

10-301/601: Introduction to Machine Learning

Lecture 14 – Backpropagation

Henry Chai

6/14/23

Front Matter

- Announcements
 - PA3 released 6/8, due 6/15 (tomorrow) at 11:59 PM
 - PA4 released 6/15 (tomorrow), due 7/13 (**4 weeks from tomorrow**) at 11:59 PM
 - We have scheduled this so that **you do not have to be working on PA4 during exam week or over break!**
 - Quiz 4: Neural Networks on 6/20 (next Tuesday)
 - No lecture **or OH** on 6/19 (next Monday) for Juneteenth
 - Midterm on 6/23, one week from Friday
 - Reminder: all of this week's material is in-scope
- Recommended Readings
 - Mitchell, [Chapters 4.1 – 4.6](#)

Recall: Gradient Descent for Learning

- Input: $\mathcal{D} = \{(\mathbf{x}^{(n)}, y^{(n)})\}_{n=1}^N, \eta^{(0)}$
- Initialize all weights $W_{(0)}^{(1)}, \dots, W_{(0)}^{(L)}$ to small, random numbers and set $t = 0$ (???)
- While TERMINATION CRITERION is not satisfied (???)
 - For $l = 1, \dots, L$
 - Compute $G^{(l)} = \nabla_{W^{(l)}} \ell_{\mathcal{D}} \left(W_{(t)}^{(1)}, \dots, W_{(t)}^{(L)} \right)$ (???)
 - Update $W^{(l)}$: $W_{(t+1)}^{(l)} = W_{(t)}^{(l)} - \eta_0 G^{(l)}$
 - Increment t : $t = t + 1$
- Output: $W_{(t)}^{(1)}, \dots, W_{(t)}^{(L)}$

Computing Gradients

$$\ell_{\mathcal{D}} \left(W_{(t)}^{(1)}, \dots, W_{(t)}^{(L)} \right) = \sum_{n=1}^N \ell_{(x^{(n)}, y^{(n)})} \left(W_{(t)}^{(1)}, \dots, W_{(t)}^{(L)} \right)$$

$$\nabla_{W^{(l)}} \ell_{\mathcal{D}} \left(W_{(t)}^{(1)}, \dots, W_{(t)}^{(L)} \right)$$

$$= \begin{bmatrix} \frac{\partial \ell_{\mathcal{D}}}{\partial w_{1,0}^{(l)}} & \frac{\partial \ell_{\mathcal{D}}}{\partial w_{1,1}^{(l)}} & \dots & \frac{\partial \ell_{\mathcal{D}}}{\partial w_{1,d^{(l-1)}}^{(l)}} \\ \frac{\partial \ell_{\mathcal{D}}}{\partial w_{2,0}^{(l)}} & \frac{\partial \ell_{\mathcal{D}}}{\partial w_{2,1}^{(l)}} & \dots & \frac{\partial \ell_{\mathcal{D}}}{\partial w_{2,d^{(l-1)}}^{(l)}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial \ell_{\mathcal{D}}}{\partial w_{d^{(l)},0}^{(l)}} & \frac{\partial \ell_{\mathcal{D}}}{\partial w_{d^{(l)},1}^{(l)}} & \dots & \frac{\partial \ell_{\mathcal{D}}}{\partial w_{d^{(l)},d^{(l-1)}}^{(l)}} \end{bmatrix}$$

$$\frac{\partial \ell_{\mathcal{D}}}{\partial w_{b,a}^{(l)}} = \sum_{n=1}^N \frac{\partial \ell_{(x^{(n)}, y^{(n)})} \left(W_{(t)}^{(1)}, \dots, W_{(t)}^{(L)} \right)}{\partial w_{b,a}^{(l)}} = \sum_{n=1}^N \frac{\partial e(\mathbf{o}^{(L)}, y^{(n)})}{\partial w_{b,a}^{(l)}}$$

Computing Gradients: Intuition

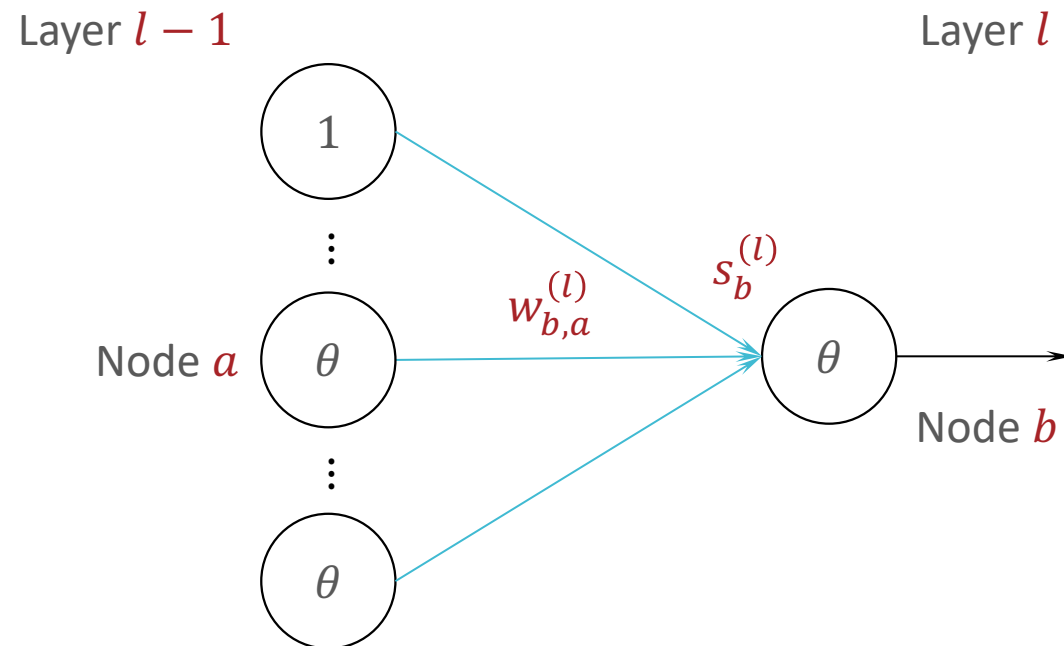
- A weight affects the prediction of the network (and therefore the error) through downstream signals/outputs
 - Use the chain rule!
- Any weight going into the same node will affect the prediction through the same downstream path
 - Compute derivatives starting from the last layer and move “backwards”
 - Store computed derivatives and reuse for efficiency (automatic differentiation)

Computing Partial Derivatives

Computing $\nabla_{W^{(l)}} \ell_{\mathcal{D}} \left(W_{(t)}^{(1)}, \dots, W_{(t)}^{(L)} \right)$ reduces to computing

$$\frac{\partial e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})}{\partial w_{b,a}^{(l)}}$$

Insight: $w_{b,a}^{(l)}$ only affects $e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})$ via $s_b^{(l)}$



