CS 190I Deep Learning Regularization

Lei Li (leili@cs)
UCSB

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Recap

- Back propagation for Feed-forward neural network
- Model evaluation
- Cross validation
- Overfitting and underfitting

Underfitting and Overfitting

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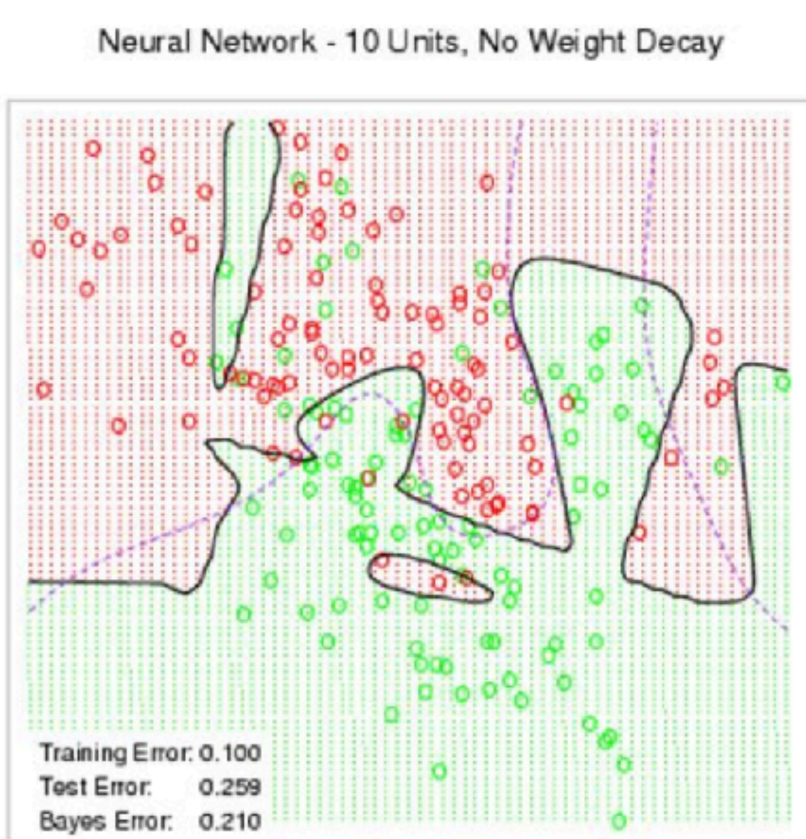
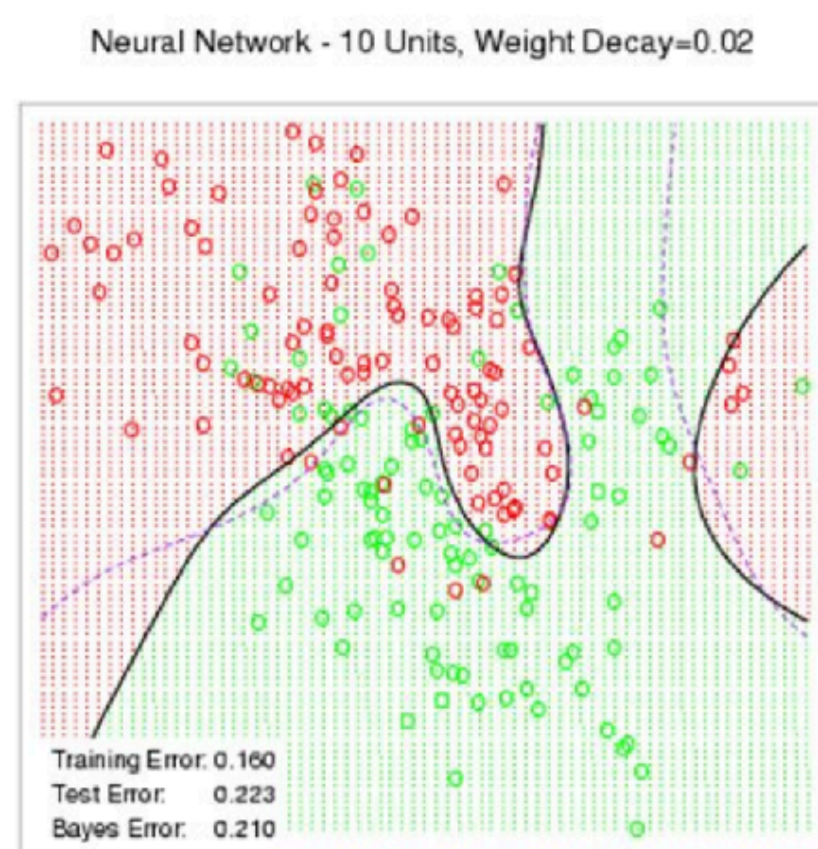
Regularization

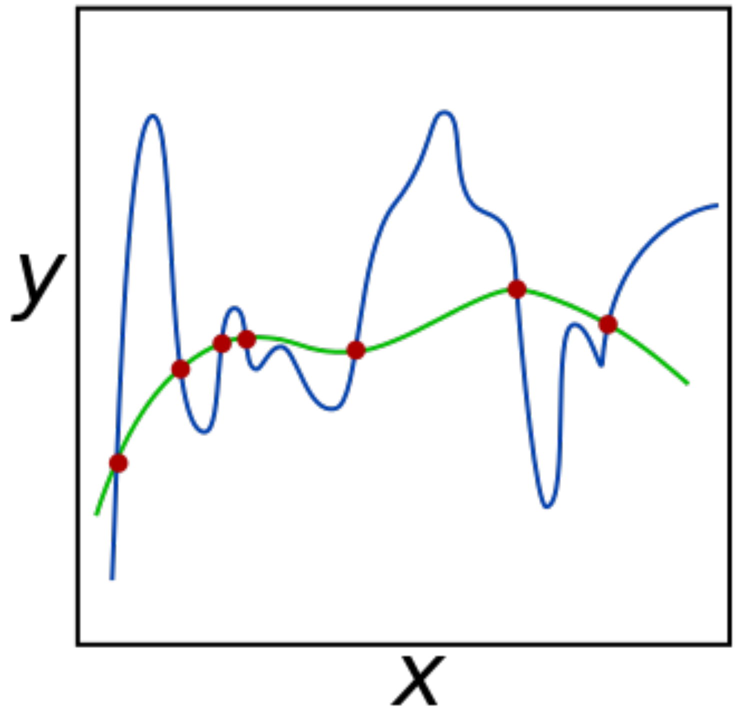




L_2 Regularization as Hard Constraint

- Reduce model complexity by limiting value range

$$\min \ \ell(\theta) \quad \text{subject to} \quad \|\theta\|^2 \leq \lambda$$



  – Often do not regularize bias *b*
    - Doing or not doing has little difference in practice
  – A small λ means more regularization

