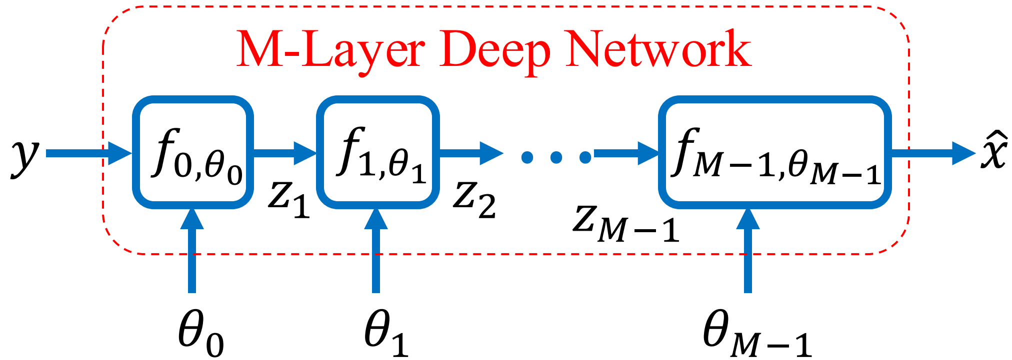
Optimization of Deep Functions

- Intro to Deep Learning
- Deep Learning Structures
- Gradient of a Deep Network
- Forward and Back Propagation

Deep Learning Background

- Shallow learning:
  - Inference function formed by 1 or 2 layers.
  - For many years, this was thought to be enough [Cybenko 1989].
- Deep learning:
  - What is it?
    - Uses many layers of inference functions in a hierarchal structure.
    - Typically 10 to 100 layers.
  - Why do people use it?
    - Over the last decade, there has been overwhelming empirical evidence that deep learning dramatically outperforms shallow learning on a wide range of real applications.
    - Intuitively, it is easier to represent complex phenomena using a hierarchy of inference functions.
  - If it's so great, then why did it take so long?
    - It was difficult to implement and no one was sure it would work, but now its easy to implement with modern software tools.
    - Must train all layers jointly $\Rightarrow$ requires automatic differentiation
    - Many more parameters to model and the problem of "vanishing gradient"
    - Requires more training data.

Deep Learning Structure



- Inference function is hierarchical.
  - For $M = 4$, we have that $\theta = [\theta_0, \theta_1, \theta_2, \theta_3]$, and

$$\hat{x} = f_\theta(y) = f_{3,\theta_3}\left(f_{2,\theta_2}\left(f_{1,\theta_1}\left(f_{0,\theta_0}(y)\right)\right)\right) \text{ (this is a mess)}$$

  - Instead write

$$f_\theta y = f_{3,\theta_3} f_{2,\theta_2} f_{1,\theta_1} f_{0,\theta_0} y = \left[\prod_{m=0}^{M-1} f_{m,\theta_m}\right] y$$

Remember the Loss Gradient

- To compute the loss gradient

$$\nabla L_{MSE}(\theta) = \frac{-2}{K}\sum_{k=0}^{K-1} \boxed{\left(x_k - f_\theta(y_k)\right)^t}\ \boxed{\nabla f_\theta(y_k)}$$

ϵ_k^t
error
vector

adjoint
gradien
t

$$\boxed{\begin{array}{c}1 \times P \\ \text{Loss gradient}\end{array}} = \frac{-2}{K}\sum_{k=0}^{K-1} \boxed{\begin{array}{c}1 \times N_x \\ \text{error vector}\end{array}}\ \boxed{\begin{array}{c}N_x \times P \\ \text{function gradient} \\ \\ \dfrac{\partial[f_\theta(y_k)]_i}{\partial\theta_j}\end{array}}$$

- For each training pair, we need to:
  - Compute the error vector
  - Multiply by the adjoint gradient ⇐ **This is the hard part!**
  - Sum them up