Computing Partial Derivatives

Computing $\nabla_{W^{(l)}} \ell_{\mathcal{D}} \left(W_{(t)}^{(1)}, \dots, W_{(t)}^{(L)} \right)$ reduces to computing

$$\frac{\partial e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})}{\partial w_{b,a}^{(l)}}$$

Insight: $w_{b,a}^{(l)}$ only affects $e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})$ via $s_b^{(l)}$

Chain rule:
$$\frac{\partial e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})}{\partial w_{b,a}^{(l)}} = \frac{\partial e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})}{\partial s_b^{(l)}} \left(\frac{\partial s_b^{(l)}}{\partial w_{b,a}^{(l)}} \right)$$

$$s_b^{(l)} = \sum_{a=0}^{d^{(l-1)}} w_{b,a}^{(l)} o_a^{(l-1)} \rightarrow \frac{\partial s_b^{(l)}}{\partial w_{b,a}^{(l)}} = o_a^{(l-1)}$$

Compute outputs $\mathbf{o}^{(l)} \forall l \in \{0, \dots, L\}$ by forward propagation

Computing Partial Derivatives

Computing $\nabla_{W^{(l)}} \ell_{\mathcal{D}} \left(W_{(t)}^{(1)}, \dots, W_{(t)}^{(L)} \right)$ reduces to computing

$$\frac{\partial e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})}{\partial w_{b,a}^{(l)}}$$

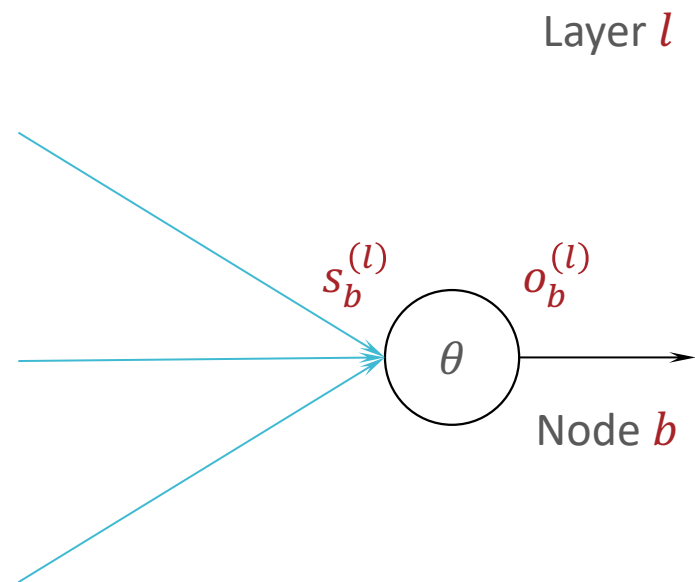
Insight: $w_{b,a}^{(l)}$ only affects $e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})$ via $s_b^{(l)}$

Chain rule:
$$\frac{\partial e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})}{\partial w_{b,a}^{(l)}} = \frac{\partial e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})}{\partial s_b^{(l)}} \left(\frac{\partial s_b^{(l)}}{\partial w_{b,a}^{(l)}} \right)$$

$$\delta_b^{(l)} := \frac{\partial e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})}{\partial s_b^{(l)}}$$

Computing Partial Derivatives

Insight: $s_b^{(l)}$ only affects $e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})$ via $o_b^{(l)}$



Computing Partial Derivatives

Insight: $s_b^{(l)}$ only affects $e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})$ via $o_b^{(l)}$

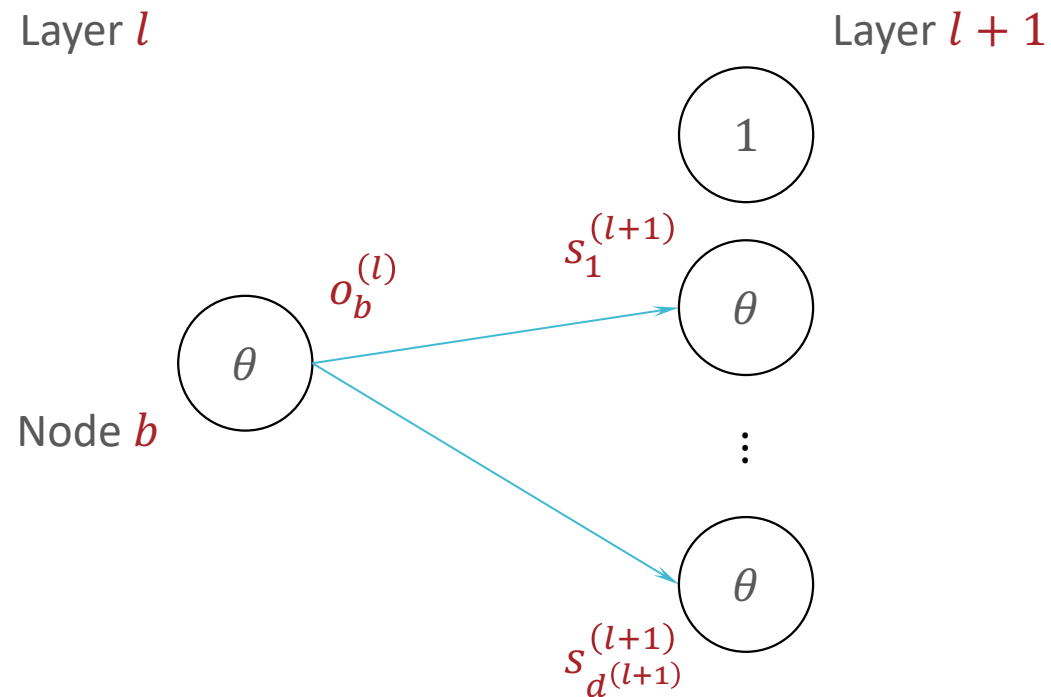
$$\text{Chain rule: } \delta_b^{(l)} = \frac{\partial e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})}{\partial o_b^{(l)}} \left(\frac{\partial o_b^{(l)}}{\partial s_b^{(l)}} \right)$$

$$\begin{aligned} o_b^{(l)} = \theta(s_b^{(l)}) &\rightarrow \frac{\partial o_b^{(l)}}{\partial s_b^{(l)}} = \frac{\partial \theta(s_b^{(l)})}{\partial s_b^{(l)}} \\ &= 1 - \left(\tanh(s_b^{(l)}) \right)^2 \end{aligned}$$

when $\theta(\cdot) = \tanh(\cdot)$

Computing Partial Derivatives

Insight: $o_b^{(l)}$ affects $e(\mathbf{o}^{(L)}, \mathbf{y}^{(n)})$ via $s_1^{(l+1)}, \dots, s_d^{(l+1)}$