L_2 Regularization as Soft Constraint

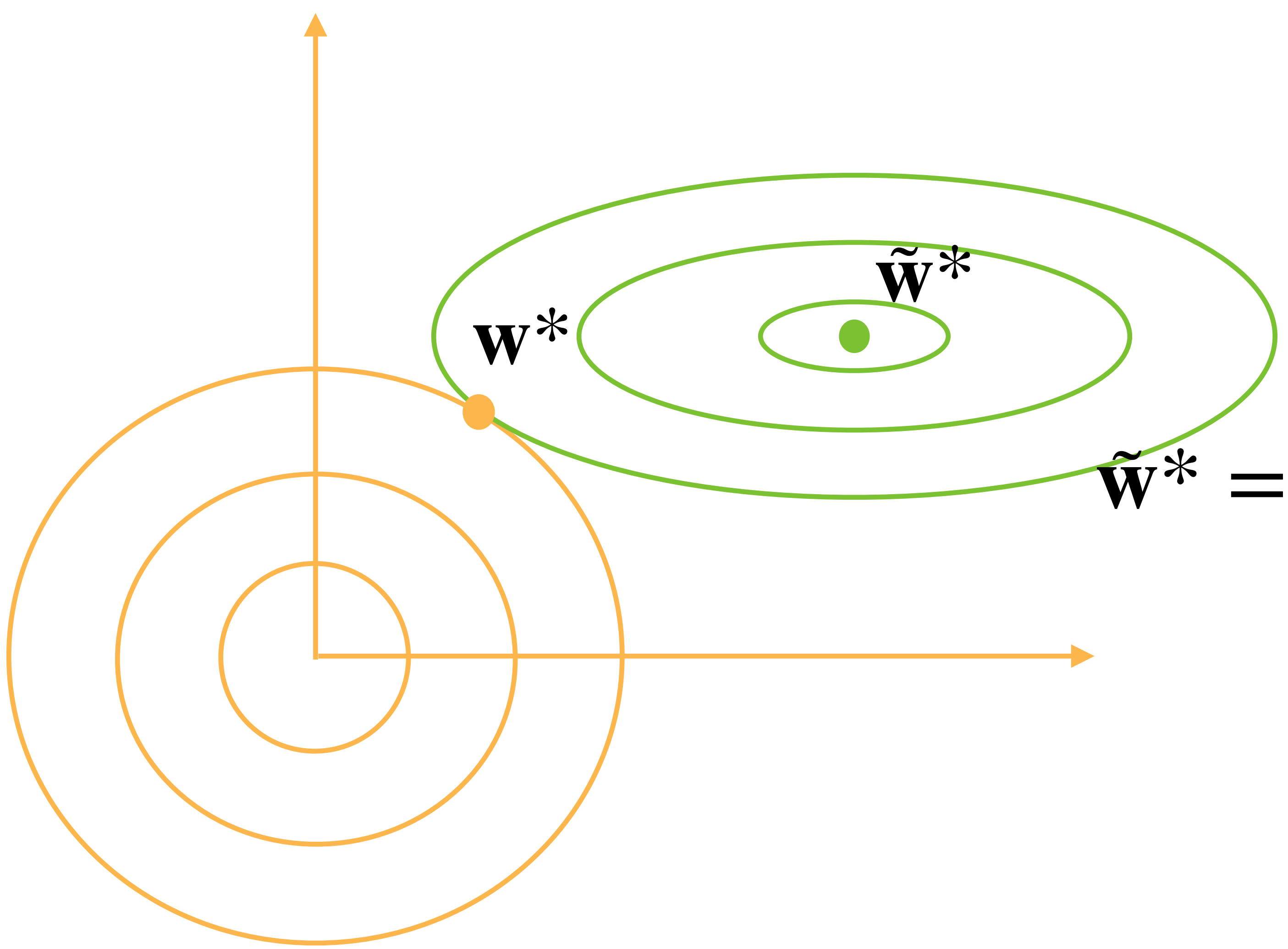
- Using Lagrangian multiplier method
- Minimizing the loss plus additional penalty

$$\min \quad \ell(\theta) + \frac{\lambda}{2} ||\theta||^2$$

  - Hyper-parameter controls regularization importance
  - $\lambda = 0$: no effect
  - $\lambda \to \infty, \theta^* \to \mathbf{0}$

Illustrate the Effect on Optimal Solutions

$$\mathbf{w}^* = \arg\min \ \frac{1}{2}\|w^T x + b - y\|_2^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$



$$\tilde{\mathbf{w}}^* = \arg\min \ \frac{1}{2}\|w^T x + b - y\|_2^2$$

Update Rule - Weight Decay

- Compute the gradient

$$\frac{\partial}{\partial \theta}\left(\ell(\theta) + \frac{\lambda}{2}\|\theta\|^2\right) = \frac{\partial \ell(\theta)}{\partial \theta} + \lambda\theta$$

- Update weight at step *t*

$$\theta_{t+1} = (1 - \eta\lambda)\theta_t - \eta\frac{\partial \ell(\theta_t)}{\partial \theta_t}$$

backprop

  – Often $\eta\lambda < 1$, so also called weight decay in deep learning

Weight Decay in Pytorch

```
import torch

learning_rate = 1e-3
weight_decay = 1.0
optimizer =
torch.optim.SGD(model.parameters()
, lr=learning_rate,
weight_decay=weight_decay)
```

