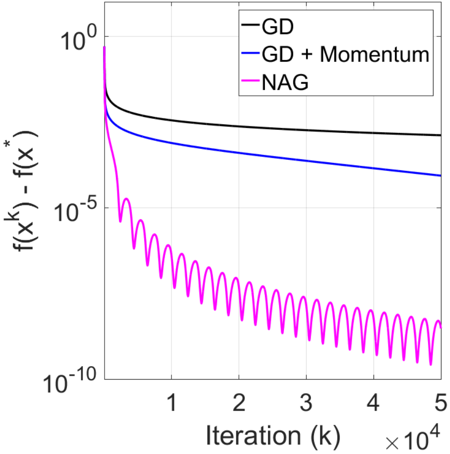
PyTorch

$$\begin{cases} \mathbf{v}_k = \mu \mathbf{v}_{k-1} + \mathbf{g}_k, \\ \mathbf{w}_k = \mathbf{w}_{k-1} - s\mathbf{v}_k. \end{cases}$$

Convex Optimization – Nesterov Accelerated Gradient (NAG)

$$\mathbf{v}_k = \mathbf{w}_{k-1} - s\nabla f(\mathbf{w}_{k-1}),$$
$$\mathbf{w}_k = \mathbf{v}_k + \frac{k-1}{k+2}(\mathbf{v}_k - \mathbf{v}_{k-1}).$$

$O(1/k^2)$ convergence rate!



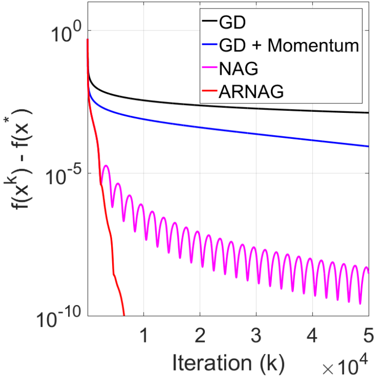
Convex Optimization – Adaptive Restart NAG (ARNAG)

$$\mathbf{v}_k = \mathbf{w}_{k-1} - s\nabla f(\mathbf{w}_{k-1}),$$

$$\mathbf{w}_k = \mathbf{v}_k + \frac{t-1}{t+2}(\mathbf{v}_k - \mathbf{v}_{k-1}),\ t \text{ increase by1 if objective decay, else } t = 1.$$

$O(e^{-\alpha k})$ convergence rate with an extra sharpness assumption!

Sharpness: $\frac{\mu}{r} d(x, X^*)^r < f(x) - f^*, \quad \mu > 0, r > 1.$



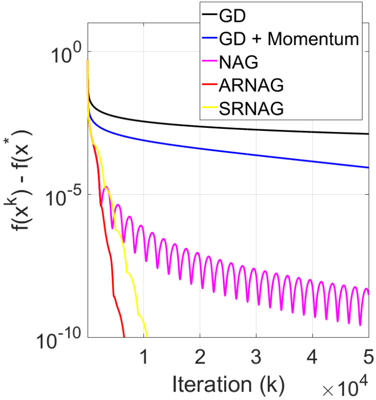
V. Roulet et al. NIPS 2017

Convex Optimization – Scheduled Restart NAG (SRNAG)

$$\mathbf{v}_k = \mathbf{w}_{k-1} - s\nabla f(\mathbf{w}_{k-1}),$$

$$\mathbf{w}_k = \mathbf{v}_k + \frac{t-1}{t+2}(\mathbf{v}_k - \mathbf{v}_{k-1}),\ t \text{ increase by1 within some iterations, else } t = 1.$$

$O(e^{-\beta k})$ convergence rate with an extra sharpness assumption!



V. Roulet et al. NIPS 2017

What If We Do Not Have Exact Gradient?

In ERM,

$$\min_{\mathbf{w}} f(\mathbf{w}) := \frac{1}{N}\sum_{i=1}^{N} f_i(\mathbf{w}) := \frac{1}{N}\sum_{i=1}^{N} \mathcal{L}(g(\mathbf{x}_i, \mathbf{w}), y_i),$$

when $N \gg 1$, compute $\nabla f(\mathbf{w})$ will be very expensive.