Computing Partial Derivatives

Insight: $o_b^{(l)}$ affects $e(\mathbf{o}^{(L)}, y^{(n)})$ via $s_1^{(l+1)}, \dots, s_{d^{(l+1)}}^{(l+1)}$

$$\text{Chain rule: } \frac{\partial e(\mathbf{o}^{(L)}, y^{(n)})}{\partial o_b^{(l)}} = \sum_{c=1}^{d^{(l+1)}} \frac{\partial e(\mathbf{o}^{(L)}, y^{(n)})}{\partial s_c^{(l+1)}} \left(\frac{\partial s_c^{(l+1)}}{\partial o_b^{(l)}} \right)$$

$$s_c^{(l+1)} = \sum_{b=0}^{d^{(l)}} w_{c,b}^{(l+1)} o_b^{(l)} \rightarrow \frac{\partial s_c^{(l+1)}}{\partial o_b^{(l)}} = w_{c,b}^{(l+1)}$$

$$= \sum_{c=1}^{d^{(l+1)}} \delta_c^{(l+1)} \left(w_{c,b}^{(l+1)} \right)$$

Computing Partial Derivatives

$$\begin{aligned}\delta_b^{(l)} &= \frac{\partial e(\mathbf{o}^{(L)}, y^{(n)})}{\partial o_b^{(l)}} \left(\frac{\partial o_b^{(l)}}{\partial s_b^{(l)}} \right) \\ &= \left(\sum_{c=1}^{d^{(l+1)}} \delta_c^{(l+1)} \left(w_{c,b}^{(l+1)} \right) \right) \left(1 - \left(o_b^{(l)} \right)^2 \right) \\ \boldsymbol{\delta}^{(l)} &:= \nabla_{\mathbf{s}^{(l)}} e(\mathbf{o}^{(L)}, y^{(n)})\end{aligned}$$

Based solely on their shape alone, which of the following could be an expression for [loading eqn.]? Here [loading eqn.] is the element-wise product operation.

$$\begin{array}{l} W^{(l+1)T} \delta^{(l+1)} \odot (1 - \mathbf{o}^{(l)}) \\ W^{(l+1)T} \delta^{(l+1)} \odot (1 - \mathbf{o}^{(l)T}) \\ \delta^{(l+1)T} W^{(l+1)} \odot (1 - \mathbf{o}^{(l)}) \end{array}$$

Computing Partial Derivatives

$$\begin{aligned}\delta_b^{(l)} &= \frac{\partial e(\mathbf{o}^{(L)}, y^{(n)})}{\partial o_b^{(l)}} \left(\frac{\partial o_b^{(l)}}{\partial s_b^{(l)}} \right) \\ &= \left(\sum_{c=1}^{d^{(l+1)}} \delta_c^{(l+1)} \left(w_{c,b}^{(l+1)} \right) \right) \left(1 - \left(o_b^{(l)} \right)^2 \right) \\ \boldsymbol{\delta}^{(l)} &= W^{(l+1)T} \boldsymbol{\delta}^{(l+1)} \odot \left(1 - \mathbf{o}^{(l)} \odot \mathbf{o}^{(l)} \right)\end{aligned}$$

where \odot is the element-wise product operation

Sanity check: $W^{(l+1)} \in \mathbb{R}^{d^{(l+1)} \times (d^{(l)}+1)}$ and

$\boldsymbol{\delta}^{(l+1)} \in \mathbb{R}^{d^{(l+1)} \times 1}$ so

$W^{(l+1)T} \boldsymbol{\delta}^{(l+1)} \in \mathbb{R}^{(d^{(l)}+1) \times 1}$, the same size as $\mathbf{o}^{(l)}$!

Computing Gradients

$$\frac{\partial e(\mathbf{o}^{(L)}, y^{(n)})}{\partial w_{b,a}^{(l)}} = \delta_b^{(l)} \left(\frac{\partial s_b^{(l)}}{\partial w_{b,a}^{(l)}} \right) = \delta_b^{(l)} \left(o_a^{(l-1)} \right)$$

$$\nabla_{W^{(l)}} e(\mathbf{o}^{(L)}, y^{(n)}) = \boldsymbol{\delta}^{(l)} \mathbf{o}^{(l-1)T}$$

Sanity check: $\mathbf{o}^{(l-1)} \in \mathbb{R}^{(d^{(l-1)}+1) \times 1}$ and

$$\boldsymbol{\delta}^{(l)} \in \mathbb{R}^{d^{(l)} \times 1} \text{ so}$$

$$\boldsymbol{\delta}^{(l)} \mathbf{o}^{(l-1)T} \in \mathbb{R}^{d^{(l)} \times (d^{(l-1)}+1)}, \text{ the same size as } W^{(l)}!$$

Computing Partial Derivatives

Can recursively compute $\delta^{(l)}$ using $\delta^{(l+1)}$; need to compute the base case: $\delta^{(L)}$

Assume the output layer is a single node and the error function is the squared error:

$$\begin{aligned}\delta^{(L)} &= \delta_1^{(L)}, \mathbf{o}^{(L)} = o_1^{(L)} \text{ and } e(o_1^{(L)}, y^{(n)}) = (o_1^{(L)} - y^{(n)})^2 \\ \delta_1^{(L)} &= \frac{\partial e(o_1^{(L)}, y^{(n)})}{\partial s_1^{(L)}} = \frac{\partial}{\partial s_1^{(L)}} (o_1^{(L)} - y^{(n)})^2 \\ &= 2(o_1^{(L)} - y^{(n)}) \frac{\partial o_1^{(L)}}{\partial s_1^{(L)}} = 2(o_1^{(L)} - y^{(n)}) (1 - (o_1^{(L)})^2)\end{aligned}$$