General Penalty

- Minimizing the loss plus additional penalty

$$\min \ \ell(\theta) + R(\theta)$$

  - $\ell(\theta)$ is the original loss
  - $R(\theta)$ is penalty (or regularization term), not necessary smooth

L1 Regularization

- Minimizing the loss plus additional penalty

$$\min \ \ell(\theta) + \lambda |\theta|$$

  - $\ell(\theta)$ is the original loss
  - using L1 norm as penalty

L1 Update Rule - Soft Thresholding

- $\ell(\theta) + \lambda|\theta|$ is not always differentiable!
- Soft-threshold (Proximal operator):

$$S_\lambda(x) = \mathrm{sign}(x)\max(0, |x| - \lambda) = \mathrm{sign}(x)\mathrm{Relu}(|x| - \lambda)$$

- Update weight at step *t*

$$\tilde{\theta}_t = \theta_t - \eta \frac{\partial \ell(\theta_t)}{\partial \theta_t}$$

$$\theta_{t+1} = S_\lambda(\tilde{\theta})$$

- Also known as Proximal Gradient Descent

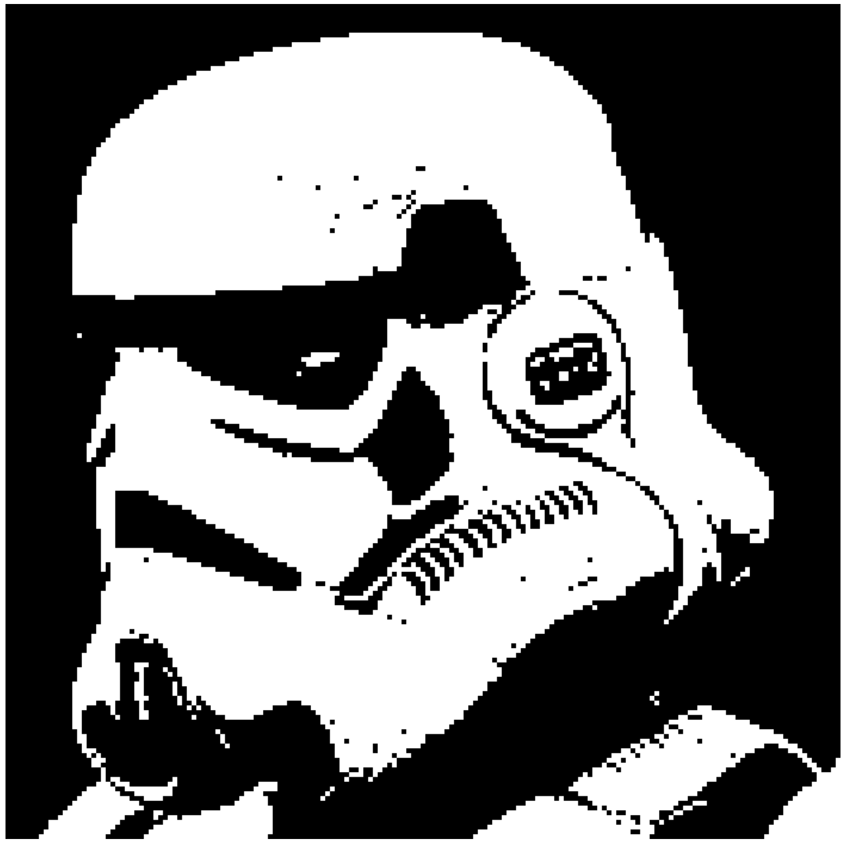
Effects of L1 and L2 Regularization

- L1 Regularization
  - will make parameters sparse (many parameters will be zeros)
  - could be useful for model pruning
- L2 Regularization
  - will make the parameter shrink towards 0, but not necessary 0.

Dropout

Motivation

- A good model should be robust under modest changes in the input
  - Dropout: inject noises into internal layers (simulating the noise)