Stochastic Gradient:

$$\nabla f(\mathbf{w}) \approx \frac{1}{n}\sum_{i=1}^{n} f_i(\mathbf{w}), \text{ with } [n] \subset [N] \text{ and } n \ll N.$$

Can NAG still accelerate convergence with Stochastic Gradient?

A Motivating Example – Gaussian Noise Corrupted Gradient – Case I

Consider

$$\min_{\mathbf{w}} f(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T\mathbf{L}\mathbf{w} - \mathbf{w}^T\mathbf{b},$$

where

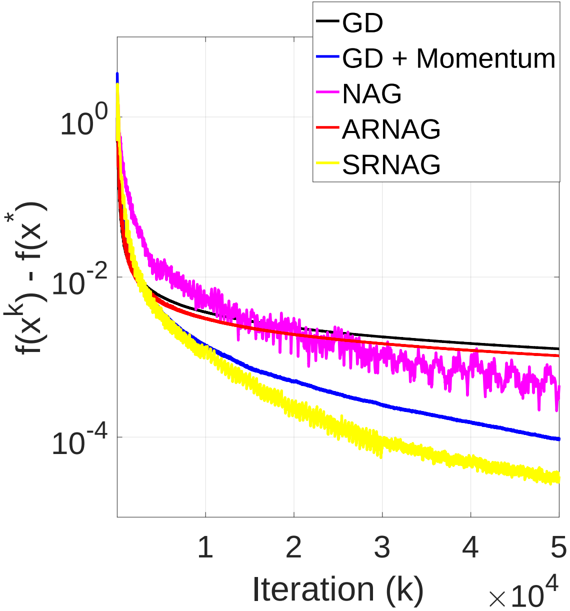
$$\mathbf{L} = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & 0 & \cdots & 0 & -1 & 2 \end{pmatrix}_{1000\times 1000},$$

and $\mathbf{b}$ is a 1000-dim vector whose first entry is 1 and all the other entries are 0.

Gaussian Noise Corrupted Gradient:

$$\nabla f(\mathbf{w}) = \mathbf{L}\mathbf{w} - \mathbf{b} + \mathbf{n}, \quad \mathbf{n} \sim \mathcal{N}(0, (\frac{0.1}{\lfloor k/100 \rfloor + 1})^2).$$

A Motivating Example – Gaussian Noise Corrupted Gradient – Case I



A Motivating Example – Gaussian Noise Corrupted Gradient – Case II

Consider

$$\min_{\mathbf{w}} f(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T\mathbf{L}\mathbf{w} - \mathbf{w}^T\mathbf{b},$$

where

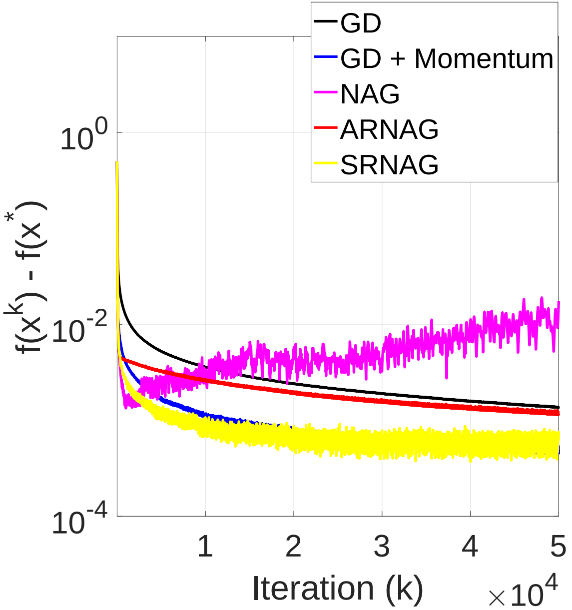
$$\mathbf{L} = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & 0 & \cdots & 0 & -1 & 2 \end{pmatrix}_{1000\times1000},$$

and $\mathbf{b}$ is a 1000-dim vector whose first entry is 1 and all the other entries are 0.

