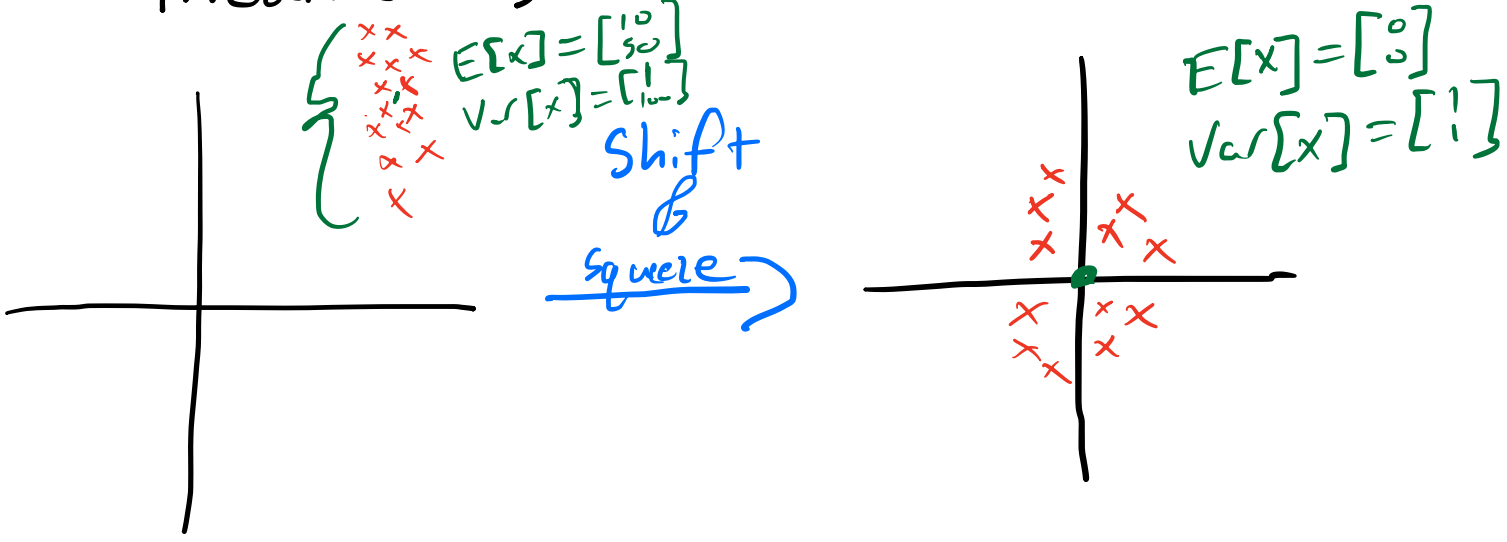
Last time

Normalization: keep data at consistent mean ($E[x]$) and variance ($Var[x]$).



Motivation

1) Gradient Scale

$$\left|\frac{dL}{dw_1}\right| = |x|\,|\sigma'(xw_1+b_1)| \prod_{i=2}^{l} \left|\frac{d\phi_i}{d\phi_{i-1}}\right| \dots$$

(Prevent scale of data from affecting gradient)

2) Scale mismatch

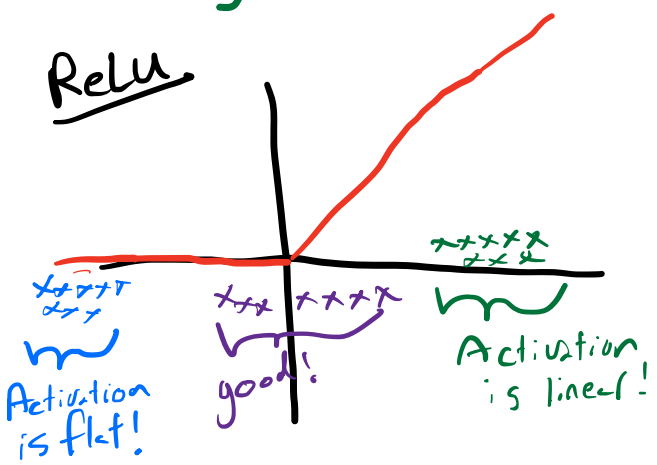
e.g. $x_1 = \begin{bmatrix} 2152 \\ 0.02 \end{bmatrix}$ $x_2 = \begin{bmatrix} 1092 \\ 0.017 \end{bmatrix}$ ...