Add Noise without Bias

- Add noise into ***x*** to get ***x'***, we hope

$$\mathbf{E}[\mathbf{x}'] = \mathbf{x}$$

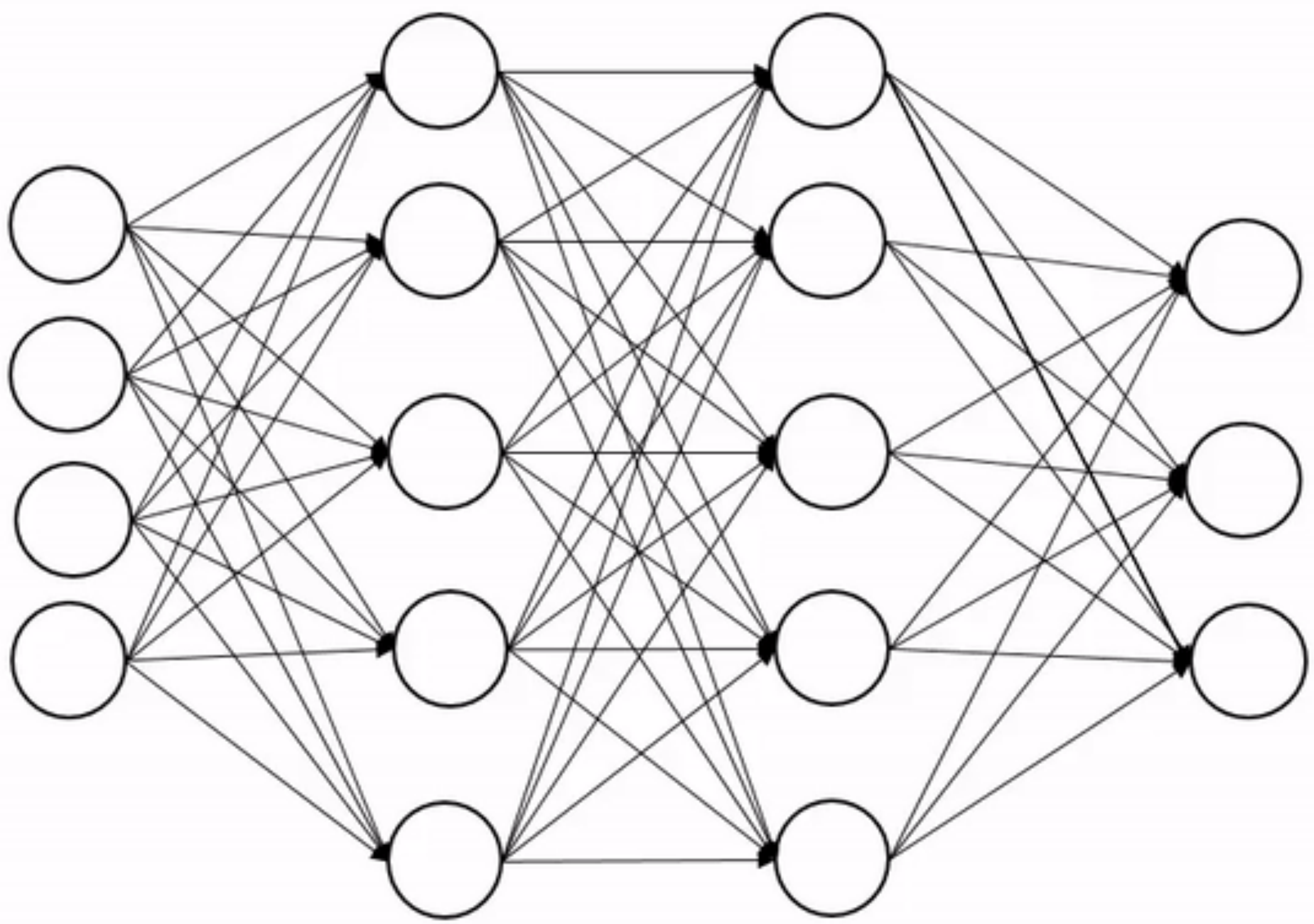
- Dropout perturbs each element by

$$x_i' = \begin{cases} 0 & \text{with probablity } p \\ \frac{x_i}{1-p} & \text{otherise} \end{cases}$$

Apply Dropout

- Often apply dropout on the output of hidden fully-connected layers

$$\mathbf{h} = \sigma(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$
$$\mathbf{h}' = \text{dropout}(\mathbf{h})$$
$$\mathbf{o} = \mathbf{W}_2\mathbf{h}' + \mathbf{b}_2$$
$$\mathbf{y} = \text{softmax}(o)$$



Dropout in Training and Inference

- Dropout is only used in training

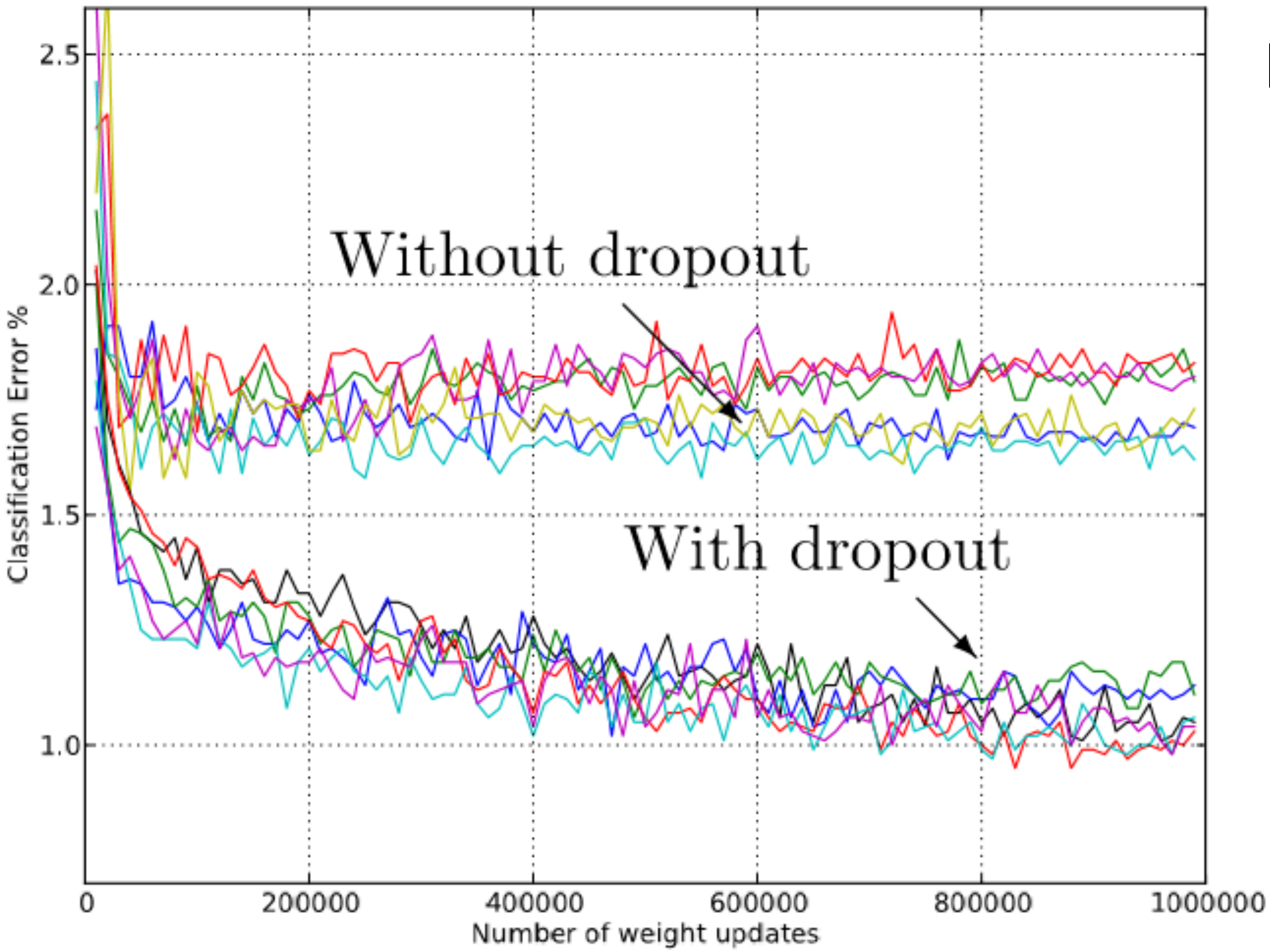
$$\mathbf{h}' = \text{dropout}(\mathbf{h})$$

