# Optimization for Deep Learning

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24.11.17


# Agenda

# Introduction

- Gradient descent is a way to minimize an objective function $J(\theta)$
  - $\theta \in \mathbb{R}^d$: model parameters
  - $\eta$: learning rate
  - $\nabla_\theta J(\theta)$: gradient of the objective function with regard to the parameters
- Updates parameters **in opposite direction** of gradient
- Update equation: $\theta = \theta - \eta \cdot \nabla_\theta J(\theta)$

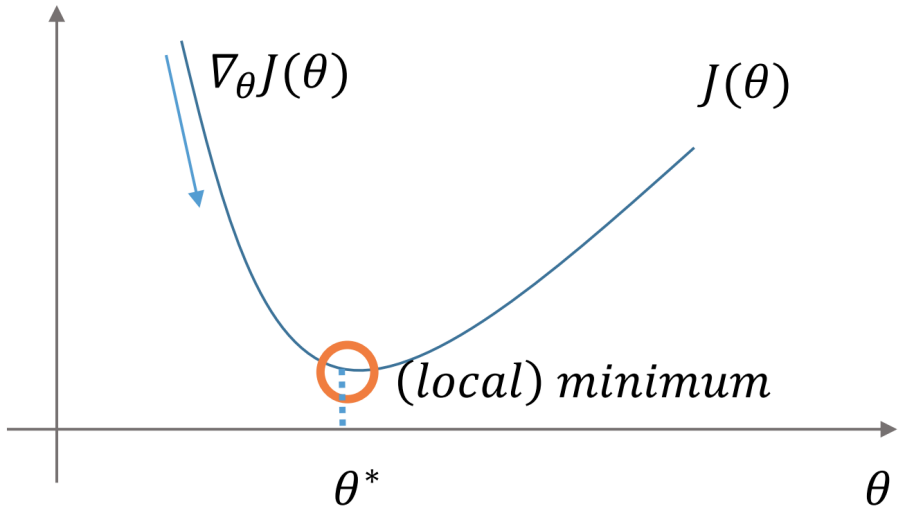



Figure: Optimization with gradient descent

# Gradient descent variants

1. Batch gradient descent
2. Stochastic gradient descent
3. Mini-batch gradient descent

Difference: Amount of data used per update

Notes:

Main difference: the number of inputs used to compute the gradient of the parameters in each step.
- Batch gives the true gradient.
- The gradient with respect to a minibatch is an approximation of the true gradient. The larger the minibatch, the better the approximation.

The number of inputs are collected into an array and computed "at the same time"
The trade-off here is purely about performance (memory/cycles).
Note that we have large number of parameters, for example VGG-16D needs calculate 15 245 800 floats (in the feature maps) for one 224x224 image

# Batch gradient descent

- Computes gradient with the **entire** dataset.
- Update equation: $\theta = \theta - \eta \cdot \nabla_\theta J(\theta)$

```
for i in range(nb_epochs):
  params_grad = evaluate_gradient(
    loss_function, data, params)
  params = params - learning_rate * params_grad
```

Listing 1: Code for batch gradient descent update

- Pros:
  - Guaranteed to converge to **global** minimum for **convex** error surfaces and to a **local** minimum for **non-convex** surfaces.
- Cons:
  - **Very slow**.
  - Intractable for datasets that **do not fit in memory**.
  - **No online learning**.

# Stochastic gradient descent

- Computes update for **each** example $x^{(i)}y^{(i)}$.
- Update equation: $\theta = \theta - \eta \cdot \nabla_\theta J(\theta; x^{(i)}; y^{(i)})$

**Shuffling: We shuffle the data to obtain a less biased estimation of the true gradient. For example, the data might be stored in chronological order.**
**To get an unbiased estimate of the true gradient, you'd like your mini batch to be a true random sample rather than examples that are highly correlated (which may be how the data is presented to you)**

```
for i in range(nb_epochs):
  np.random.shuffle(data)
  for example in data:
    params_grad = evaluate_gradient(
      loss_function, example, params)
    params = params - learning_rate * params_grad
```

Listing 2: Code for stochastic gradient descent update

- Pros
  - **Much faster** than batch gradient descent.
  - Allows **online learning**.
- Cons
  - **High variance** updates.

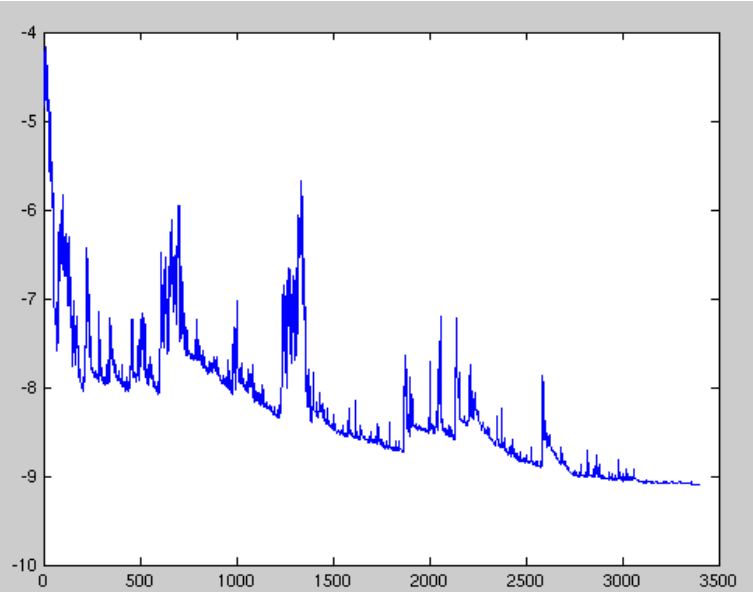



Figure: SGD fluctuation (Source: Wikipedia)