We saw why this is a problem!

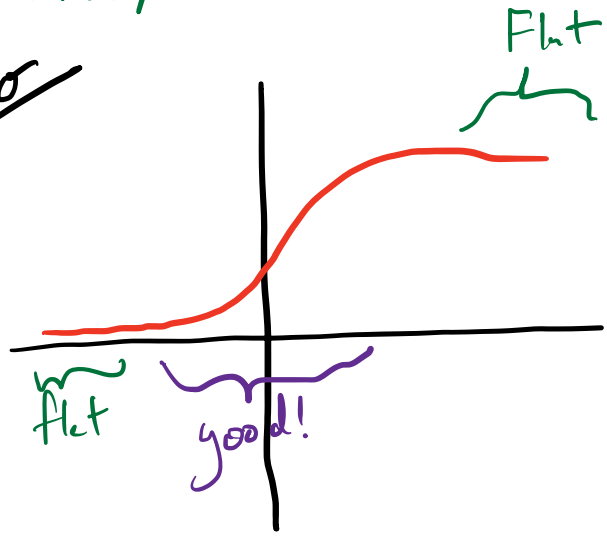
Motivation

3) Activations only make sense near 0

ReLU



or



Normalization

$$\text{Norm}(x) = \frac{x - E[x]}{\sqrt{\text{Var}[x] + \epsilon}}$$

Prevent div. by 0! $\epsilon \ll 1$

Estimate $E[x]$, $\text{Var}[x]$ from dataset or Batch

$$E[x] \approx \bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

$$\text{Var}[x] \approx s^2 = \frac{1}{N-1} \sum_{i=1}^{N} \left(x_i - \bar{x} \right)^2$$

Unbiased estimator

$$E[Norm(x)] = E\left[\frac{x - E[x]}{\sqrt{Var[x] + \epsilon}}\right]$$

$$= \frac{1}{\sqrt{Var[x] + \epsilon}}\left[E[x] - E[x]\right] = 0$$

Batch Normalization

$$\text{BatchNorm}(x) = \frac{x - E[x]}{\sqrt{Var[x] + \epsilon}}$$

ϵ: prevent div. by 0!

Estimate $E[x]$, $Var[x]$ from dataset or **Batch**

← Batch sampled for SGD

$$E[x] \approx \bar{x} = \frac{1}{B}\sum_{i=1}^{B} x_i$$

$$Var[x] \approx s^2 = \frac{1}{B-1}\sum_{i=1}^{B}\left(x_i - \bar{x}\right)^2$$

$B-1$: Unbiased estimator

Deep Network

$$f(x) = \phi_\ell(\phi_{\ell-1}(\dots \phi_1(x)))w_0 + b_0$$

Composing feature transforms

e.g.

$$f(x) = \sigma(\sigma(\dots\sigma(x^T W_1 + b_1)^T W_2 + b_2)\dots)^T W_\ell + b_\ell)w_0 + b_0$$