- No dropout is applied during inference!
- Pytorch Layer:

```
torch.nn.Dropout(p=0.5)
```

Dropout: Typical results

- From Sr r different architect ropout
  - 2-4 hidc



Recap

- Regularization
  - to avoid model overfitting
  - L1 ==> more sparse parameters
  - L2/Weight decay ==> shrink parameters
  - Dropout, equivalent to L2, but as a network Layer

Numerical Stability

Gradients for Neural Networks

- Consider a network with *d* layers

$$\mathbf{h}^t = f_t(\mathbf{h}^{t-1}) \quad \text{and} \quad y = \ell \circ f_d \circ \ldots \circ f_1(\mathbf{x})$$

- Compute the gradient of the loss ℓ w.r.t. $\mathbf{W}_t$

$$\frac{\partial \ell}{\partial \mathbf{W}^t} = \frac{\partial \ell}{\partial \mathbf{h}^d} \underbrace{\frac{\partial \mathbf{h}^d}{\partial \mathbf{h}^{d-1}} \ldots \frac{\partial \mathbf{h}^{t+1}}{\partial \mathbf{h}^t}}_{\text{Multiplication of } d\text{-}t \text{ matrices}} \frac{\partial \mathbf{h}^t}{\partial \mathbf{W}^t}$$

Two Issues for Deep Neural Networks

- Two common issues with $\prod_{i=t}^{d-1} \frac{\partial \mathbf{h}^{i+1}}{\partial \mathbf{h}^{i}}$

Gradient Exploding

$1.5^{100} \approx 4 \times 10^{17}$

Gradient Vanishing

$0.8^{100} \approx 2 \times 10^{-10}$

Example: FFN

- Assume FFN (without bias for simplicity)

$$f_t(\mathbf{h}^{t-1}) = \sigma(\mathbf{W}^t\mathbf{h}^{t-1})$$ σ is the activation function

$$\frac{\partial \mathbf{h}^t}{\partial \mathbf{h}^{t-1}} = \text{diag}\left(\sigma'(\mathbf{W}^t\mathbf{h}^{t-1})\right)(W^t)^T$$ σ' is the gradient function of σ

$$\prod_{i=t}^{d-1} \frac{\partial \mathbf{h}^{i+1}}{\partial \mathbf{h}^i} = \prod_{i=t}^{d-1} \text{diag}\left(\sigma'(\mathbf{W}^i\mathbf{h}^{i-1})\right)(W^i)^T$$

Gradient Exploding

- Use ReLU as the activation function

$$\sigma(x) = \max(0,x) \quad \text{and} \quad \sigma'(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases}$$

- Elements of $\prod_{i=t}^{d-1} \frac{\partial \mathbf{h}^{i+1}}{\partial \mathbf{h}^i} = \prod_{i=t}^{d-1} \text{diag}\left(\sigma'(\mathbf{W}^i \mathbf{h}^{i-1})\right)(W^i)^T$ may from $\prod_{i=t}^{d-1} (W^i)^T$
  - Leads to large values when *d-t* is large

