Stochastic Gradient Descent

- Batches and Epochs
- Learning Rate and Momentum
- Nesterov Momentum
- ADAM optimizer

Batches, Epochs, and Stochastic Gradient Descent (SGD)

- Partition training set into randomized batches

$$S = \{1, \cdots, K\} = \bigcup_{b=1}^{B} S_b \qquad K_b = |S_b|$$

$= $ (# of sampler per batch)

  - For each batch you compute a separate gradient

$\nabla L(\theta; S_b) \Leftarrow$ Gradient for b^{th} batch of training data

```
Repeat until converged {
  Repeat $b = 1$ to $B$ {
    $d \leftarrow -\nabla L(\theta; S_b)$
    $\theta \leftarrow \theta + \alpha d^t$
  }
}
```

One epoch

One batch

Stochastic Gradient Descent (SGD)

Theoretical Analysis of SGD

- Assume simple sampling (sampling with replacement)

$$g_k = \nabla L_k(\theta) = (\text{gradient from } k^{th} \text{ training sample})$$

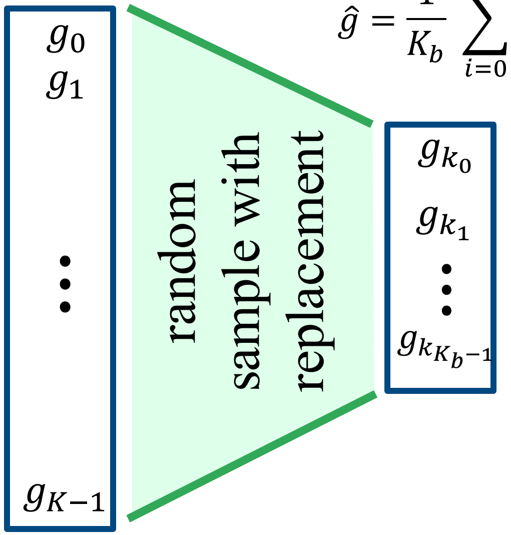
  - Each sample, g_{k_i}, is i.i.d. with distribution $p(g) = \frac{histogram(g)}{K}$

True gradient:

$$g = \frac{1}{K}\sum_{k=0}^{K-1} g_k$$

Batch gradient:

$$\hat{g} = \frac{1}{K_b}\sum_{i=0}^{K_b-1} g_{k_i}$$



g_0

g_1

$\vdots$

g_{K-1}

random sample with replacement

g_{k_0}

g_{k_1}

$\vdots$

$g_{k_{K_b-1}}$

- Then

$$\underset{\text{Batch Gradient}}{\hat{g}} = \underset{\text{True Gradient}}{g} + \underset{\text{Noise}}{\frac{w}{\sqrt{K_b}}}$$

where

$$E[w] = 0$$

$$Var[w] \approx \frac{1}{K}\sum_{k=0}^{K-1}(g_k - g)(g_k - g)^t$$

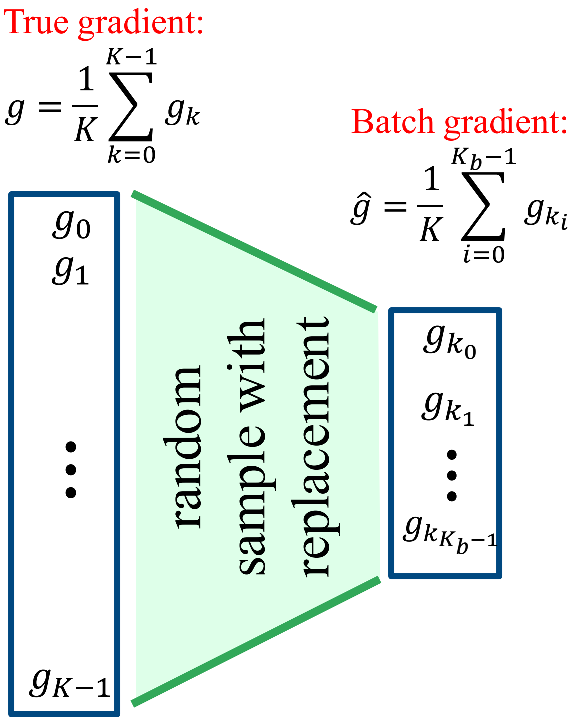
Effect of Batch Size on SGD

$$\hat{g} = g + \frac{w}{\sqrt{K_b}}$$

Batch Gradient

True Gradien t

Noise



True gradient:

$$g = \frac{1}{K}\sum_{k=0}^{K-1} g_k$$

Batch gradient:

$$\hat{g} = \frac{1}{K}\sum_{i=0}^{K_b-1} g_{k_i}$$

- Then we have that:
  - As $K_b \rightarrow \infty$ (batch size goes up) ⇒
    - Noise decreases and computation increases
  - As $K_b \rightarrow 0$ (batch size goes down) ⇒
    - Noise increases and computation decreases