or

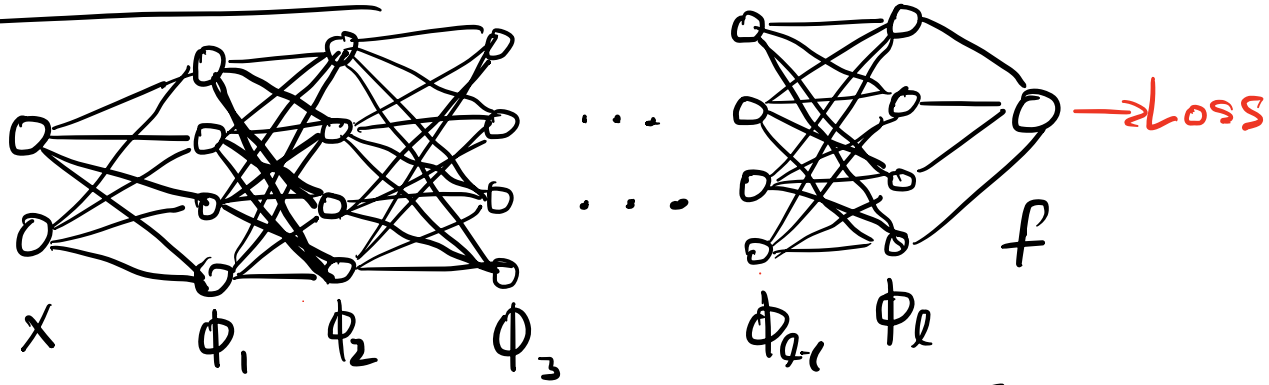
$$\phi_1 = \sigma(x^T W_1 + b_1)$$
$$\phi_2 = \sigma(\phi_1^T W_2 + b_2)$$
$$\vdots$$
$$\phi_\ell = \sigma(\phi_{\ell-1}^T W_\ell + b_\ell)$$

$$f = \phi_\ell^T w_0 + b_0$$
$$L = \text{Loss}(f, y)$$

e.g. $(f-y)^2$ MSE

Deep Network

ℓ-Layer network



or

$$\phi_1 = \sigma(x^T W_1 + b_1)$$
$$\phi_2 = \sigma(\phi_1^T W_2 + b_2)$$
$$\vdots$$
$$\phi_\ell = \sigma(\phi_{\ell-1}^T W_\ell + b_\ell)$$

$$f = \phi_\ell^T W_0 + b_0$$
$$L = \text{Loss}(f, y)$$

e.g. $(f-y)^2$

$E[x] = 0$ $\quad Var[x] = 1$ $\quad$ w/ Norm.

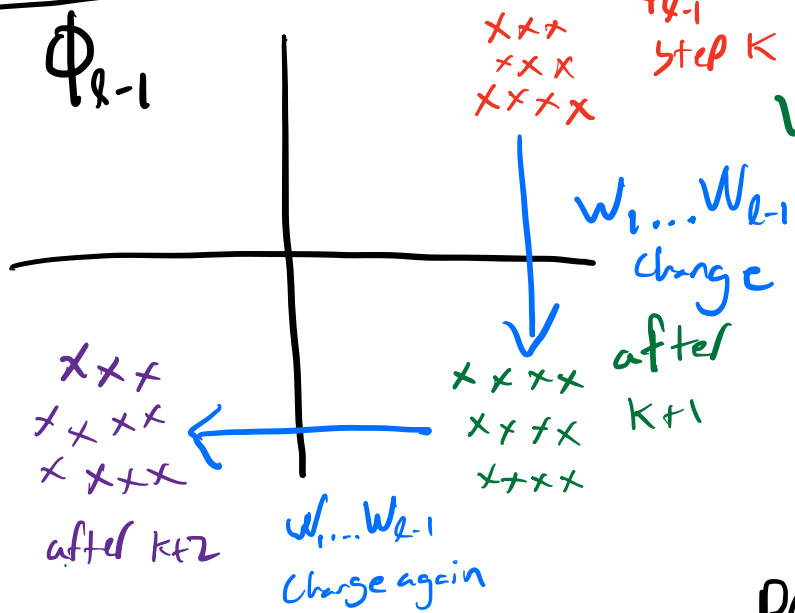
$E[\phi_{\ell-1}] = ?$ $\quad Var[\phi_{\ell-1}] = ?$