$$1.5^{100} \approx 4 \times 10^{17}$$

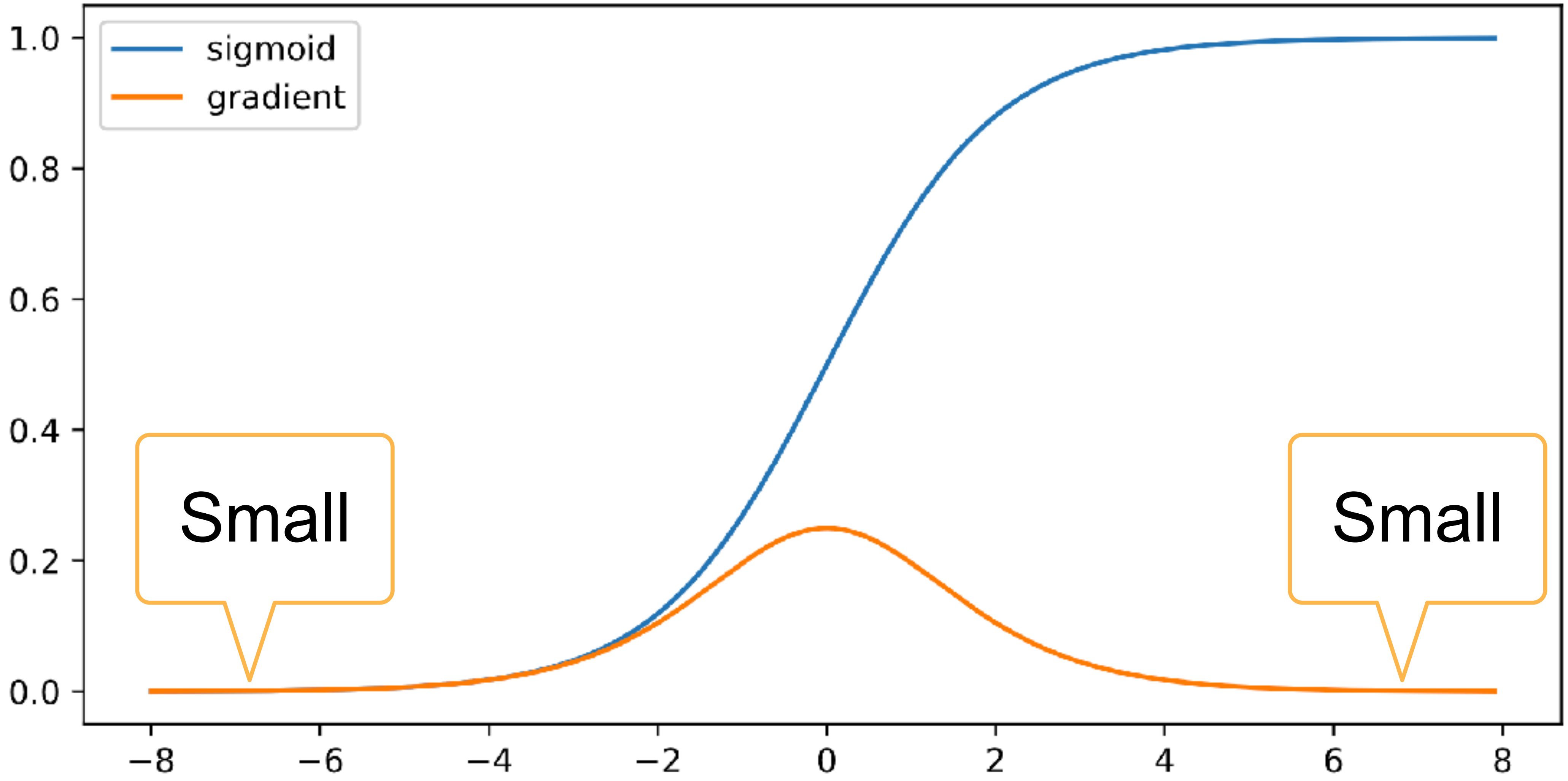
Issues with Gradient Exploding

- Value out of range: infinity value
  - Severe for using 16-bit floating points
    - Range: 6E-5 ~ 6E4
- Sensitive to learning rate (LR)
  - Not small enough LR -> large weights -> larger gradients
  - Too small LR -> No progress
  - May need to change LR dramatically during training

Gradient Vanishing

- Use sigmoid as the activation function

$$\sigma(x) = \frac{1}{1 + e^{-x}} \qquad \sigma'(x) = \sigma(x)(1 - \sigma(x))$$



Gradient Exploding

- Use sigmoid as the activation function

$$\sigma(x) = \frac{1}{1+e^{-x}} \qquad \sigma'(x) = \sigma(x)(1-\sigma(x))$$

- Elements $\prod_{i=t}^{d-1} \frac{\partial \mathbf{h}^{i+1}}{\partial \mathbf{h}^{i}} = \prod_{i=t}^{d-1} \text{diag}\left(\sigma'(\mathbf{W}^i \mathbf{h}^{i-1})\right)(W^i)^T$ are products of *d-t* small values

$$0.8^{100} \approx 2 \times 10^{-10}$$

Issues with Gradient Vanishing

- Gradients with value 0
  - Severe with 16-bit floating points
- No progress in training
  - No matter how to choose learning rate
- Severe with bottom layers
  - Only top layers are well trained
  - No benefit to make networks deeper