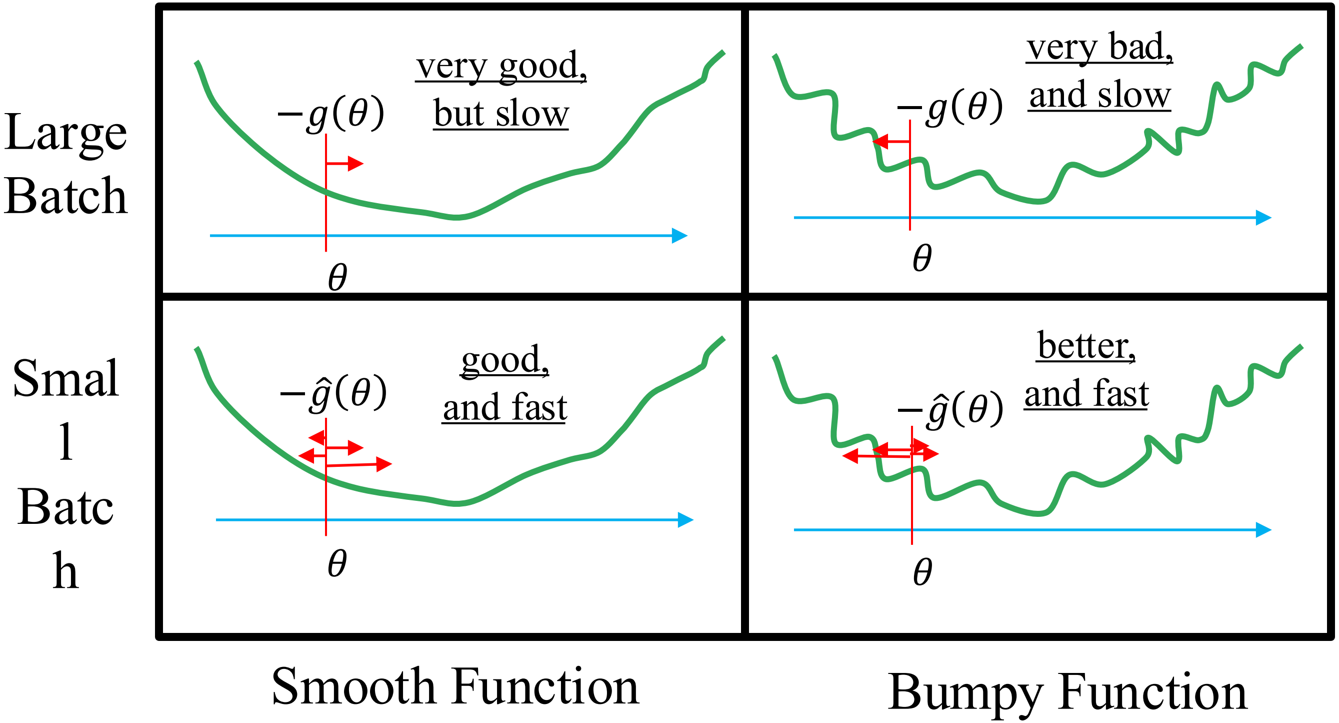
Effect of Gradient Noise: Exploration

$$\hat{g} = g + \frac{w}{\sqrt{K_b}}$$

Batch Gradient

True Gradien t

Noise



Large Batch

Smal l Batc h

very good, but slow

very bad, and slow

good, and fast

better, and fast

Smooth Function

Bumpy Function

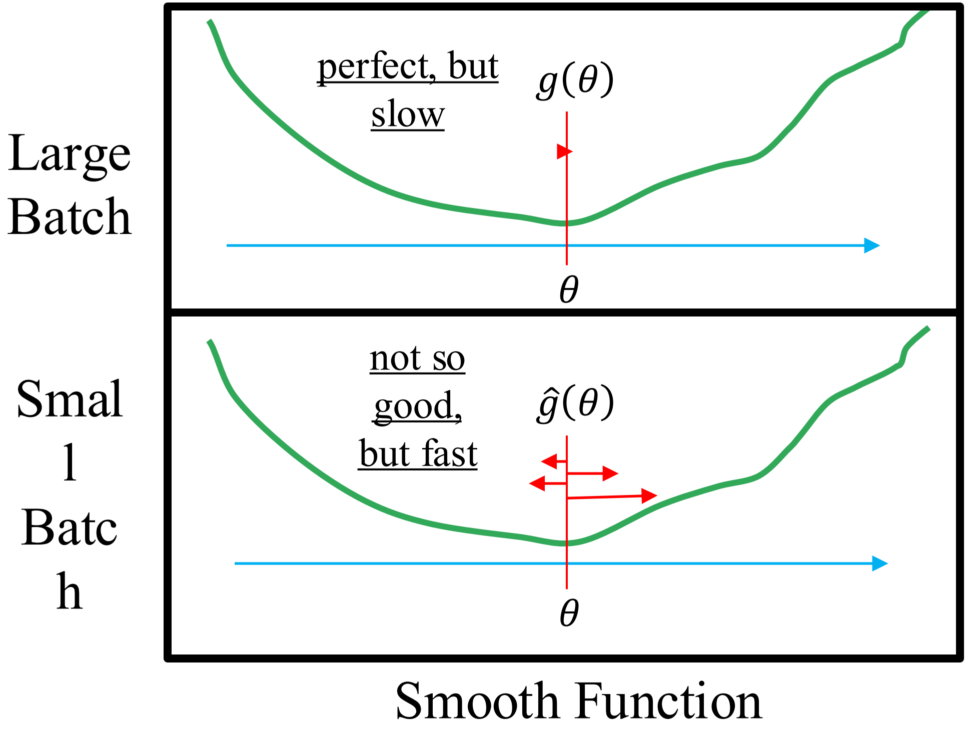
Effect of Gradient Noise: Exploitation

$$\hat{g} = g + \frac{w}{\sqrt{K_b}}$$

Batch Gradient

True Gradien t

Noise

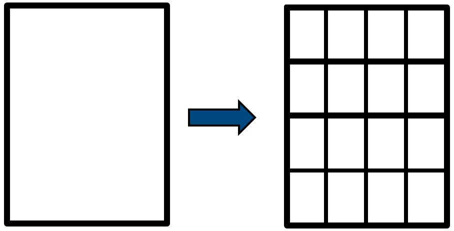


SGD Issues and Tradeoffs

- Why SGD works?
  - The gradient for a small batch is much faster to compute and almost as good as the full gradient.
  - If $K = 10{,}000$ and $K_b = |S_b| = 32$, then one iteration of SGD is approximately $\frac{10{,}000}{32} \approx 312$ times faster than GD.
- Batch size
  - Larger batches: less "noise" in gradient ⇒
    - *Worse*: slower updates; less exploration.
    - *Better:* better local convergence.
  - Smaller batches: more "noise" in gradient ⇒