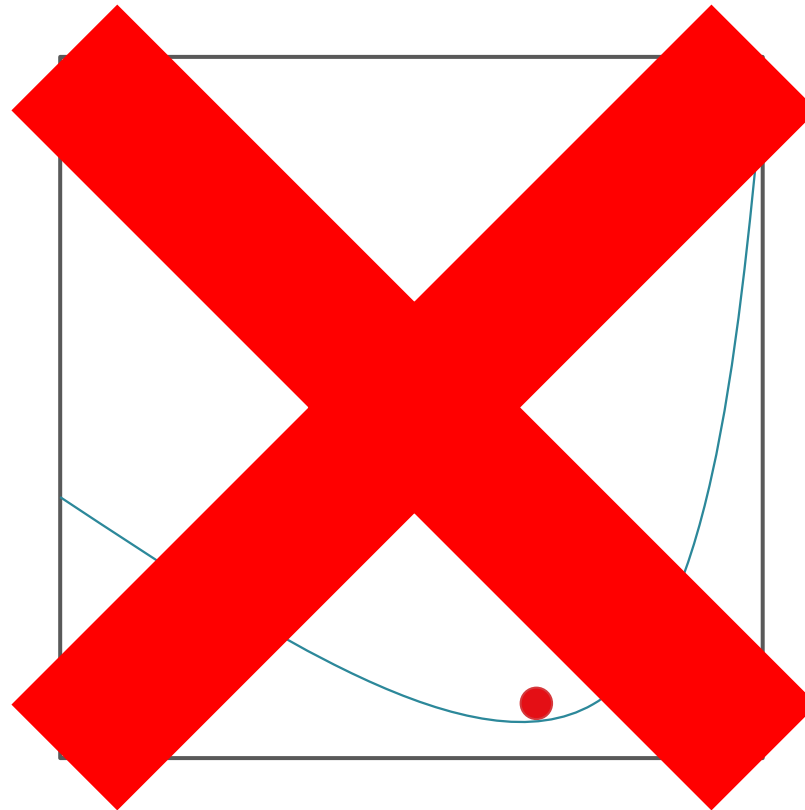
when $\theta(\cdot) = \tanh(\cdot)$

Back- propagation

- Input: $W^{(1)}, \dots, W^{(L)}$ and $\mathcal{D} = \{(\mathbf{x}^{(n)}, y^{(n)})\}_{n=1}^N$
- Initialize: $\ell_{\mathcal{D}} = 0$ and $G^{(l)} = 0 \odot W^{(l)} \forall l = 1, \dots, L$
- For $n = 1, \dots, N$
 - Run forward propagation with $\mathbf{x}^{(n)}$ to get $\mathbf{o}^{(1)}, \dots, \mathbf{o}^{(L)}$
 - (Optional) Increment $\ell_{\mathcal{D}}$: $\ell_{\mathcal{D}} = \ell_{\mathcal{D}} + (o^{(L)} - y^{(n)})^2$
 - Initialize: $\delta^{(L)} = 2 (o_1^{(L)} - y^{(n)}) (1 - (o_1^{(L)})^2)$
 - For $l = L - 1, \dots, 1$
 - Compute $\delta^{(l)} = W^{(l+1)T} \delta^{(l+1)} \odot (1 - \mathbf{o}^{(l)} \odot \mathbf{o}^{(l)})$
 - Increment $G^{(l)}$: $G^{(l)} = G^{(l)} + \delta^{(l)} \mathbf{o}^{(l-1)T}$
- Output: $G^{(1)}, \dots, G^{(L)}$, the gradients of $\ell_{\mathcal{D}}$ w.r.t $W^{(1)}, \dots, W^{(L)}$

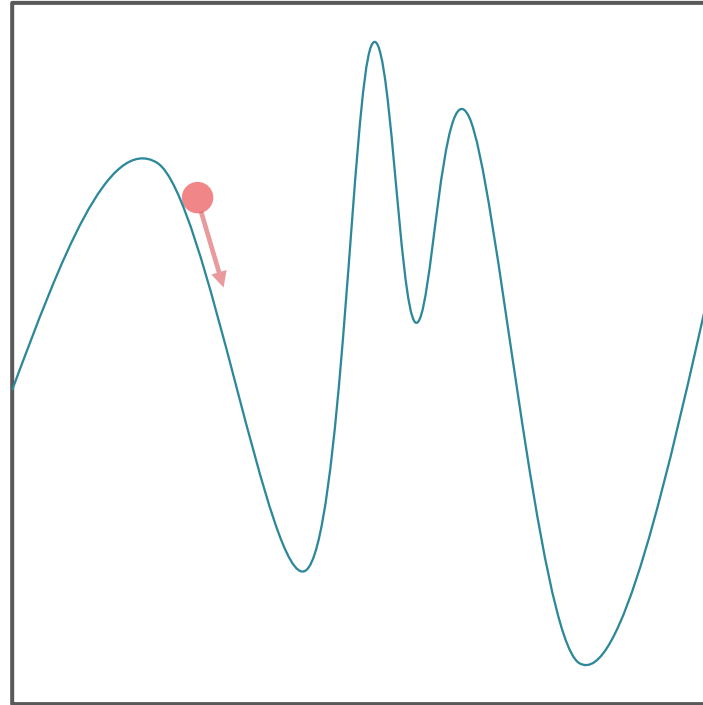
Recall: Gradient Descent

- Iterative method for minimizing functions
- Requires the gradient to exist everywhere



Non-convexity

- Gradient descent is not guaranteed to find a global minimum on non-convex surfaces



Stochastic Gradient Descent for Neural Networks

- Input: $\mathcal{D} = \{(\mathbf{x}^{(n)}, y^{(n)})\}_{n=1}^N, \eta_{SGD}^{(0)}$
- 1. Initialize all weights $W_{(0)}^{(1)}, \dots, W_{(0)}^{(L)}$ to small, random numbers and set $t = 0$
- 2. While TERMINATION CRITERION is not satisfied
 - a. Randomly sample a data point from \mathcal{D} , $(\mathbf{x}^{(n)}, y^{(n)})$
 - b. Compute the pointwise gradient,
$$G^{(l)} = \nabla_{W^{(l)}} e(\mathbf{o}^{(L)}, y^{(n)}) \quad \forall l$$
 - c. Update $W^{(l)}$: $W_{t+1}^{(l)} \leftarrow W_t^{(l)} - \eta_{SGD}^{(0)} G^{(l)} \quad \forall l$
 - d. Increment t : $t \leftarrow t + 1$
- Output: $W_t^{(1)}, \dots, W_t^{(L)}$