Gaussian Noise Corrupted Gradient:

$$\nabla f(\mathbf{w}) = \mathbf{L}\mathbf{w} - \mathbf{b} + \mathbf{n}, \quad \mathbf{n} \sim \mathcal{N}(0, 0.001^2).$$

A Motivating Example – Gaussian Noise Corrupted Gradient – Case II



A Motivating Example – Logistic Regression – Case III

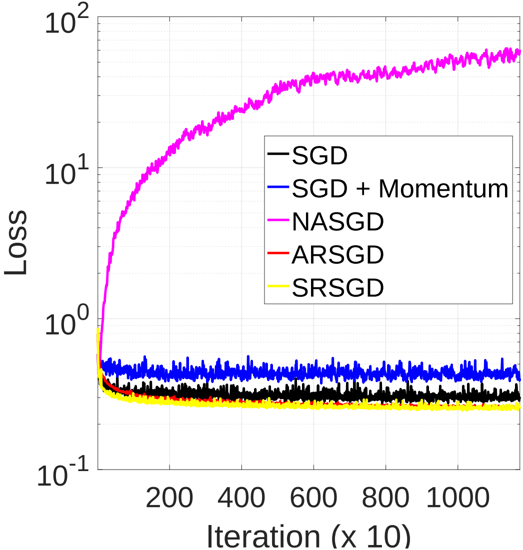


Figure: Training loss of logistic regression for MNIST classification.

Analysis

NAG:

Given a convex function $f : \mathbb{R}^d \to \mathbb{R}$ with smoothness parameter L. Given any point $\mathbf{w} \in \mathbb{R}^d$ an exact first order oracle returns a pair $(f_L(\mathbf{x}), g_L(\mathbf{w})) \in \mathbb{R} \times \mathbb{R}^d$ so that for all $\mathbf{u} \in \mathbb{R}^d$, we have

$$0 \leq f(\mathbf{u}) - (f_L(\mathbf{w}) + \langle g_L(\mathbf{w}), \mathbf{u} - \mathbf{w} \rangle) \leq \frac{L}{2} \|\mathbf{u} - \mathbf{w}\|^2.$$

The first inequality follows from convexity and the second from the smoothness condition.
An inexact oracle returns for any given point $\mathbf{w} \in \mathbb{R}^d$ a pair $(f_{\delta,L}(\mathbf{x}), g_{\delta,L}(\mathbf{w})) \in \mathbb{R} \times \mathbb{R}^d$ so that for all $\mathbf{u} \in \mathbb{R}^d$ we have

$$0 \leq f(\mathbf{u}) - (f_{\delta,L}(\mathbf{w}) + \langle g_{\delta,L}(\mathbf{w}), \mathbf{u} - \mathbf{w} \rangle) \leq \frac{L}{2} \|\mathbf{u} - \mathbf{w}\|^2 + \delta.$$

It has the same picture as before except now there is some δ slack between the linear and parabola approximations.

Theorem Given access to δ-inexact first-order oracle GD spits out a point $\mathbf{w}^k$ after k steps so that

$$f(\mathbf{w}^k) - f(\mathbf{w}^*) \leq O(L/k) + \delta.$$

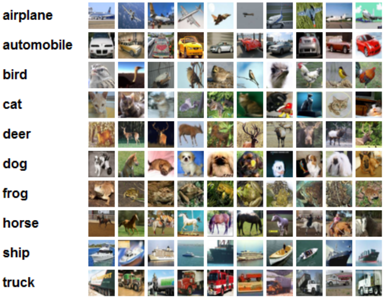
NAG on the other hand gives

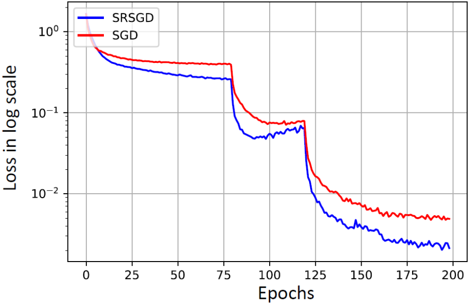
$$f(\mathbf{w}^k) - f(\mathbf{w}^*) \leq O(L/k^2) + O(k\delta).$$

Adaptive Restart NAG: restart too often, degenerates to GD.