# Batch gradient descent vs. SGD fluctuation

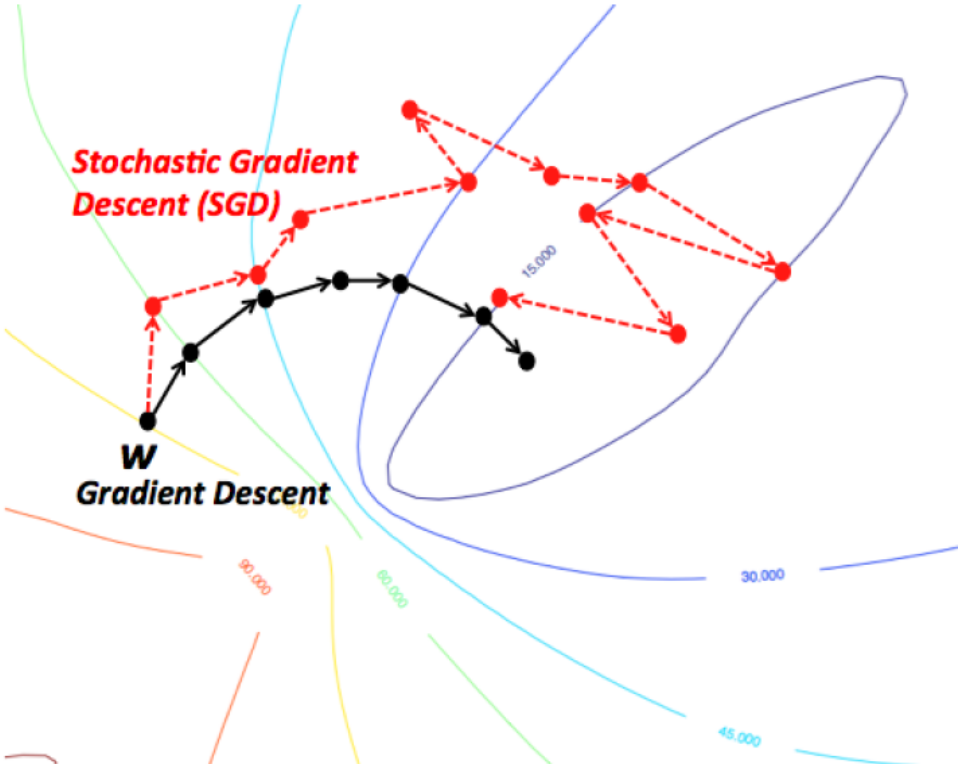



Figure: Batch gradient descent vs. SGD fluctuation (Source: wikidocs.net)

- SGD shows same convergence behaviour as batch gradient descent if learning rate is **slowly decreased (annealed)** over time.

# Mini-batch gradient descent

- Performs update for every **mini-batch** of $n$ examples.
- Update equation: $\theta = \theta - \eta \cdot \nabla_\theta J(\theta; x^{(i:i+n)}; y^{(i:i+n)})$

```
for i in range(nb_epochs):
  np.random.shuffle(data)
  for batch in get_batches(data, batch_size=50):
    params_grad = evaluate_gradient(
      loss_function, batch, params)
    params = params - learning_rate * params_grad
```

Listing 3: Code for mini-batch gradient descent update

- Pros
  - **Reduces variance** of updates.
  - Can exploit **matrix multiplication** primitives.
- Cons
  - **Mini-batch size** is a hyperparameter. Common sizes are 50-256.
- Typically the algorithm of choice.
- Usually referred to as SGD even when mini-batches are used.

| Method | Accuracy | Update Speed | Memory Usage | Online Learning |
|---|---|---|---|---|
| **Batch** gradient descent | Good | Slow | High | No |
| **Stochastic** gradient descent | Good (with annealing) | High | Low | Yes |
| **Mini-batch** gradient descent | Good | Medium | Medium | Yes |

Table: Comparison of trade-offs of gradient descent variants

# Challenges

- Choosing a **learning rate**.
- Defining an **annealing schedule**.
- Updating features to **different extent**.
- **Avoiding suboptimal minima**.