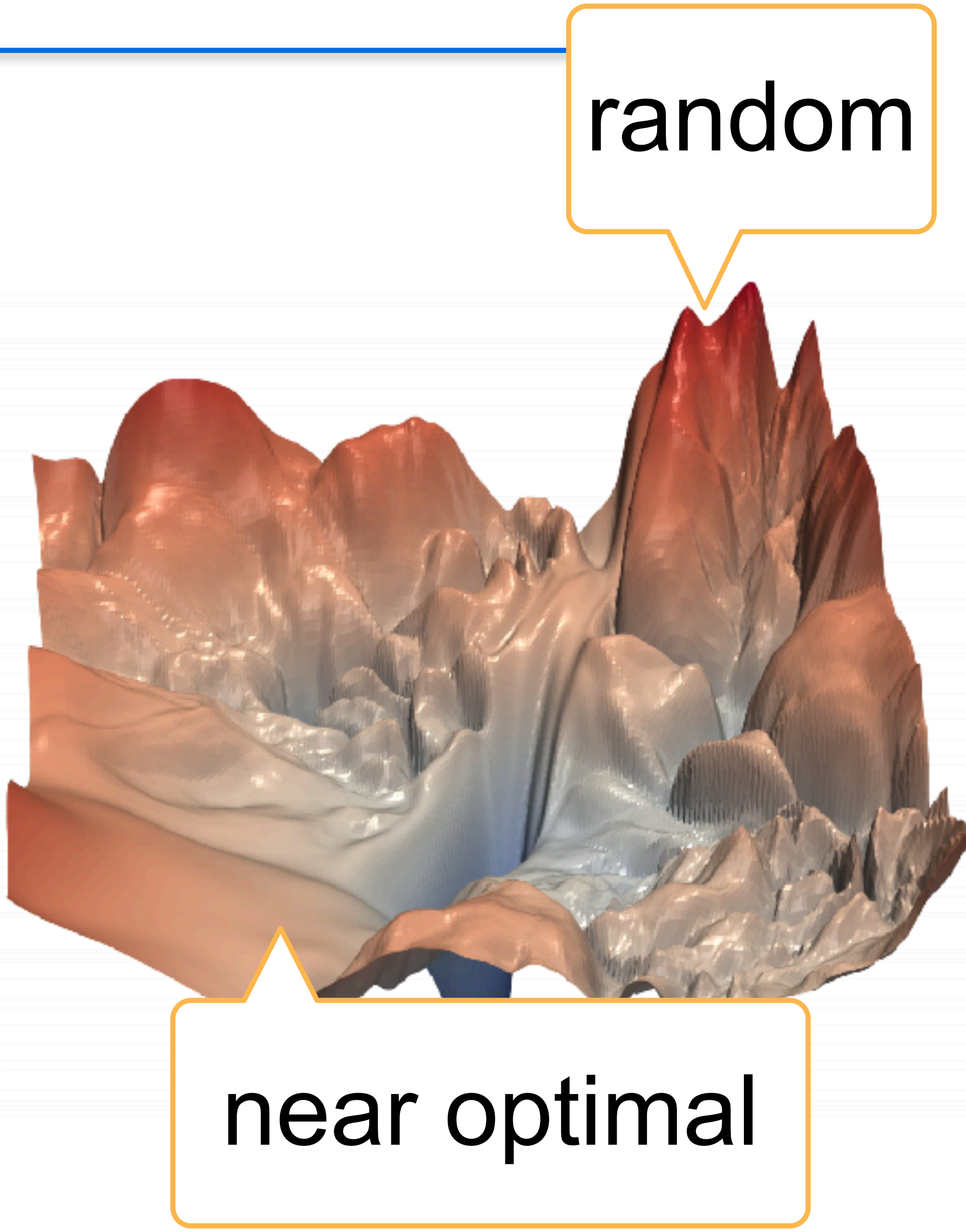
Stabilize Training

Stabilize Training

- Goal: make sure gradient values are in a proper range
  - E.g. in [1e-6, 1e3]
- Multiplication -> plus
  - ResNet, LSTM (later lecture)
- Normalize
  - Gradient clipping
  - Batch Normalization / Layer Normalization (later)
- Proper weight initialization and activation functions

Weight Initialization

- Initialize weights with random values in a proper range
- The beginning of training easily suffers to numerical instability
  - The surface far away from an optimal can be complex
  - Near optimal may be flatter
- Initializing according to $\mathcal{N}(0, 0.01)$ works well for small networks, but not guarantee for deep neural networks



Constant Variance for each Layer

- Treat both layer outputs and gradients are random variables
- Make the mean and variance for each layer's output are same, similar for gradients

Forward

$$\mathbb{E}[h_i^t] = 0$$

$$\mathrm{Var}[h_i^t] = a$$

Backward

$$\mathbb{E}\left[\frac{\partial \ell}{\partial h_i^t}\right] = 0 \quad \mathrm{Var}\left[\frac{\partial \ell}{\partial h_i^t}\right] = b \qquad \forall i, t$$

a and *b* are constants

Example: FFN

- Assumptions $\mathbb{E}[w_{i,j}^t] = 0,\ \mathrm{Var}[w_{i,j}^t] = \gamma_t$
  - i.i.d $w_{i,j}^t$
  - h_i^{t-1} is independent to $w_{i,j}^t$
  - identity activation: $\mathbf{h}^t = \mathbf{W}^t \mathbf{h}^{t-1}$ with $\mathbf{W}^t \in \mathbb{R}^{n_t \times n_{t-1}}$

$$\mathbb{E}[h_i^t] = \mathbb{E}\left[\sum_j w_{i,j}^t h_j^{t-1}\right] = \sum_j \mathbb{E}[w_{i,j}^t]\mathbb{E}[h_j^{t-1}] = 0$$

Forward Variance

$$\mathrm{Var}[h_i^t] = \mathbb{E}[(h_i^t)^2] - \mathbb{E}[h_i^t]^2 = \mathbb{E}\left[\left(\sum_j w_{i,j}^t h_j^{t-1}\right)^2\right]$$

$$= \mathbb{E}\left[\sum_j \left(w_{i,j}^t\right)^2 \left(h_j^{t-1}\right)^2 + \sum_{j \neq k} w_{i,j}^t w_{i,k}^t h_j^{t-1} h_k^{t-1}\right]$$

$$= \sum_j \mathbb{E}\left[\left(w_{i,j}^t\right)^2\right] \mathbb{E}\left[\left(h_j^{t-1}\right)^2\right]$$

$$= \sum_j \mathrm{Var}[w_{i,j}^t]\mathrm{Var}[h_j^{t-1}] = n_{t-1}\gamma_t \mathrm{Var}[h_j^{t-1}] \quad \Rightarrow \quad n_{t-1}\gamma_t = 1$$

n_{t-1} is the number of units in t-1 layer

Backward Mean and Variance

- Apply forward analysis as well

$$\frac{\partial \ell}{\partial \mathbf{h}^{t-1}} = \frac{\partial \ell}{\partial \mathbf{h}^{t}} \mathbf{W}^{t} \quad \text{leads to} \quad \left(\frac{\partial \ell}{\partial \mathbf{h}^{t-1}}\right)^{T} = (W^{t})^{T} \left(\frac{\partial \ell}{\partial \mathbf{h}^{t}}\right)^{T}$$

$$\mathbb{E}\left[\frac{\partial \ell}{\partial h_i^{t-1}}\right] = 0$$

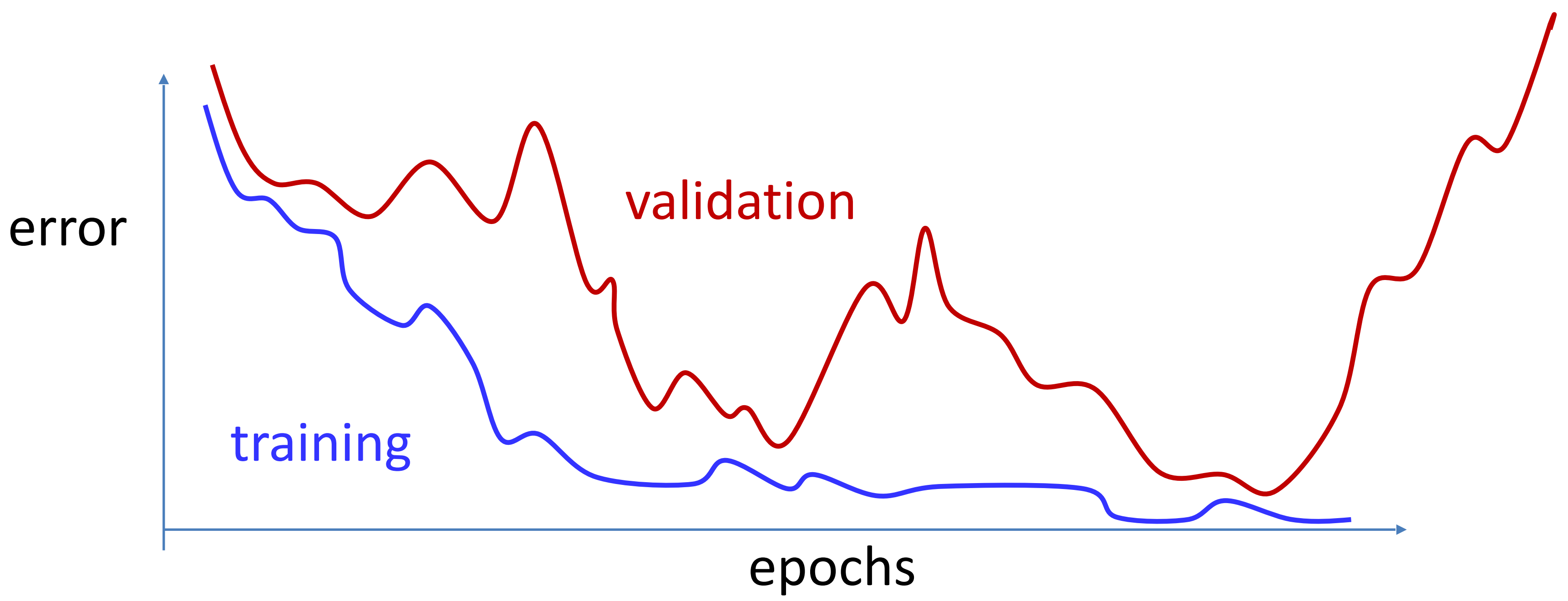
$$\mathrm{Var}\left[\frac{\partial \ell}{\partial h_i^{t-1}}\right] = n_t \gamma_t \mathrm{Var}\left[\frac{\partial \ell}{\partial h_j^{t}}\right] \quad \Rightarrow \quad n_t \gamma_t = 1$$