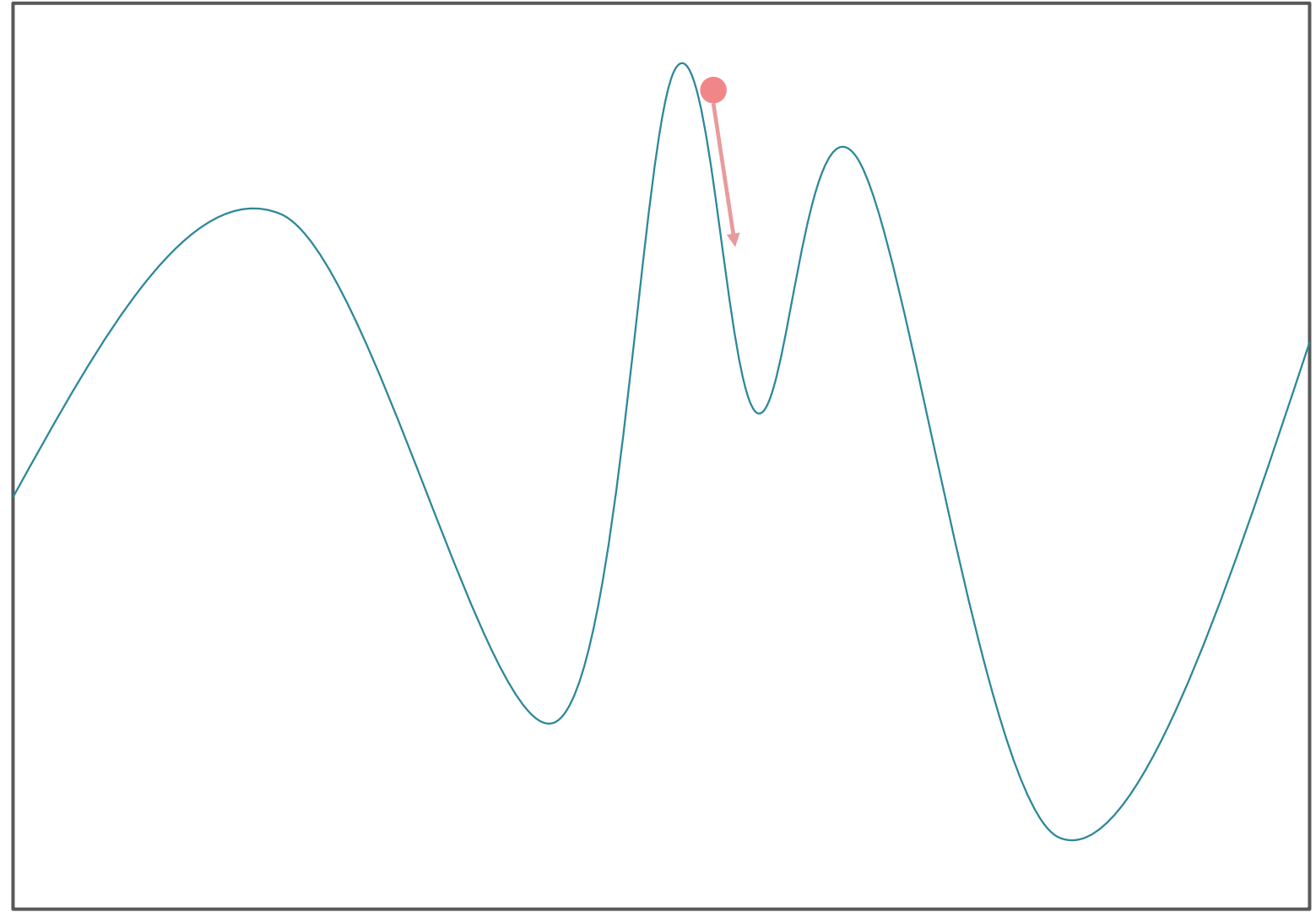
Mini-batch Stochastic Gradient Descent for Neural Networks

- Input: $\mathcal{D} = \{(\mathbf{x}^{(n)}, y^{(n)})\}_{n=1}^N, \eta_{MB}^{(0)}, B$
- 1. Initialize all weights $W_{(0)}^{(1)}, \dots, W_{(0)}^{(L)}$ to small, random numbers and set $t = 0$
- 2. While TERMINATION CRITERION is not satisfied
 - a. Randomly sample B data points from \mathcal{D} , $\{(\mathbf{x}^{(b)}, y^{(b)})\}_{b=1}^B$
 - b. Compute the gradient w.r.t. the sampled *batch*,
$$G^{(l)} = \frac{1}{B} \sum_{b=1}^B \nabla_{W^{(l)}} e(\mathbf{o}^{(L)}, y^{(b)}) \quad \forall l$$
 - c. Update $W^{(l)}$: $W_{t+1}^{(l)} \leftarrow W_t^{(l)} - \eta_{MB}^{(0)} G^{(l)} \quad \forall l$
 - d. Increment t : $t \leftarrow t + 1$
- Output: $W_t^{(1)}, \dots, W_t^{(L)}$

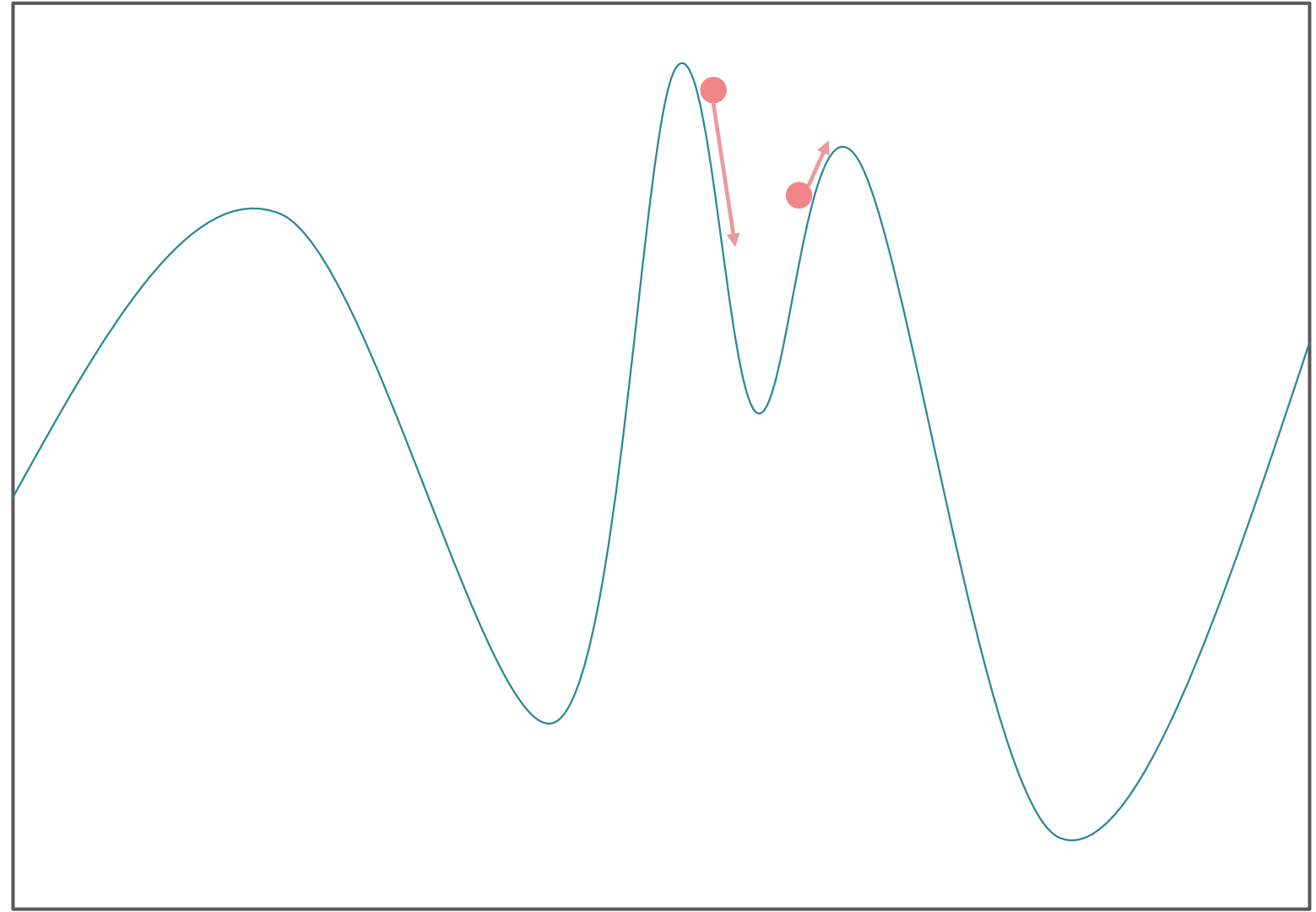
Mini-batch Stochastic Gradient Descent with Momentum for Neural Networks