Depend on $W_1 \ldots W_{\ell-1}$ which could change

Distribution Shift

Layer ℓ

$$\phi_\ell = \sigma(\phi_{\ell-1} W_\ell + b_\ell)$$



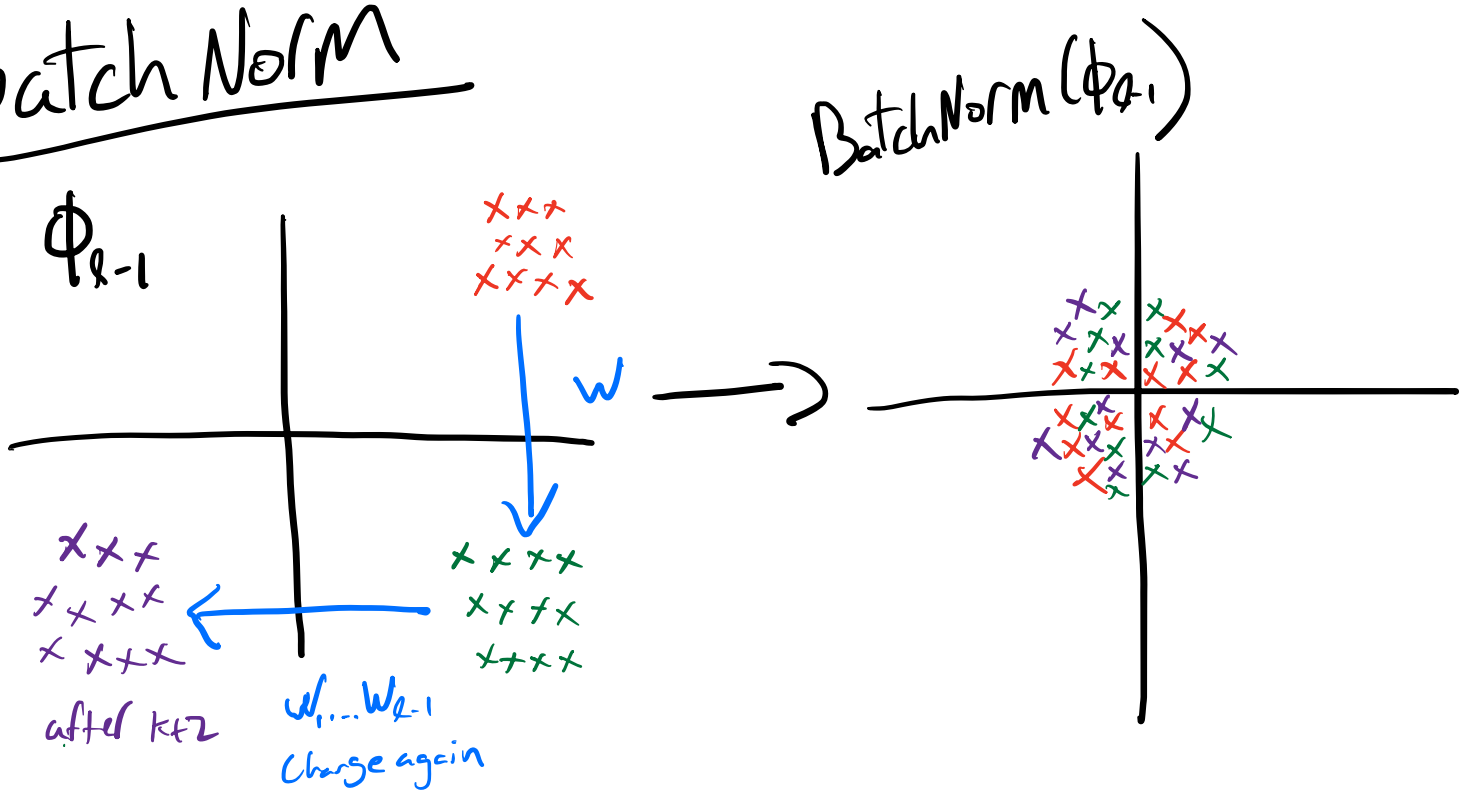
$$W_\ell^{(k+1)} \leftarrow W_\ell^{(k)} - \alpha \phi_{\ell-1}^{(k)} \sigma'\left(\phi_{\ell-1}^{(k)} W_\ell^{(k)} + b_\ell\right)$$