The Adjoint of the Loss Gradient

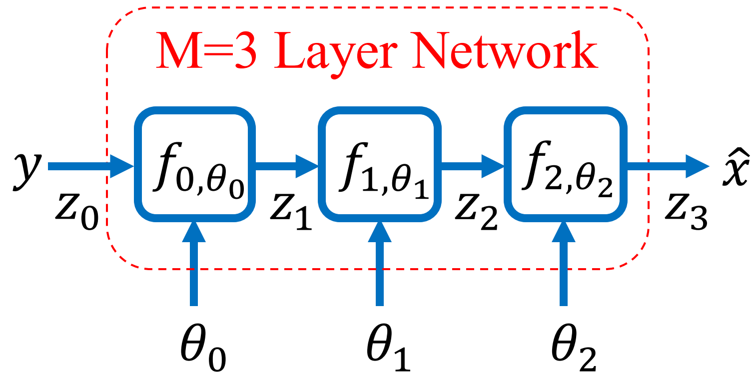
- To compute the loss gradient

$$[\nabla L_{MSE}(\theta)]^t = \frac{-2}{K}\sum_{k=0}^{K-1} \underbrace{\boxed{[\nabla f_\theta(y_k)]^t}}_{\text{adjoint gradien t}} \underbrace{\boxed{\left(x_k - f_\theta(y_k)\right)}}_{\epsilon_k \text{ error vector}}$$

$$\boxed{\begin{array}{c} P \times 1 \\ \text{Loss gradient} \end{array}} = \frac{-2}{K}\sum_{k=0}^{K-1} \boxed{\begin{array}{c} P \times N_x \\ \text{adjoint function} \\ \text{gradient} \\ \dfrac{\partial[f_\theta(y_k)]_j}{\partial \theta_i} \end{array}} \boxed{\begin{array}{c} N_x \times 1 \\ \text{error vector} \end{array}}$$

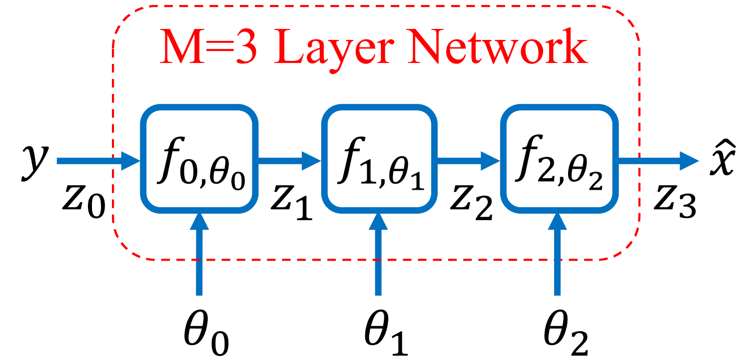
- The adjoint gradient of the loss function:
  - Input and output are exchanged
  - Reverses flow of network

Example Deep Network



- For $M = 3$,
  - Inference function $f_\theta y = f_{2,\theta_2} f_{1,\theta_1} f_{0,\theta_0} y$
  - Parameter vectors is $\theta = [\theta_0, \theta_1, \theta_2\ ]$
  - Hidden states $z_{m+1} = f_{\theta_m}\ z_m$ with dimension $z_m \in \Re^{N_m}$
- How do we compute the gradient of this inference function?

Gradients of Deep Network



- By the chain rule:
  - Gradient with respect to z_0

$$\nabla_{z_0} f_\theta = [\nabla_{z_2} f_2][\nabla_{z_1} f_1][\nabla_{z_0} f_0]$$

  - Adjoint gradient with respect to z_0

$$[\nabla_{z_0} f_\theta]^t = [\nabla_{z_0} f_0]^t [\nabla_{z_1} f_1]^t [\nabla_{z_2} f_2]^t$$

  - Gradient with respect to θ_0

$$\nabla_{\theta_0} f_\theta = [\nabla_{z_2} f_2][\nabla_{z_1} f_1][\nabla_\theta f_0]$$

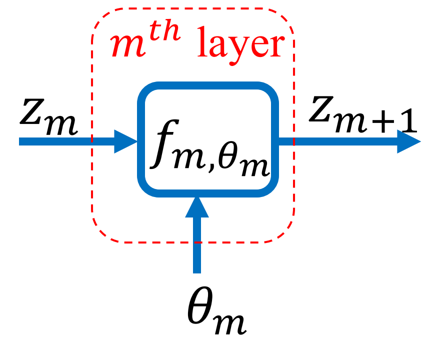
  - Adjoint gradient with respect to θ_0

$$[\nabla_{\theta_0} f_\theta]^t = [\nabla_\theta f_0]^t [\nabla_{z_1} f_1]^t [\nabla_{z_2} f_2]^t$$