- Input: $\mathcal{D} = \{(\mathbf{x}^{(n)}, y^{(n)})\}_{n=1}^N, \eta_{MB}^{(0)}, B, \beta$
- 1. Initialize all weights $W_{(0)}^{(1)}, \dots, W_{(0)}^{(L)}$ to small, random numbers and set $t = 0, G_{-1}^{(l)} = 0 \odot W^{(l)} \forall l = 1, \dots, L$
- 2. While TERMINATION CRITERION is not satisfied
 - a. Randomly sample B data points from $\mathcal{D}, \{(\mathbf{x}^{(b)}, y^{(b)})\}_{b=1}^B$
 - b. Compute the gradient w.r.t. the sampled *batch*,
$$G_t^{(l)} = \frac{1}{B} \sum_{b=1}^B \nabla_{W^{(l)}} e(\mathbf{o}^{(L)}, y^{(b)}) \forall l$$
 - c. Update $W^{(l)}$: $W_{t+1}^{(l)} \leftarrow W_t^{(l)} - \eta_{MB}^{(0)} (\beta G_{t-1}^{(l)} + G_t^{(l)}) \forall l$
 - d. Increment t : $t \leftarrow t + 1$
- Output: $W_t^{(1)}, \dots, W_t^{(L)}$

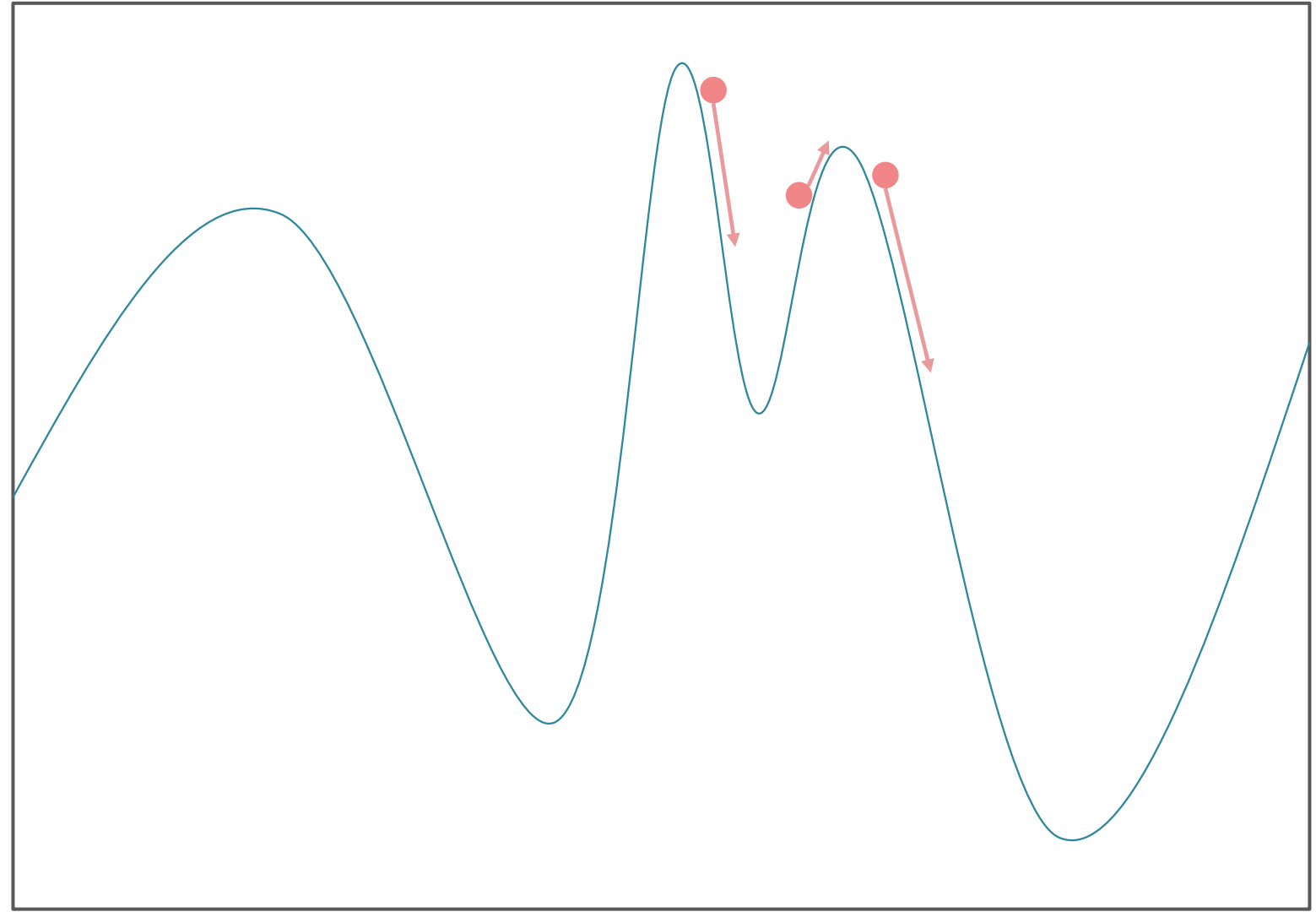
Mini-batch Stochastic Gradient Descent with Momentum for Neural Networks