update using old $\phi_{\ell-1}^{(k)}$

$$f(x) = \sigma\left(\phi_{\ell-1}^{(k+1)} W_\ell^{(k+1)} + b_\ell\right) \dots$$

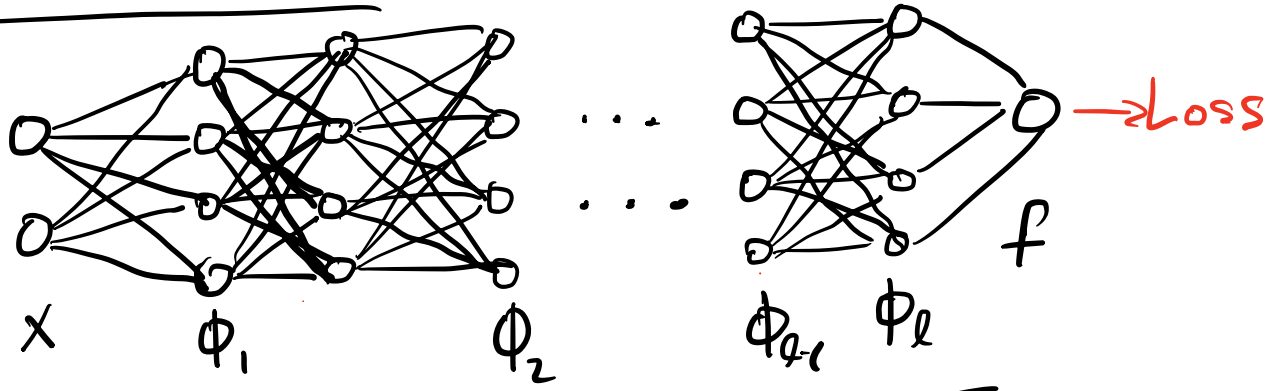
Predict using new $\phi_{\ell-1}^{(k+1)}$

Batch Norm



Can apply BatchNorm In the network

Deep Network w/ Batch Norm!



or

$$\phi_1 = \sigma(BN(x)^T W_1 + b_1) \qquad f = BN(\phi_\ell)^T W_0 + b_0$$

$$\phi_2 = \sigma(BN(\phi_1)^T W_2 + b_2) \qquad L = \text{Loss}(f, y)$$

$$\vdots$$

$$\phi_\ell = \sigma(BN(\phi_{\ell-1})^T W_\ell + b_\ell)$$

e.g. $(f-y)^2$

$E[x] = 0 \quad Var[x] = 1$ w/ Norm.

$E[BN(\phi_{\ell-1})] = 0 \quad Var[BN(\phi_{\ell-1})] = 1$

Deep Network w/ Batch Norm

$E[BN(\phi_{l-1})] = 0 \quad Var[BN(\phi_{l-1})] = 1$

$E[\phi_{l-1}]$, $Var[\phi_{l-1}]$ still change every step

∴ We need to use Batch Norm and update $\bar{x} \approx E[x]$ and $s^2 \approx Var[x]$ at every step

($E[\phi_{l-1}]$ for layer l)

Test time

Problem: At test time we might want to make a prediction on a single obs.

Single obs. → $B = 1$

$\bar{x} = \frac{1}{1} x_1$ $\quad s^2 = \frac{1}{1-1}(x_1 - \bar{x})^2$

$x_1 - \bar{x} = 0$! $\quad$ $= 0 \rightarrow$ divide by 0!

Batch Norm at test time

In practice: Maintain Running Average of mean and variance estimates as we go. (using EMA!)