    - *Worse:* hunts around local minimum.
    - *Better:* faster updates; better exploration.
- Patch size:
  - Many algorithms train on image "patches"
  - Apocryphal: Smaller patches speed training. Not true!!!!
  - However, smaller patches might fit better into GPU cache
- Step size α
  - Too large ⇒ hunts around local minimum
  - Too small ⇒ slow convergence

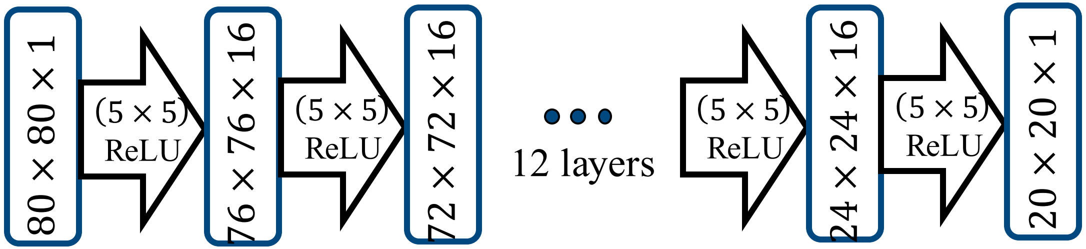
Training with Patches

- Concept:
  - Break training images into patches
  - Often used in training denoising, deblurring, or reconstruction algorithms



  - Typically, may be $N \times N$ where $N = 80$ patches (DNCNN)
  - Typically, use a stride of $N_s = N/2$ so that patches overlap

- Patch size issues:
  - Apocryphal:
    - Smaller patches increase amount of training data. Not true!!
    - Smaller patches speed training. Not true!!!!
  - Advantages:
    - Smaller patches might fit better into GPU cache
  - Disadvantages:
    - Valid region tends towards 0 for deep CNNs