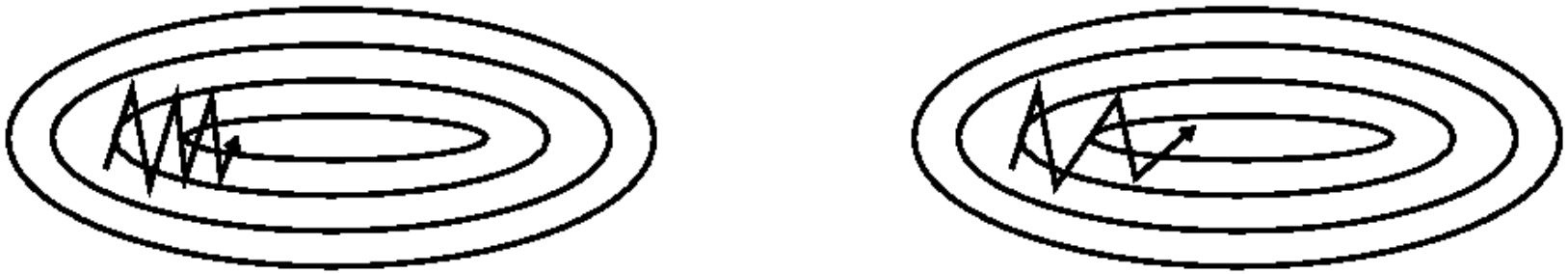
# Gradient descent optimization algorithms

1. Momentum
2. Nesterov accelerated gradient
3. Adagrad
4. Adadelta
5. RMSprop
6. Adam
7. Adam extensions

# Momentum

- SGD has trouble navigating **ravines**.
- Momentum [Qian, 1999] helps SGD **accelerate**.
- Adds a fraction $\gamma$ of the update vector of the past step $v_{t-1}$ to current update vector $v_t$. Momentum term $\gamma$ is usually set to 0.9.

$$\begin{aligned} v_t &= \gamma v_{t-1} + \eta \nabla_\theta J(\theta) \\ \theta &= \theta - v_t \end{aligned} \tag{1}$$



(a) SGD without momentum

(b) SGD with momentum

Figure: Source: Genevieve B. Orr

- **Reduces updates** for dimensions whose gradients **change directions**.
- **Increases updates** for dimensions whose gradients **point in the same directions**.

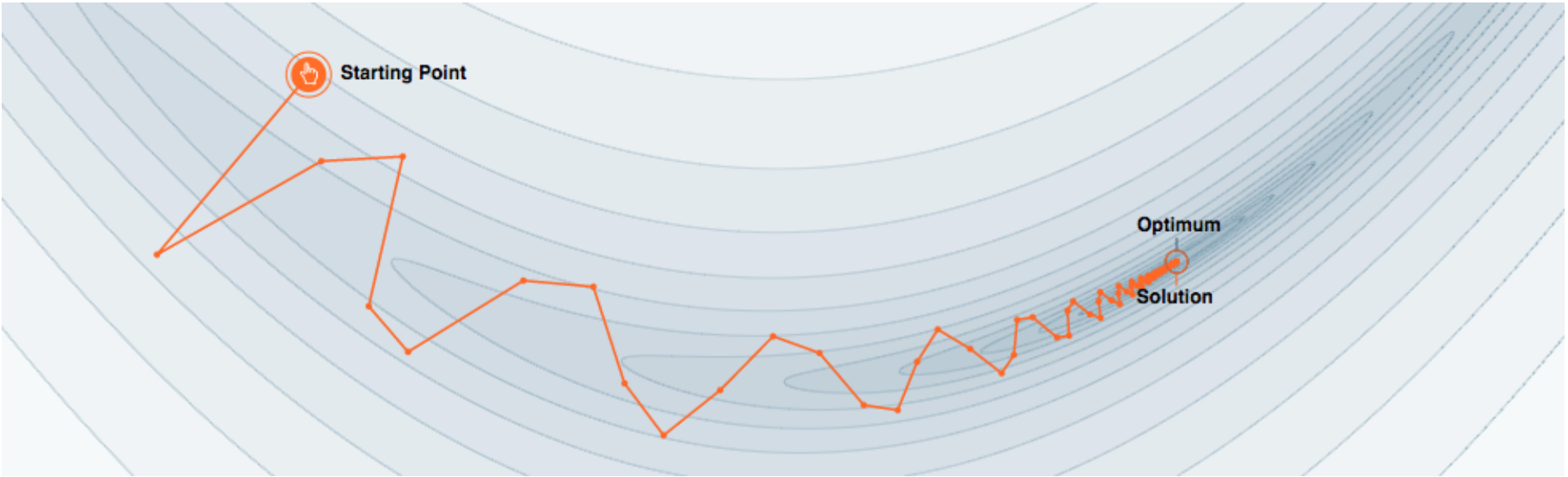



Figure: Optimization with momentum (Source: distill.pub)

# Nesterov accelerated gradient

- Momentum **blindly accelerates** down slopes: First computes gradient, then makes a big jump.
  Nesterov accelerated gradient (NAG) [Nesterov, 1983] first makes a big jump in the direction of the previous accumulated gradient $\theta - \gamma v_{t-1}$. Then measures where it ends up and makes a correction, resulting in the complete update vector.

$$
\begin{aligned}
v_t &= \gamma\, v_{t-1} + \eta \nabla_\theta J(\theta - \gamma v_{t-1}) \\
\theta &= \theta - v_t
\end{aligned}
\tag{2}
$$