At step k: $\bar{X}^{(k)}_{Avg.} \leftarrow \beta \bar{X}^{(k-1)}_{Avg.} + (1-\beta)\bar{X}^{(k)}$ $\beta \in [0,1]$ typically ≥ 0.9

Est. using current batch

$S^{2\,(k)}_{Avg.} \leftarrow \beta S^{2\,(k-1)}_{Avg.} + (1-\beta) S^{2\,(k)}$

At test:

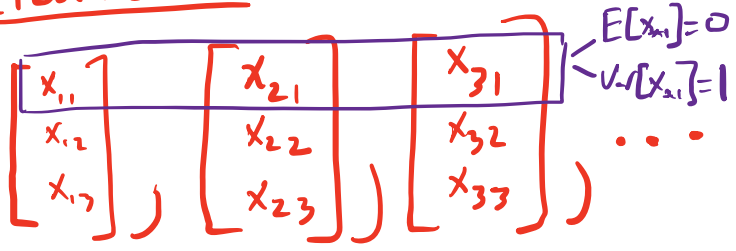
$$\underset{\text{test}}{\text{BatchNorm}}(x) = \frac{x - \bar{X}_{Avg.}}{\sqrt{S^2_{Avg.} + \varepsilon}}$$

Use the same estimates every time we evaluate

LayerNorm

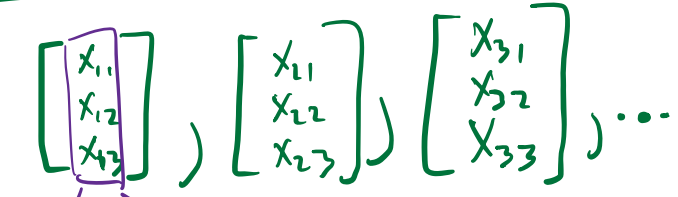
What if we don't want to do separate things at train and test time?

Batch norm



Find $\bar{x} \approx E[x]$, $s \approx Var[x]$ by Averaging over observations for each dimension

LayerNorm



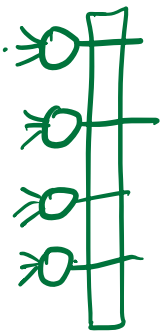
Alt. Average over dimensions within an observation

Layer Norm

$$\text{LayerNorm}(x_i) = \frac{x_i - \bar{x}_i}{\sqrt{s_i^2 + \varepsilon}}$$

$$\bar{x}_i = \frac{1}{d}\sum_{j=1}^{d} x_{ij} \qquad s^2 = \frac{1}{d-1}\sum_{j=1}^{d}(x_{ij} - \bar{x}_i)^2$$

In network



$E[x] = 0, \text{Var}[x] = 1$

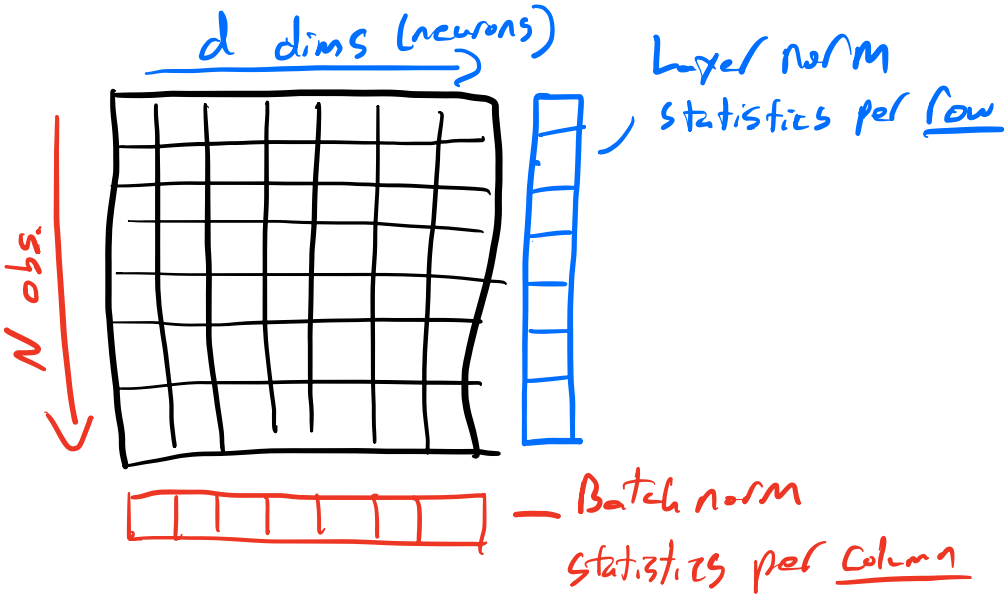
Can be applied w/ Batch size 1! As long as $d > 1$