Mini-batch Stochastic Gradient Descent with Momentum for Neural Networks



Mini-batch Stochastic Gradient Descent with Momentum for Neural Networks



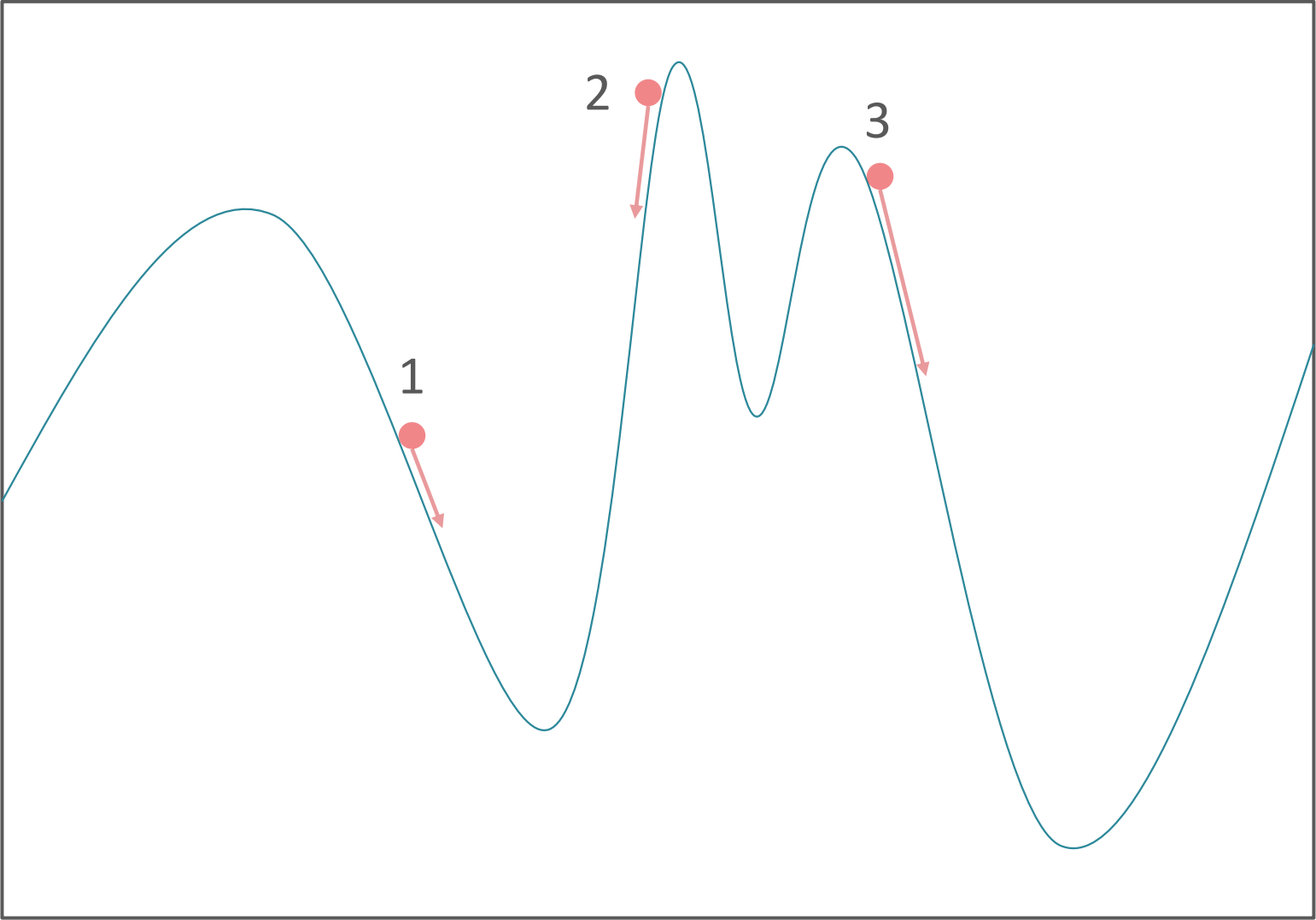
Mini-batch Stochastic Gradient Descent with Adaptive Gradients for Neural Networks

- Input: $\mathcal{D} = \{(\mathbf{x}^{(n)}, y^{(n)})\}_{n=1}^N, \eta_{MB}^{(0)}, B, \epsilon$
- 1. Initialize all weights $W_{(0)}^{(1)}, \dots, W_{(0)}^{(L)}$ to small, random numbers and set $t = 0, S_{-1}^{(l)} = 0 \odot W^{(l)} \forall l = 1, \dots, L$
- 2. While TERMINATION CRITERION is not satisfied
 - a. Randomly sample B data points from $\mathcal{D}, \{(\mathbf{x}^{(b)}, y^{(b)})\}_{b=1}^B$
 - b. Compute the gradient w.r.t. the sampled *batch*,
$$G_t^{(l)} = \frac{1}{B} \sum_{b=1}^B \nabla_{W^{(l)}} e(\mathbf{o}^{(L)}, y^{(b)}) \quad \forall l$$
 - c. Update $S^{(l)}$: $S_t^{(l)} = S_{t-1}^{(l)} + G_t^{(l)} \odot G_t^{(l)} \quad \forall l$
 - d. Update $W^{(l)}$: $W_{t+1}^{(l)} \leftarrow W_t^{(l)} - \frac{\eta_{MB}^{(0)}}{\sqrt{S_t^{(l)} + \epsilon}} \odot G_t^{(l)} \quad \forall l$
 - e. Increment t : $t \leftarrow t + 1$
- Output: $W_t^{(1)}, \dots, W_t^{(L)}$