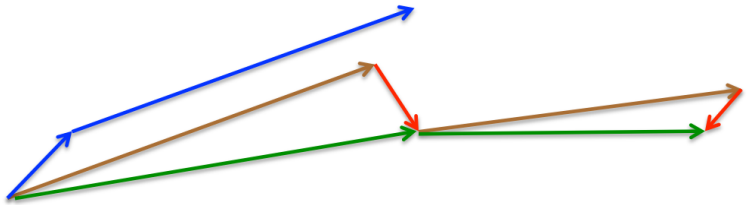


Figure: Nesterov update (Source: G. Hinton's lecture 6c)

# Adagrad

- Previous methods: **Same learning rate** $\eta$ for all parameters $\theta$.
- Adagrad [Duchi et al., 2011] **adapts** the learning rate to the parameters (**large** updates for **infrequent** parameters, **small** updates for **frequent** parameters).
- SGD update: $\theta_{t+1} = \theta_t - \eta \cdot g_t$
  - $g_t = \nabla_{\theta_t} J(\theta_t)$
- Adagrad divides the learning rate by the **square root of the sum of squares of historic gradients**.
- Adagrad update:

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t \tag{3}$$

  - $G_t \in \mathbb{R}^{d \times d}$: diagonal matrix where each diagonal element $i, i$ is the sum of the squares of the gradients w.r.t. $\theta_i$ up to time step $t$
  - $\epsilon$: smoothing term to avoid division by zero
  - $\odot$: element-wise multiplication

- Pros
  - Well-suited for dealing with **sparse data**.
  - Significantly **improves robustness** of SGD.
  - Lesser need to manually tune learning rate.
- Cons
  - **Accumulates squared gradients** in denominator. Causes the learning rate to **shrink** and become **infinitesimally small**.

# Adadelta

- Adadelta [Zeiler, 2012] restricts the window of accumulated past gradients to a **fixed size**. SGD update:

$$\begin{aligned} \Delta\theta_t &= -\eta \cdot g_t \\ \theta_{t+1} &= \theta_t + \Delta\theta_t \end{aligned} \tag{4}$$

- Defines **running average** of squared gradients $E[g^2]_t$ at time $t$:

$$E[g^2]_t = \gamma E[g^2]_{t-1} + (1-\gamma) g_t^2 \tag{5}$$

  - $\gamma$: fraction similarly to momentum term, around 0.9
- Adagrad update:

$$\Delta\theta_t = -\frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t \tag{6}$$

- Preliminary Adadelta update:

$$\Delta\theta_t = -\frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t \tag{7}$$

$$\Delta\theta_t = -\frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t \tag{8}$$

- Denominator is just root mean squared (RMS) error of gradient:

$$\Delta\theta_t = -\frac{\eta}{RMS[g]_t} g_t \tag{9}$$

- Note: **Hypothetical units do not match**.
- Define **running average of squared parameter updates** and RMS:

$$\begin{aligned} E[\Delta\theta^2]_t &= \gamma E[\Delta\theta^2]_{t-1} + (1-\gamma)\Delta\theta_t^2 \\ RMS[\Delta\theta]_t &= \sqrt{E[\Delta\theta^2]_t + \epsilon} \end{aligned} \tag{10}$$

- Approximate with $RMS[\Delta\theta]_{t-1}$, replace $\eta$ for **final Adadelta update**:

$$\begin{aligned} \Delta\theta_t &= -\frac{RMS[\Delta\theta]_{t-1}}{RMS[g]_t} g_t \\ \theta_{t+1} &= \theta_t + \Delta\theta_t \end{aligned} \tag{11}$$

# RMSprop

- Developed independently from Adadelta around the same time by Geoff Hinton.
- Also divides learning rate by a **running average of squared gradients**.
- RMSprop update:

$$E[g^2]_t = \gamma E[g^2]_{t-1} + (1-\gamma) g_t^2$$
$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t \tag{12}$$

  - $\gamma$: decay parameter; typically set to 0.9
  - $\eta$: learning rate; a good default value is 0.001

# Adam

- Adaptive Moment Estimation (Adam) [Kingma and Ba, 2015] also stores **running average of past squared gradients** $v_t$ like Adadelta and RMSprop.
- Like Momentum, stores **running average of past gradients** $m_t$.

$$\begin{aligned} m_t &= \beta_1 m_{t-1} + (1 - \beta_1) g_t \\ v_t &= \beta_2 v_{t-1} + (1 - \beta_2) g_t^2 \end{aligned} \tag{13}$$

  - $m_t$: first moment (mean) of gradients
  - $v_t$: second moment (uncentered variance) of gradients
  - $\beta_1, \beta_2$: decay rates

- $m_t$ and $v_t$ are initialized as 0-vectors. For this reason, they are biased towards 0.
- Compute bias-corrected first and second moment estimates:

$$\hat{m}_t = \frac{m_t}{1 - \beta_1^t}$$
$$\hat{v}_t = \frac{v_t}{1 - \beta_2^t} \tag{14}$$

- Adam update rule:

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t \tag{15}$$

# Adam extensions

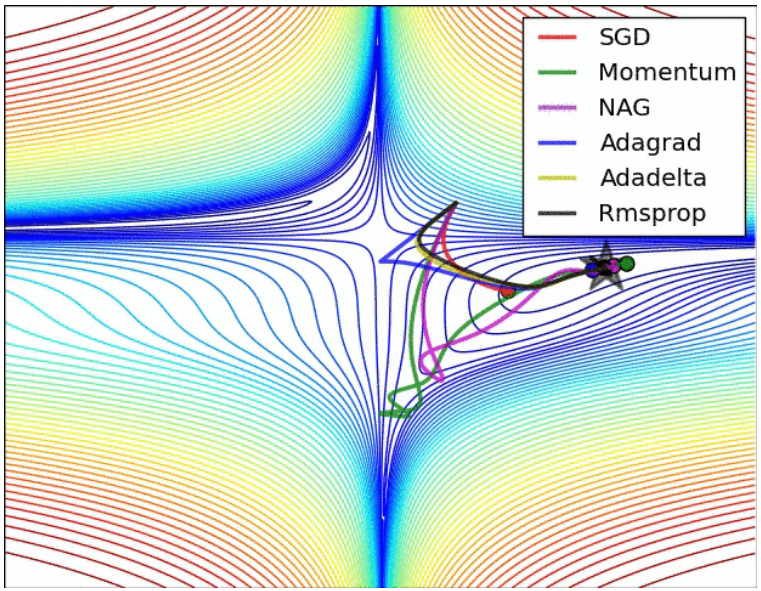
1. AdaMax [Kingma and Ba, 2015]
   - Adam with $\ell_\infty$ norm
2. Nadam [Dozat, 2016]
   - Adam with Nesterov accelerated gradient

# Update equations

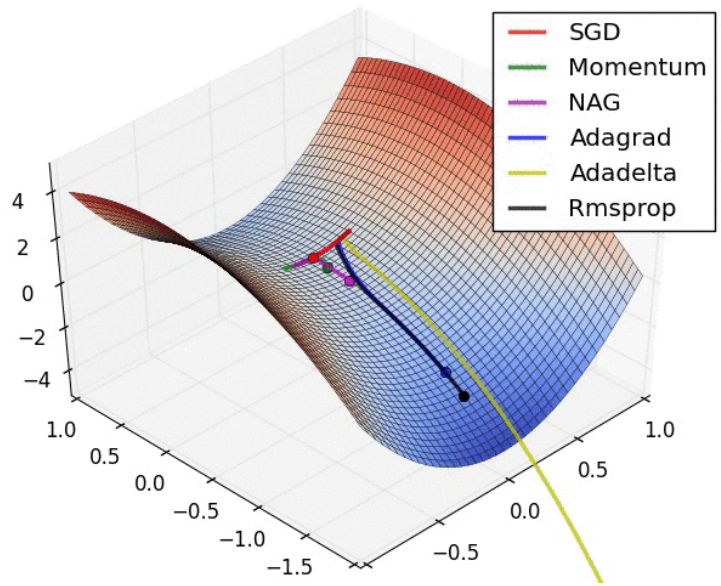
| Method | Update equation |
|---|---|
| | $g_t = \nabla_{\theta_t} J(\theta_t)$ |
| SGD | $\Delta\theta_t = -\eta \cdot g_t$ |
| | $\theta_t = \theta_t + \Delta\theta_t$ |
| Momentum | $\Delta\theta_t = -\gamma\, v_{t-1} - \eta g_t$ |
| NAG | $\Delta\theta_t = -\gamma\, v_{t-1} - \eta \nabla_\theta J(\theta - \gamma v_{t-1})$ |
| Adagrad | $\Delta\theta_t = -\frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t$ |
| Adadelta | $\Delta\theta_t = -\frac{RMS[\Delta\theta]_{t-1}}{RMS[g]_t} g_t$ |
| RMSprop | $\Delta\theta_t = -\frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t$ |
| Adam | $\Delta\theta_t = -\frac{\eta}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t$ |

Table: Update equations for the gradient descent optimization algorithms.

# Visualization of algorithms




(a) SGD optimization on loss surface contours

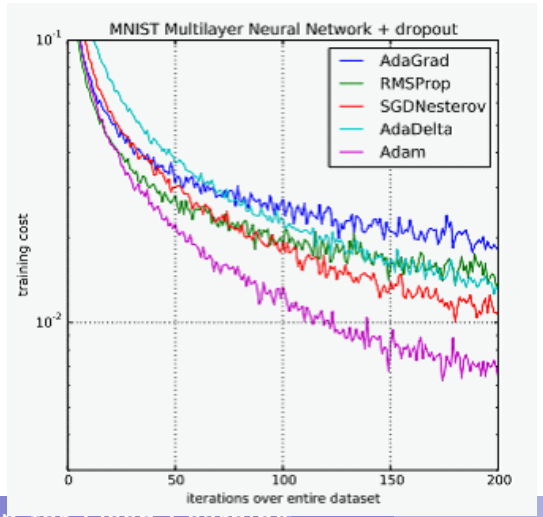



(b) SGD optimization on saddle point

Figure: Source and full animations: Alec Radford

# Which optimizer to choose?

- Adaptive learning rate methods (Adagrad, Adadelta, RMSprop, Adam) are **particularly useful for sparse features**.
- Adagrad, Adadelta, RMSprop, and Adam work well in similar circumstances.
- [Kingma and Ba, 2015] show that bias-correction helps Adam **slightly outperform RMSprop**.