Batch Norm Vs. Layer Norm

Input matrix

X

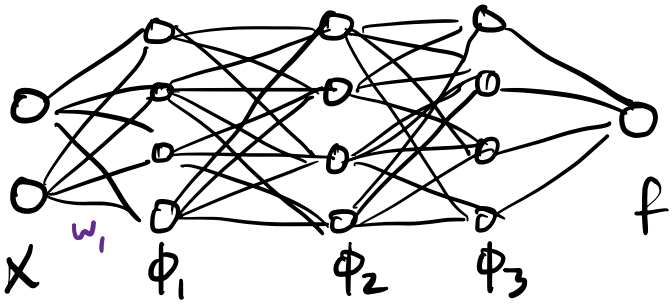
$N \times d$

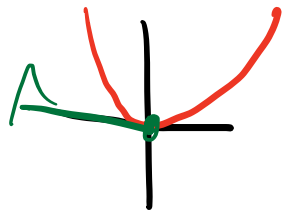


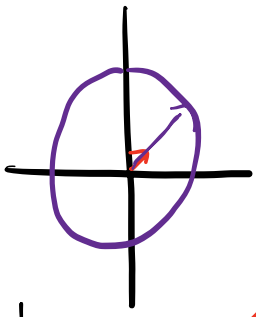
Batch Norm Usually preferred, but not always possible

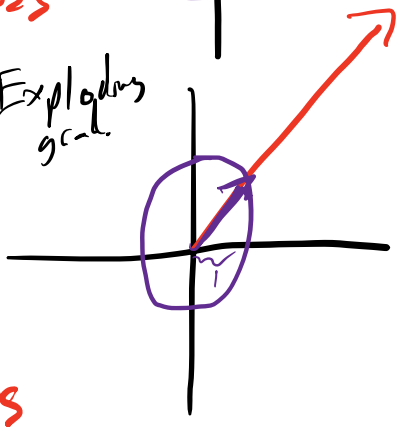
[preserves more info about each observation]

Residual Networks

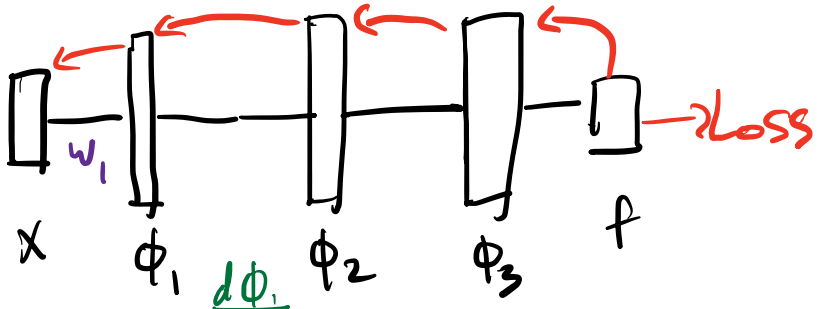








Simplified



$$\frac{dL}{dw_1} = \underbrace{x\sigma'(x^T w_1)}_{\frac{d\phi_1}{dw_1}} \frac{d\phi_2}{d\phi_1} \cdot \frac{d\phi_3}{d\phi_2} \cdots \frac{df}{d\phi_\ell} \cdot \frac{dLoss}{df}$$