Gradients for Each Node

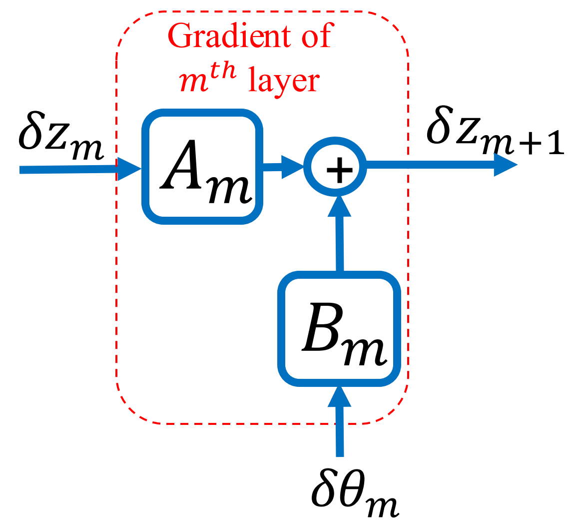
- Input gradient of layer:

$$A_m \leftarrow \nabla_z f_{\theta_m}(z_m) = \begin{array}{c|c} & \text{j index} \\ \hline \text{i index} & \left[\begin{array}{c} \text{input gradient} \\ \dfrac{\partial [f_{\theta_m}]_i}{\partial [z_m]_j} \end{array} \right] \end{array}$$



- Parameter gradient of layer:

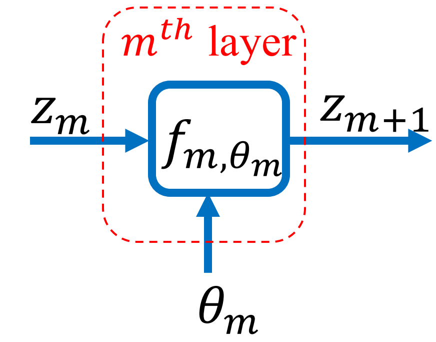
$$B_m \leftarrow \nabla_\theta f_{\theta_m}(z_m) = \begin{array}{c|c} & \text{j index} \\ \hline \text{i index} & \left[\begin{array}{c} \text{parameter gradient} \\ \dfrac{\partial [f_{\theta_m}]_i}{\partial [\theta_m]_j} \end{array} \right] \end{array}$$



Adjoint Gradients for Each Node

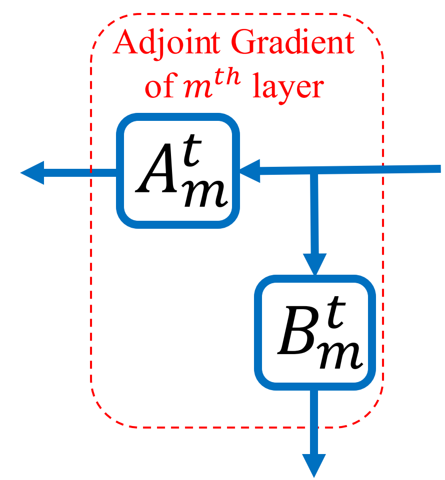
- Input gradient of layer:

$$A_m^t \leftarrow \left[\nabla_z f_{\theta_m}(z_m)\right]^t = \begin{array}{c|c} & j \text{ index} \\ \hline i \text{ index} & \underbrace{\left[\frac{\partial [f_{\theta_m}]_j}{\partial [z_m]_i}\right]}_{\text{input gradient}} \end{array}$$