# Parallelizing and distributing SGD

1. Hogwild! [Niu et al., 2011]
   - Parallel SGD updates on CPU
   - Shared memory access **without parameter lock**
   - Only works for **sparse input data**
2. Downpour SGD [Dean et al., 2012]
   - **Multiple replicas** of model on subsets of training data run in parallel
   - Updates sent to parameter server; **updates fraction of model parameters**
3. Delay-tolerant Algorithms for SGD [Mcmahan and Streeter, 2014]
   - Methods also adapt to **update delays**
4. TensorFlow [Abadi et al., 2015]
   - Computation graph is split into a **subgraph for every device**
   - Communication takes place using Send/Receive node pairs
5. Elastic Averaging SGD [Zhang et al., 2015]
   - **Links parameters elastically** to a center variable stored by parameter server

# Additional strategies for optimizing SGD

1. Shuffling and Curriculum Learning [Bengio et al., 2009]
   - Shuffle training data after every epoch to **break biases**
   - Order training examples to **solve progressively harder problems**; infrequently used in practice
2. Batch normalization [Ioffe and Szegedy, 2015]
   - **Re-normalizes every mini-batch** to zero mean, unit variance
   - Must-use for computer vision
3. Early stopping
   - "*Early stopping (is) beautiful free lunch*" (Geoff Hinton)
4. Gradient noise [Neelakantan et al., 2015]
   - Add Gaussian noise to gradient
   - Makes model **more robust to poor initializations**

# Outlook

1. Tuned SGD vs. Adam
2. SGD with restarts
3. Learning to optimize
4. Understanding generalization in Deep Learning
5. Case studies

# Tuned SGD vs. Adam

- Many recent papers use **SGD with learning rate annealing**.
- SGD with tuned learning rate and momentum is **competitive with Adam** [Zhang et al., 2017b].
- Adam **converges faster**, but **underperforms SGD** on some tasks, e.g. Machine Translation [Wu et al., 2016].
- Adam with **2 restarts and SGD-style annealing** converges faster and outperforms SGD [Denkowski and Neubig, 2017].
- **Increasing the batch size** may have the same effect as decaying the learning rate [Smith et al., 2017].

# SGD with restarts

- At each restart, the learning rate is initialized to some value and decreases with cosine annealing [Loshchilov and Hutter, 2017].
- Converges 2× to 4× faster with comparable performance.