Momentum

- SGD with momentum
  - α is step size, and γ is momentum typically with $\gamma = 0.9$

```
init $v \leftarrow 0$
Repeat until converged {
    Repeat $b = 1$ to $B$ {
        $d \leftarrow -\nabla L(\theta; S_b)$
        $\boxed{v \leftarrow \gamma v + \alpha(1-\gamma)d}$
        $\theta \leftarrow \theta + v^t$
    }
}
```

momentum term

Stochastic Gradient Descent (SGD) with momentum

  - Interpretation
    - θ is like position
    - v is like velocity
    - Friction $= 1 - \gamma$

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Stochastic Gradient Descent (SGD) with momentum

for each epoch

for each batch

momentum term

  - Interpretation
    - θ is like position
    - v is like velocity
    - Friction $= 1 - \gamma$

Interpretation of Momentum

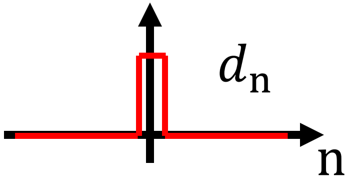
- Special case of impulsive input: If $d_{\mathrm{n}} = \delta_n$

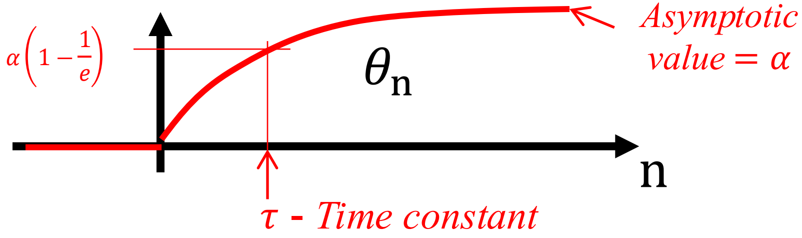
```
init $v \leftarrow 0$; $\theta_{-1} \leftarrow 0$
Repeat $n = 0$ to $N-1$ {
    $v \leftarrow \gamma v + \alpha(1-\gamma)\delta_n$
    $\theta_n \leftarrow \theta_{n-1} + v^t$
}
```

Momentum

  - Then

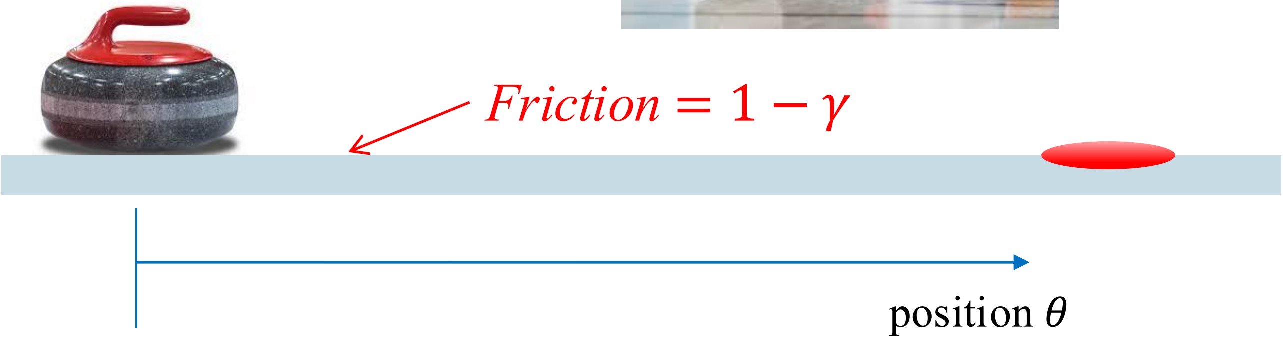
$$\theta_n = \begin{cases} \alpha(1-\gamma^{n+1}) & n \geq 0 \\ 0 & n < 0 \end{cases}$$





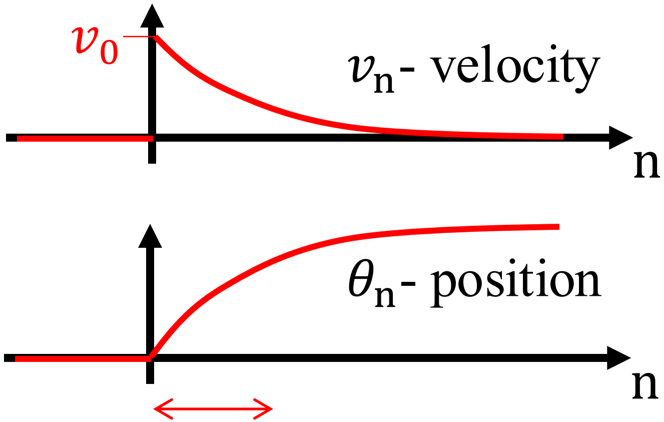
$$\tau = -1 - \frac{1}{\log \gamma} \qquad \gamma = \exp\left\{-\frac{1}{\tau+1}\right\}$$