O. Devolder, F. Glineur, and Y. Nesterov, First-Order Methods of Smooth Convex Optimization With Inexact Oracle. Math Prog A, 2014.

SRNAG for Deep Learning – ResNet for CIFAR10 and CIFAR100 Classification





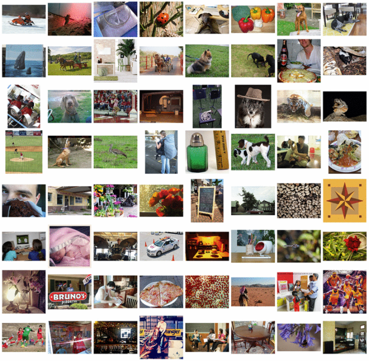
SRNAG for Deep Learning – ResNet for CIFAR10 and CIFAR100 Classification

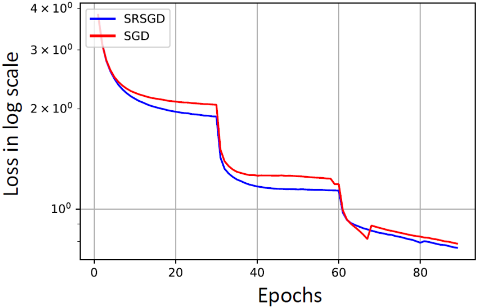
Network	# Params	SGD (baseline)	SRSGD (linear)	SRSGD (exponential)	Improvement(linear/exponential)
PreResNet-110	1.1M	94.75 ± 0.14 (93.63 (He et al., 2016))	95.07 ± 0.13	95.00 ± 0.47	0.32/0.25
PreResNet-290	3.0M	94.95 ± 0.23	95.63 ± 0.15	95.50 ± 0.18	0.68/0.55
PreResNet-470	4.9M	95.08 ± 0.10	95.82 ± 0.09	95.51 ± 0.19	0.74/0.43
PreResNet-650	6.7M	95.13 ± 0.14	96.00 ± 0.07	95.60 ± 0.13	0.87/0.47
PreResNet-830	8.6M	95.00 ± 0.23	95.91 ± 0.10	95.71 ± 0.13	0.91/0.71
PreResNet-1001	10.3M	95.16 ± 0.19 (95.08 (He et al., 2016))	96.13 ± 0.07	95.87 ± 0.10	0.97/0.71

Network	# Params	SGD (baseline)	SRSGD (linear)	SRSGD (exponential)	Improvement(linear/exponential)
PreResNet-110	1.2M	76.25 ± 0.20	76.51 ± 0.23	76.50 ± 0.39	0.26/0.25
PreResNet-290	3.0M	78.22 ± 0.21	78.51 ± 0.27	78.42 ± 0.20	0.29/0.20
PreResNet-470	4.9M	78.57 ± 0.30	79.29 ± 0.32	79.36 ± 0.18	0.72/0.79
PreResNet-650	6.7M	78.73 ± 0.14	79.64 ± 0.25	79.59 ± 0.21	0.91/0.86
PreResNet-830	8.6M	78.81 ± 0.22	79.78 ± 0.23	79.80 ± 0.25	0.97/0.99
PreResNet-1001	10.4M	79.13 ± 0.20 (77.29 (He et al., 2016))	80.25 ± 0.11	80.47 ± 0.19	1.12/1.34

Figure: Top: CIFAR10; Bottom: CIFAR100

SRNAG for Deep Learning – ResNet for ImageNet Classification





ImageNet Classification

Network	# Params	SGD	SRSGD	Improvement
ResNet-50	25.56M	75.83	76.24	0.41
ResNet-101	44.55M	77.6	78.06	0.44
ResNet-152	60.19M	78.10	78.71	0.61
ResNet-200	64.67M	77.82	78.92	1.10