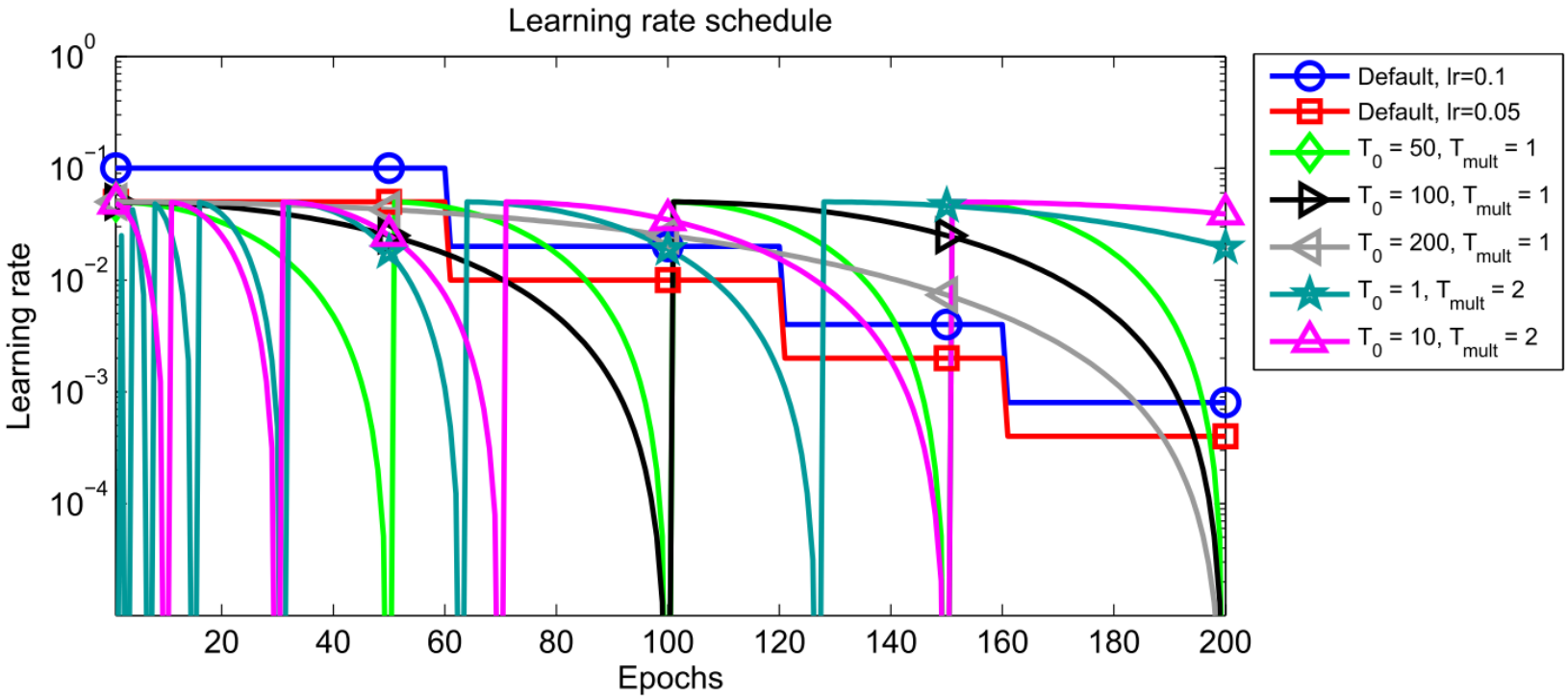



Figure: Learning rate schedules with warm restarts [Loshchilov and Hutter, 2017]

# Snapshot ensembles

1. Train model until convergence with cosine annealing schedule.
2. Save model parameters.
3. Perform warm restart and repeat steps 1-3 $M$ times.
4. Ensemble saved models.

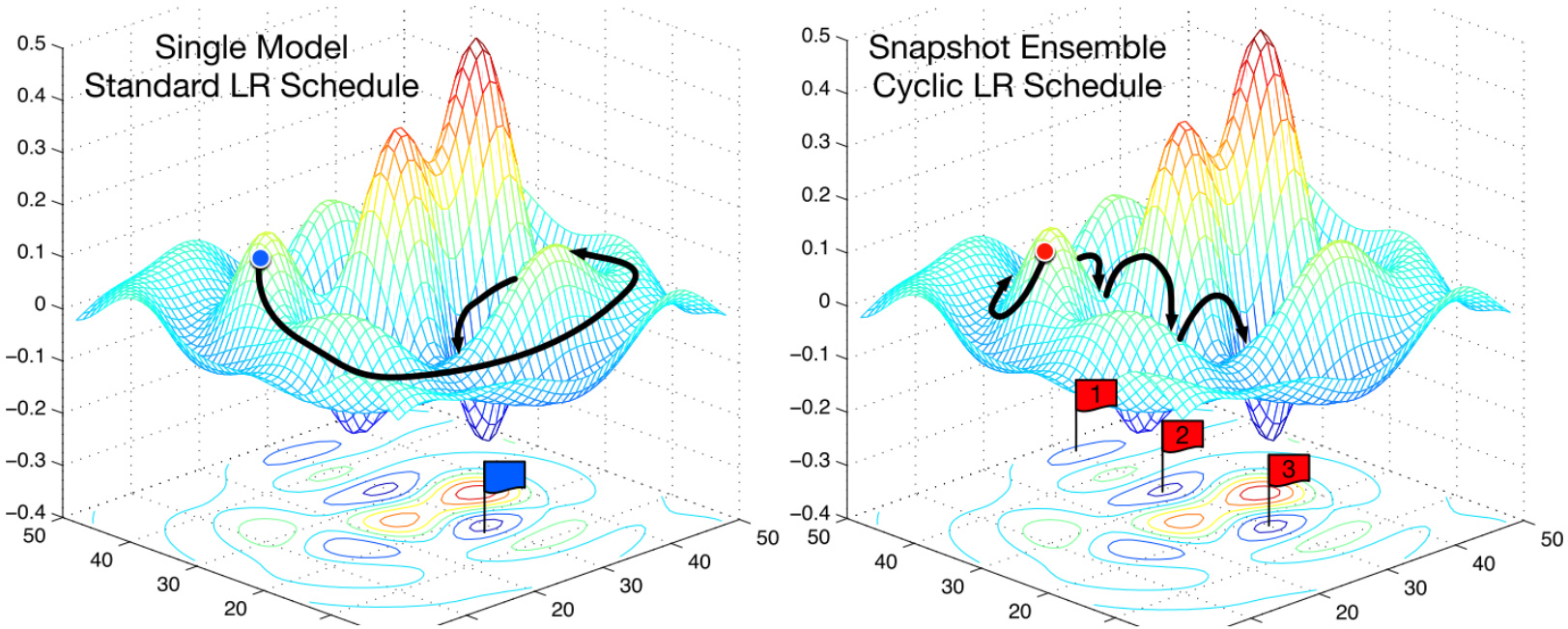



Figure: SGD vs. snapshot ensemble [Huang et al., 2017]

# Learning to optimize

- Rather than manually defining an update rule, **learn it**.
- Update rules outperform existing optimizers and transfer across tasks.