Intuition



$Friction = 1 - \gamma$

position θ



Time constant
$= -1 - 1/\log\gamma$

Nesterov Momentum*

> "I skate to where the puck is going to be,
> not where it has been." - Wayne Gretzky

- SGD with momentum
  - α is step size, and γ is momentum typically with $\gamma \approx 0.9$

```
init $v \leftarrow 0$
Repeat until converged {
   Repeat $b = 1$ to $B$ {
      $d \leftarrow \boxed{-\nabla L(\theta + \gamma v^t; S_b)}$
      $v \leftarrow \gamma v + \alpha d$
      $\theta \leftarrow \theta + v^t$
   }
}
```

Stochastic Gradient Descent (SGD) with Nesterov momentum

Nesterov gradient

  - Intuition:
    - Even if $d_n = 0$, we have that $\theta_{n+1} = \theta_n + \gamma v^t$ because of momentum
    - So compute the gradient at $\theta_n + \gamma v^t$

*Yu. E. Nesterov, "A method of solving a convex programming problem with convergence rate O(1/k^2)", Doklady ANSSSR (translated as Soviet.Math.Docl.), vol. 269, no. 3, pp. 543– 547.

Preconditioned Gradient Descent

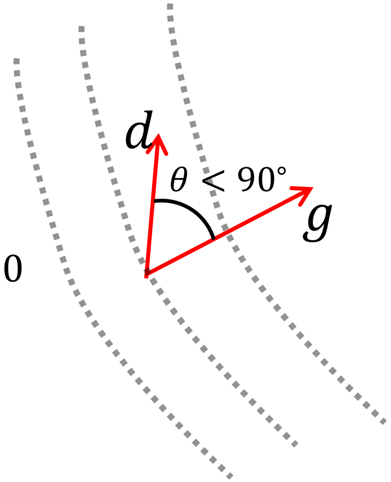
- Pick any positive definite matrix, M.
- Then Preconditioned Gradient Descent is

```
Repeat until converged {
    $g \leftarrow -[\nabla L(\theta)]^t$
    $d \leftarrow Mg$
    $\theta \leftarrow \theta + \alpha d$
}
```

  - Notice that then

$$\langle d, g\rangle = \langle Mg, g\rangle = (Mg)^t g = g^t M g > 0$$

  - This means that the angle between d and g is $< 90°$
  - So we see that PGD always goes down hill!



- How to pick M?
  - $M = B^t B$
  - $M = diag(a_0, \ldots, a_{N-1})$ where $a_i > 0$

ADAM (Adaptive Moment Estimation)*

- SGD with ADAM optimization = Momentum + Preconditioning

```
init $v \leftarrow 0$; $r \leftarrow 0$;
init $t \leftarrow 0$
Repeat until converged {
    Repeat $b = 1$ to $B$ {
        $t \leftarrow t + 1$
        $d \leftarrow -\nabla L(\theta; S_b)$
        $v \leftarrow \beta_1 v + (1 - \beta_1) d$
        $r \leftarrow \beta_2 r + (1 - \beta_2) d^2$
        $\hat{v} \leftarrow v / (1 - \beta_1^t)$
        $\hat{r} \leftarrow r / (1 - \beta_2^t)$
        $\theta \leftarrow \theta + \alpha \left( \sqrt{\hat{r}} + \epsilon \right)^{-1} \hat{v}$
    }
}
```

ADAM Optimization

  – Typical parameters: $\alpha = 0.001$; $\beta_1 = 0.9$; $\beta_2 = 0.999$; $\epsilon = 10^{-8}$

*Diederik P. Kingma and Jimmy Ba, "Adam: A Method for Stochastic Optimization", The 3rd International Conference for Learning Representations (ICLR), San Diego, 2015.

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  }
}
```

ADAM Optimization

These are all interpreted as element-wise operations on vectors

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    }
}
```

ADAM Optimization

momentum

estimate of the average squared gradient

bias correction at the start

normalizes by RMS variation of each gradient component

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