Info from Loss gets diluted (Vanishing gradients)

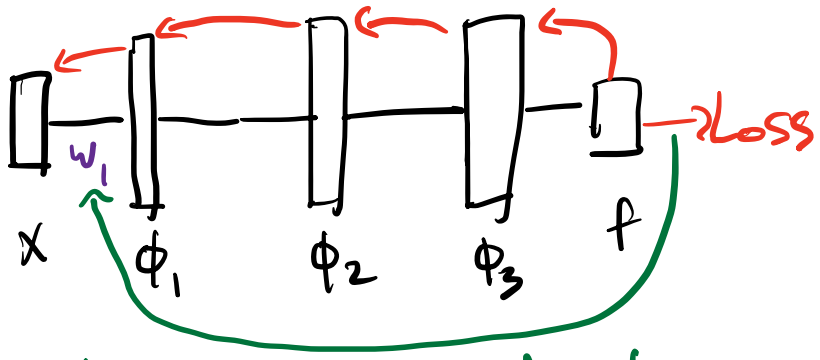
$$\rightarrow \frac{dL}{dw_1} = \frac{d\phi_1}{dw_1}\left(\frac{d\hat{\phi}_2}{d\phi_1}+1\right)\left(\frac{d\hat{\phi}_3}{d\phi_2}+1\right)\cdots\frac{df}{d\phi_\ell}\cdot\frac{dLoss}{df}$$

$$\frac{dL}{dw_1} = \frac{d\phi_1}{dw_1}\cdot\left[\underbrace{\cdots}_{\to 0}+1\right]\frac{df}{d\phi_\ell}\cdot\frac{dLoss}{df} \qquad \prod_{i=c}^{\ell}\left(\frac{d\hat{\phi}_i}{d\phi_{i-1}}+1\right)\cdot\frac{df}{d\phi_1}\frac{dLoss}{df}$$

$$\frac{d\phi_1}{dw_1}(1)\left(\frac{df}{d\phi_\ell}\cdot\frac{dLoss}{df}\right) \qquad \left(\frac{d\hat{\phi}_\ell}{d\phi_{\ell-1}}+1\right)\left(\frac{d\hat{\phi}_3}{d\phi_2}+1\right)$$

+1

Residual Networks



What if we had a direct connection?

$$\frac{dL}{dw_1} = x\sigma'(x^T w_1)\underbrace{\frac{d\phi_2}{d\phi_1}\cdot\frac{d\phi_3}{d\phi_2}\cdots\frac{df}{d\phi_n}}\cdot\frac{dLoss}{df} + \underbrace{\frac{dL}{d\phi_1}\cdot\frac{d\phi_1}{dw_1}}$$

$\left|\frac{d\phi_i}{d\phi_{i-1}}\right| < 1 \rightarrow 0$

Loss depends directly on ϕ_1

Residual function

$$\hat{f}(x) \rightarrow f(x) = \hat{f}(x) + x$$

Add input back to output!

Residual Layer

Layer: $\phi_i = \sigma(\phi_{i-1}^T w_i + b_i)$

Next value

Residual Layer: $\phi_i = \sigma(\phi_{i-1}^T w_i + b_i) + \phi_{i-1}$

$$\frac{d\phi_i}{d\phi_{i-1}} = \frac{d}{d\phi_{i-1}}\left[\sigma(\phi_{i-1}^T w_i + b_i) + \phi_{i-1}\right]$$

$$= \sigma'(\phi_{i-1}^T w_i + b_i) w_i + 1$$

$$\frac{d\phi_i}{d\phi_{i-1}} = \frac{d\hat{\phi}_i}{d\phi_{i-1}} + 1$$