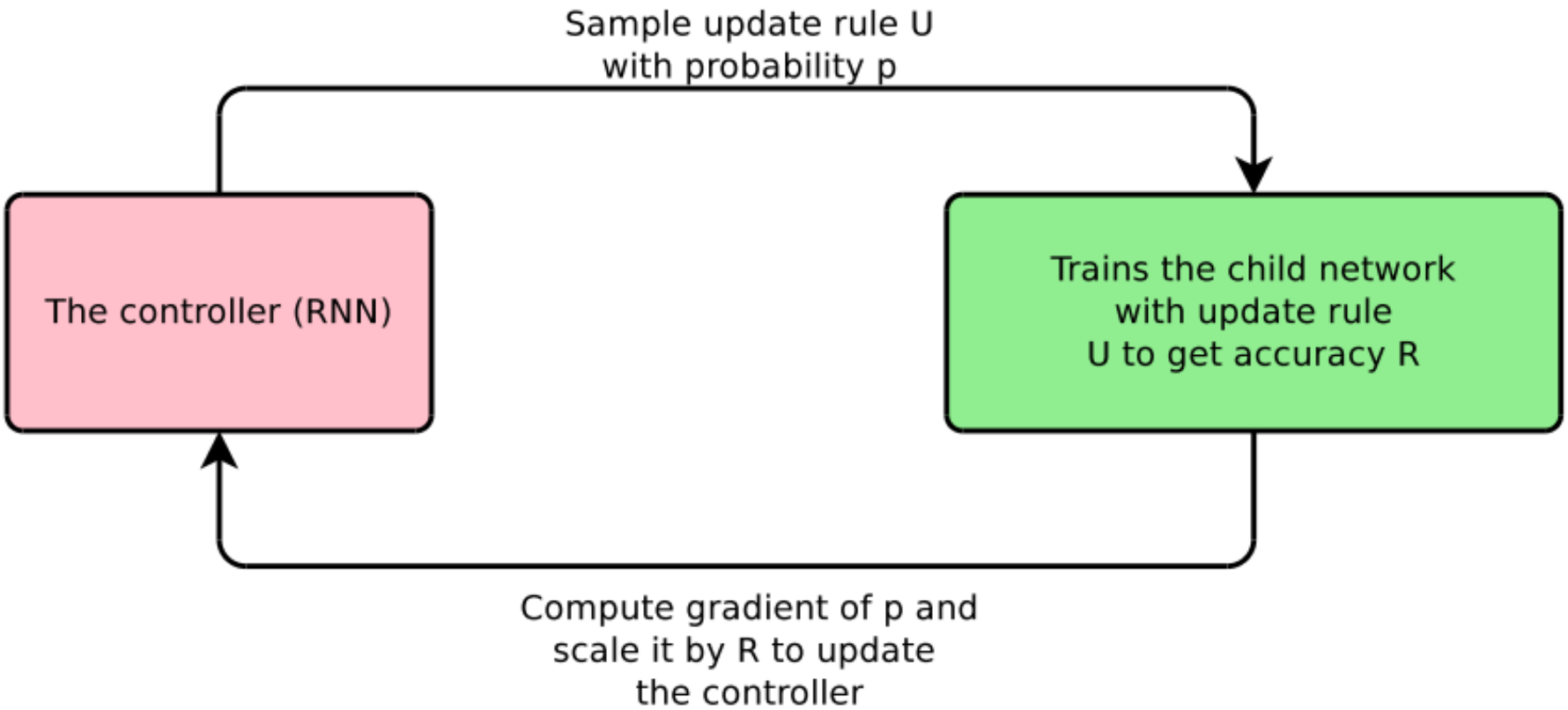



Figure: Neural Optimizer Search [Bello et al., 2017]

# Discovered update rules

- **PowerSign**:

$$\alpha^{f(t)*\text{sign}(g)*\text{sign}(m)} * g \tag{16}$$

  - $\alpha$: often $e$ or 2
  - $f$: either 1 or a decay function of the training step $t$
  - $m$: moving average of gradients
  - Scales update by $\alpha^{f(t)}$ or $1/\alpha^{f(t)}$ depending on whether the direction of the gradient and its running average agree.

- **AddSign**:

$$(\alpha + f(t) * \text{sign}(g) * \text{sign}(m)) * g \tag{17}$$

  - $\alpha$: often 1 or 2
  - Scales update by $\alpha + f(t)$ or $\alpha - f(t)$.

# Understanding generalization in Deep Learning

- **Optimization** is closely tied to **generalization**.
- The number of possible local minima **grows exponentially with the number of parameters** [Kawaguchi, 2016].
- Different local minima **generalize to different extents**.
- Recent insights in understanding generalization:
  - Neural networks can **completely memorize random inputs** [Zhang et al., 2017a].
  - Sharp minima found by batch gradient descent have **high generalization error** [Keskar et al., 2017].
  - Local minima that generalize well can be **made arbitrarily sharp** [Dinh et al., 2017].
- Several submissions at ICLR 2018 on understanding generalization.

# Case studies

- Deep Biaffine Attention for Neural Dependency Parsing [Dozat and Manning, 2017]
  - Adam with $\beta_1 = 0.9$, $\beta_2 = 0.9$
  - Report large positive impact on final performance of lowering $\beta_2$
- Attention is All You Need [Vaswani et al., 2017]
  - Adam with $\beta_1 = 0.9$, $\beta_2 = 0.98$, $\epsilon = 10^{-9}$, learning rate $\eta$
  - $\eta = d_{\text{model}}^{-0.5} \cdot \min(\mathit{step\_num}^{-0.5}, \mathit{step\_num} \cdot \mathit{warmup\_steps}^{-1.5})$
  - $\mathit{warmup\_steps} = 4000$

Thank you for attention!
For more details and derivations of the gradient descent optimization algorithms, refer to [Ruder, 2016].

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