Image Classification

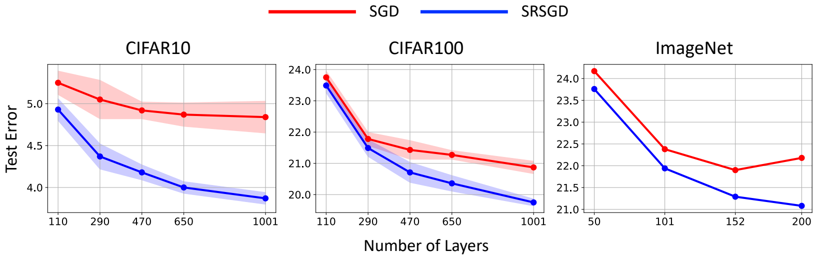


Figure: Error vs. depth of ResNet.

Momentum in Deep Neural Nets

Rethinking Deep Residual Nets (ResNets)

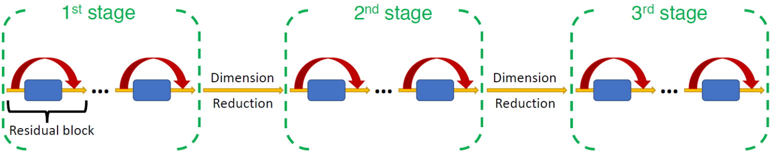
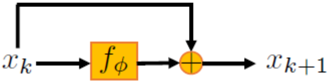


Figure: ResNet

Residual mapping: $x_{k+1} = x_k + f(x_k, w_k)$.

Residual block



How about $x_{k+1} = x_k - \mu f(x_k, w_k)$?