Xavier Initialization

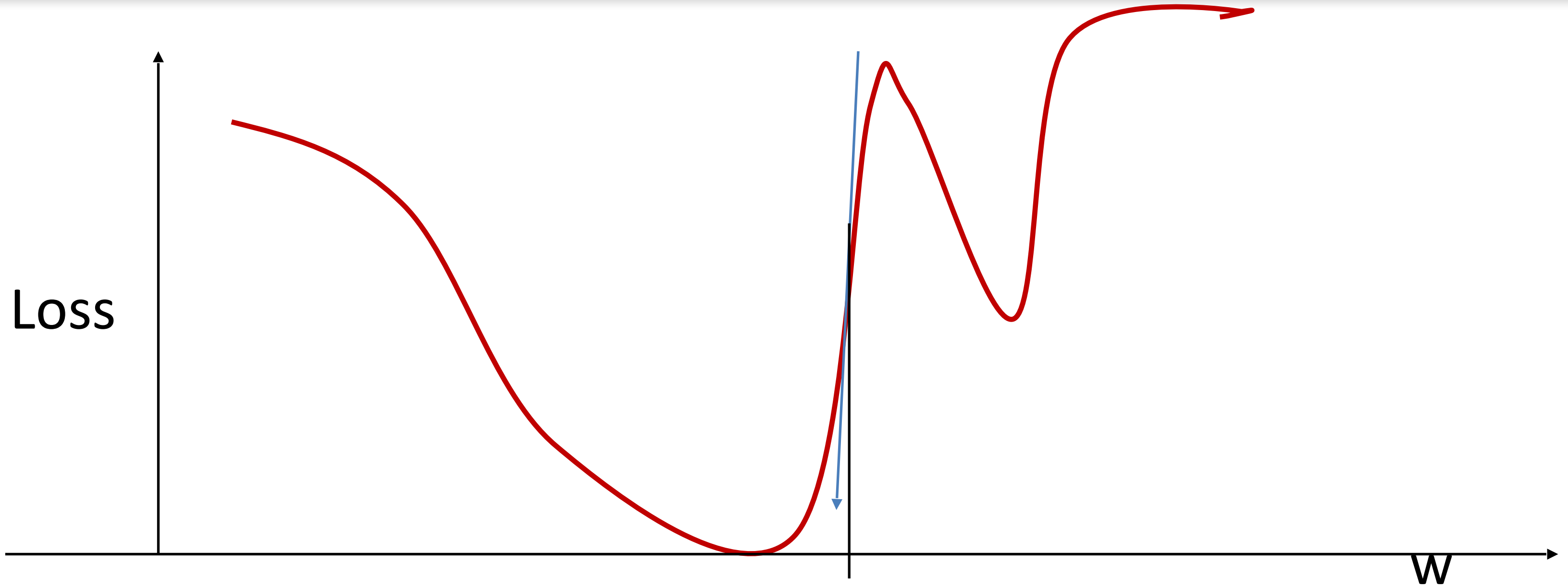
- Conflict goal to satisfies both $n_{t-1}\gamma_t = 1$ and $n_t\gamma_t = 1$
- Xavier $\gamma_t(n_{t-1} + n_t)/2 = 1 \quad \rightarrow \quad \gamma_t = 2/(n_{t-1} + n_t)$
  - Normal distribution $\mathcal{N}\left(0, \sqrt{2/(n_{t-1} + n_t)}\right)$
  - Uniform distribution $\mathcal{U}\left(-\sqrt{6/(n_{t-1} + n_t)}, \sqrt{6/(n_{t-1} + n_t)}\right)$
    - Variance of $\mathcal{U}[-a, a]$ is $a^2/3$
- Adaptive to weight shape, especially when n_t varies

Other heuristics: Early stopping

- Continued training can result in over fitting to training data
  - Track performance on a held-out validation set
  - Apply one of several early-stopping criterion to terminate training when performance on validation set degrades significantly



Additional heuristics: Gradient clipping



- Often the derivative will be too high
  - When the divergence has a steep slope
  - This can result in instability
- **Gradient clipping**: set a ceiling on derivative value

$$if\ \partial_w D > \theta\ then\ \partial_w D = \theta$$

  - Typical θ value is 5

– Can be easily set in pytorch/tensorflow

Recap

- Numerical issues in training
  - gradient explosion
  - gradient vanishing
- Proper initialization of parameters

Next Up

- Convolutional Neural Networks
- Visual perception:
  - Image classification
  - Object recognition
  - Face detection