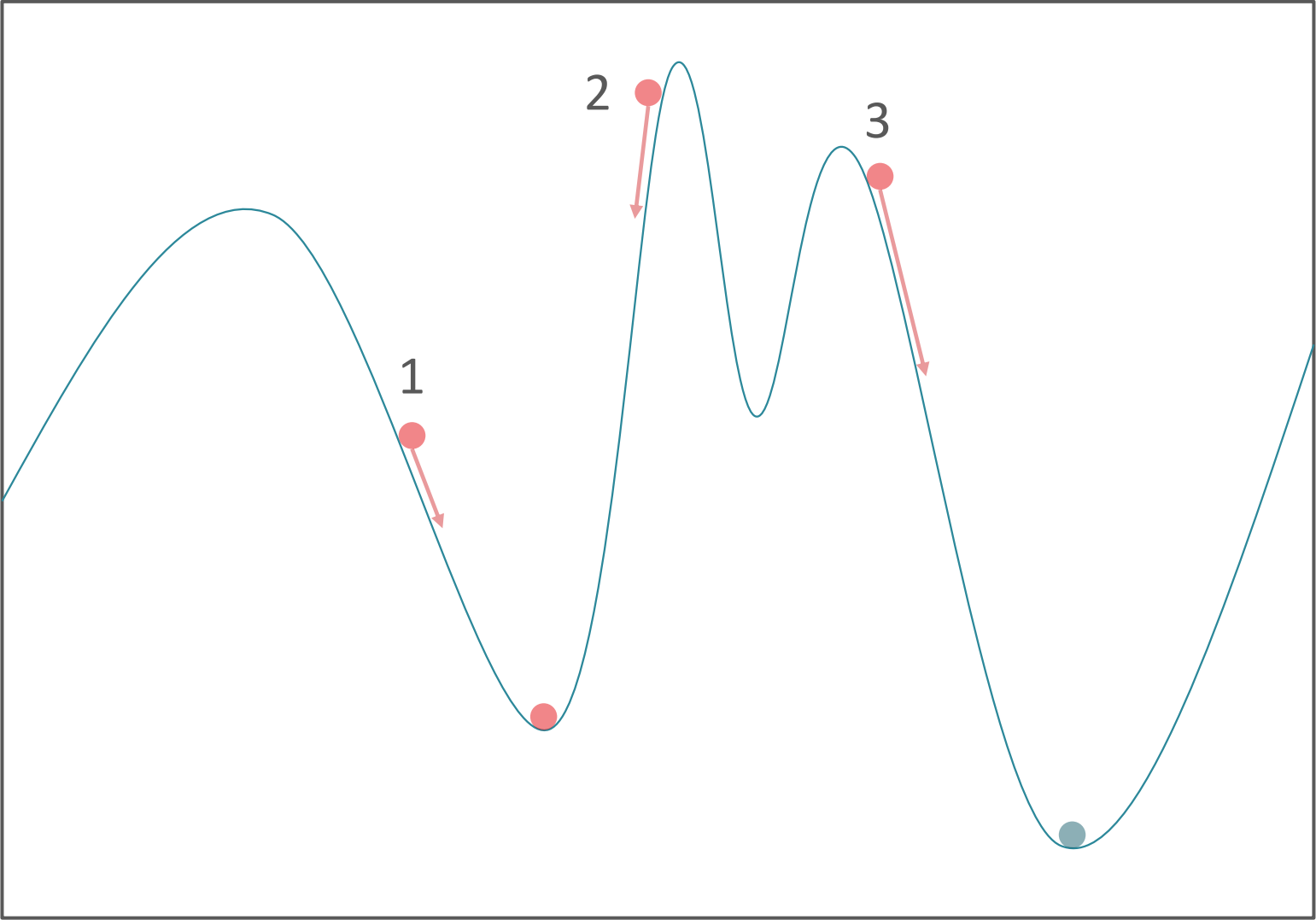
Random Restarts

- Run mini-batch gradient descent (with momentum & adaptive gradients) multiple times, each time starting with a *different, random* initialization for the weights.
- Compute the training error of each run at termination and return the set of weights that achieves the lowest training error.

Random Restarts

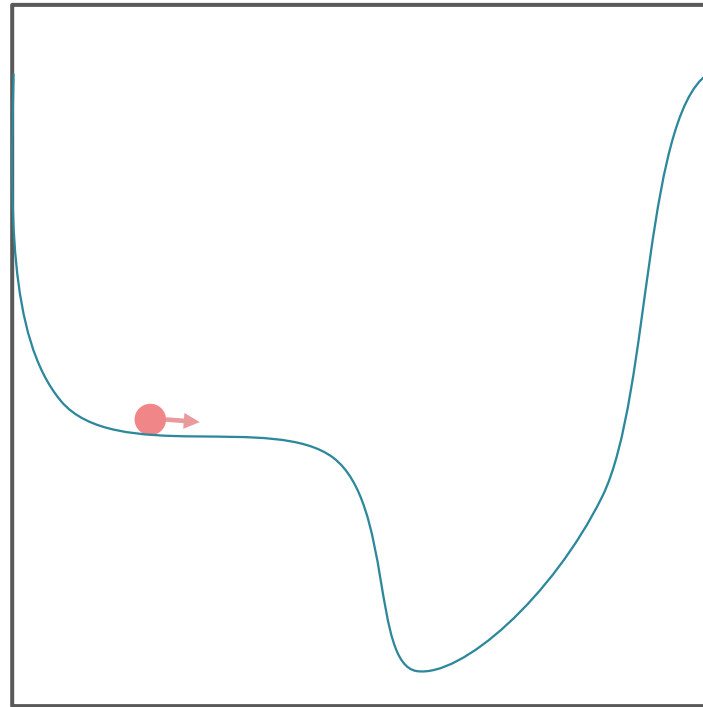


Random Restarts



Terminating Gradient Descent

- For non-convex surfaces, the gradient's magnitude is often not a good metric for proximity to a minimum



Terminating Gradient Descent “Early”

- For non-convex surfaces, the gradient’s magnitude is often not a good metric for proximity to a minimum
- Combine multiple termination criteria e.g. only stop if enough iterations have passed and the improvement in error is small
- Alternatively, terminate early by using a validation data set: if the validation error starts to increase, just stop!
 - Early stopping asks like regularization by **limiting how much of the hypothesis set** is explored

Neural Networks and Regularization

- Minimize $\ell_D^{AUG}(W^{(1)}, \dots, W^{(L)}, \lambda_C)$
 $= \ell_D(W^{(1)}, \dots, W^{(L)}) + \lambda_C \Omega(W^{(1)}, \dots, W^{(L)})$

e.g. L2 regularization

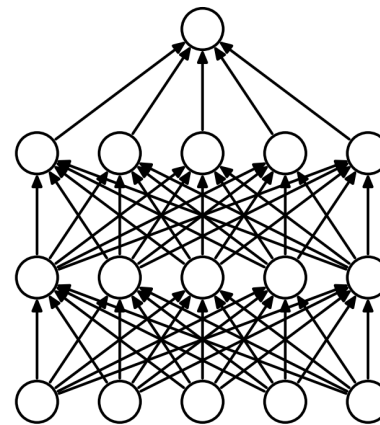
$$\Omega(W^{(1)}, \dots, W^{(L)}) = \sum_{l=1}^L \sum_{i=0}^{d^{(l-1)}} \sum_{j=1}^{d^{(l)}} (w_{j,i}^{(l)})^2$$

Neural Networks and “Strange” Regularization (Bishop, 1995)

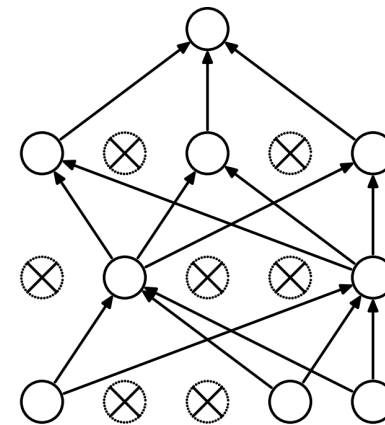
- Jitter
 - In each iteration of gradient descent, add some random noise or “jitter” to each training data point
 - Instead of computing the gradient w.r.t. $(\mathbf{x}^{(n)}, y^{(n)})$, use $(\mathbf{x}^{(n)} + \boldsymbol{\epsilon}, y^{(n)})$ where $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \sigma^2 I)$
 - Makes neural networks resilient to input noise
 - Has been proven to be equivalent to using a certain kind of regularizer Ω for some error metrics

Neural Networks and “Strange” Regularization (Srivastava et al., 2014)

- Dropout
 - In each iteration of gradient descent, randomly remove some of the nodes in the network
 - Compute the gradient using only the remaining nodes
 - The weights on edges going into and out of “dropped out” nodes are not updated



(a) Standard Neural Net



(b) After applying dropout.

Key Takeaways

- Backpropagation for efficient gradient computation
- Advanced optimization and regularization techniques for neural networks
 - Momentum can be used to break out of local minima
 - Adagrad helps when parameters behave differently w.r.t. step sizes
 - Random restarts
 - Jitter & dropout act like regularization for neural networks by preventing them fitting the training dataset perfectly