What if

$$y_{k+1} = x_k - \mu f(x_k, w_k),$$

$$x_{k+1} = y_{k+1} + \nu(y_{k+1} - y_k)?$$

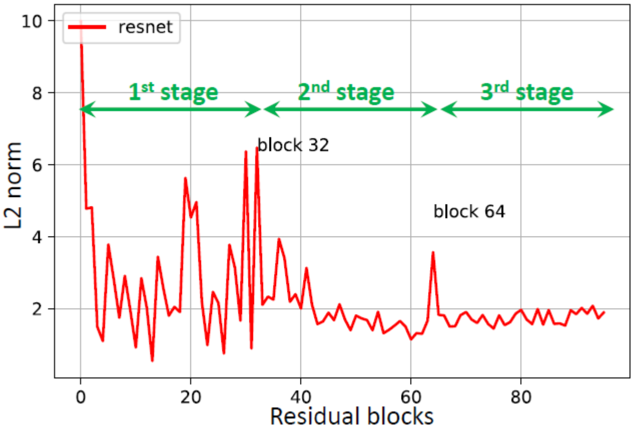
ResNet vs. Gradient Descent

Gradient descent

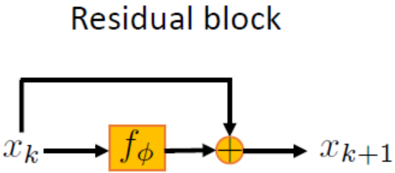
$$x_{k+1} = x_k - \mu \nabla f(x_k),$$

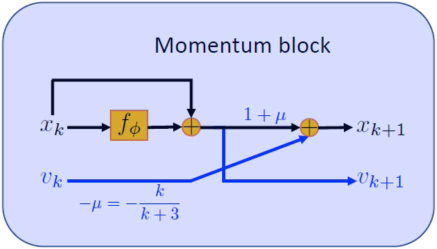
and we have

$$\lim_{k \to \infty} \|\nabla f(x_k)\|_2 = 0.$$

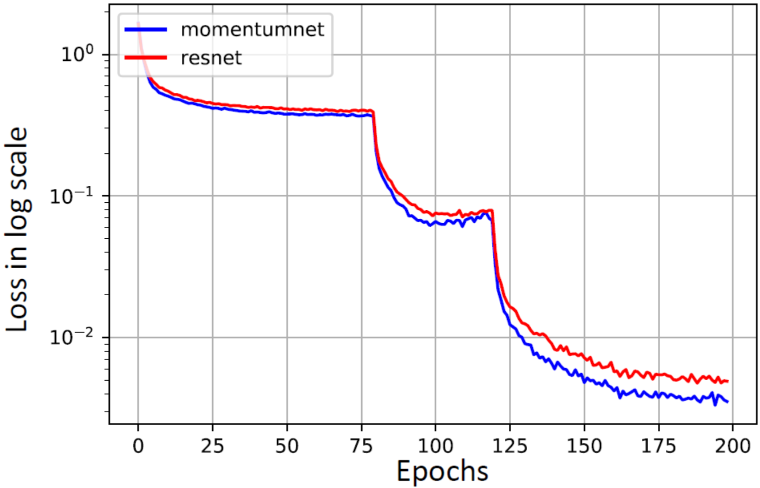


Deep Momentum Nets





Deep Momentum Nets Versus Deep Residual Nets



CIFAR10 Classification

Network	# Params	ResNet (baseline)	MomentumNet (linear)	Improvement(linear/exponential)
PreResNet-110	1.1M	94.75 ± 0.14 (93.63 (He et al., 2016))	94.69 ± 0.12	-0.06
PreResNet-290	3.0M	94.95 ± 0.23	95.09 ± 0.11	0.14
PreResNet-470	4.9M	95.08 ± 0.10	95.09 ± 0.12	0.01
PreResNet-650	6.7M	95.13 ± 0.14	95.21 ± 0.13	0.08
PreResNet-830	8.6M	95.00 ± 0.23	95.31 ± 0.22	0.31
PreResNet-1001	10.3M	95.16 ± 0.19 (95.08 (He et al., 2016))	95.35 ± 0.15	0.19

ODE Models

$$\dot{X} + \nabla f(X) = 0,$$

vs.

$$\ddot{X} + \frac{3}{t}\dot{X} + \nabla f(X) = 0.$$

Su, Boyd, Candes, NIPS, 2014

Future Directions

Optimal restart scheduling in SRSGD.

How to generalize SRSGD to adaptive step size settings.

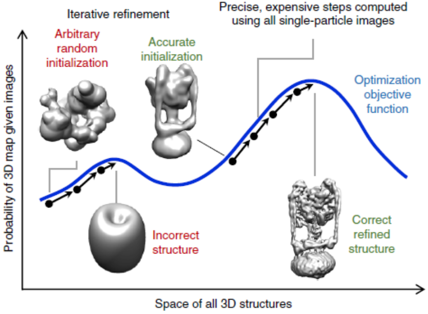
Neural architecture search with momentum units.

Microscopic Imaging (Cryo-EM)

RELION: Bayesian likelihood framework for cryo-EM structure determination:

$$\arg\max_{V_{1,\cdots,K}} \log p(V_{1,\cdots,K}|X_{1,\cdots,N}) =$$
$$\arg\max_{V_{1,\cdots,K}} \sum_{i=1}^{N} \log \sum_{j=1}^{K} \frac{1}{K} \int p(X_i, \phi_i | V_j) d\phi_i + \log p(V_{1,\cdots,K}).$$

The aim of the optimization is to find the 3D structures (V_1 to V_K) that best explain the observed images (X_1 to X_N) by marginalizing over class assignment (j) and the unknown pose variable (ϕ_i) which describes a 3D rotation and a 2D translation for each single-particle image.



Stochastic Gradient Descent!

A. Punjani, J. Rubinstein, D. Fleet, and M. Brubaker, Nature Methods, 2017.

Thank You

I. Scheduled Restart NAG Momentum

- I.1 Accelerate convergence
- I.2 Better generalization accuracy

II. Momentum in Neural Architecture Design

- II.1 Speed-up training
- II.2 Better generalization accuracy
- II.3 Mathematically mechanistic design

References:

1. B. Wang*, T. Nguyen*, A. Bertozzi[#], R. Baraniuk[#], and S. Osher[#], Scheduled Restart Momentum for Accelerated Stochastic Gradient Descent, Submitted, 2020.

2. T. Nguyen*, B. Wang*, A. Bertozzi[#], R. Baraniuk[#], and S. Osher[#], Deep Momentum Networks, Submitted, 2020.