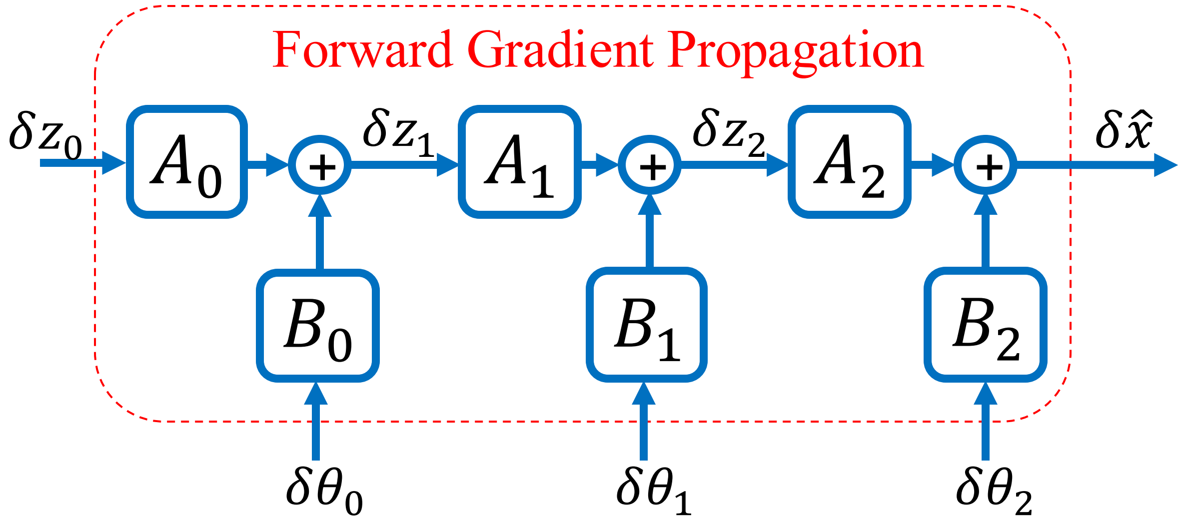


- Parameter gradient of layer:

$$B_m^t \leftarrow \left[\nabla_\theta f_{\theta_m}(z_m)\right]^t = \begin{array}{c|c} & j \text{ index} \\ \hline i \text{ index} & \underbrace{\left[\frac{\partial [f_{\theta_m}]_j}{\partial [\theta_m]_i}\right]}_{\text{parameter gradient}} \end{array}$$



Forward Propagation of Gradient



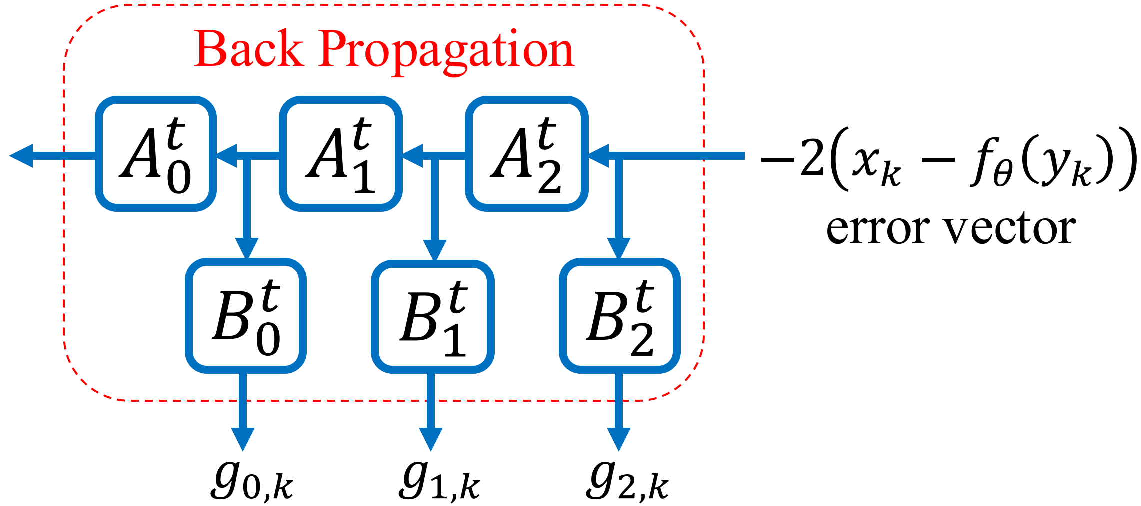
- By the chain rule, the gradients with respect to inputs are

$$\nabla_{z_2} f_\theta = A_2$$
$$\nabla_{z_1} f_\theta = A_2 A_1$$
$$\nabla_{z_0} f_\theta = A_2 A_1 A_0$$

- By the chain rule, the gradients with respect to parameters are

$$\nabla_{\theta_2} f_\theta = B_2$$
$$\nabla_{\theta_1} f_\theta = A_2 B_1$$
$$\nabla_{\theta_0} f_\theta = A_2 A_1 B_0$$

Back Propagation of Adjoint Gradient



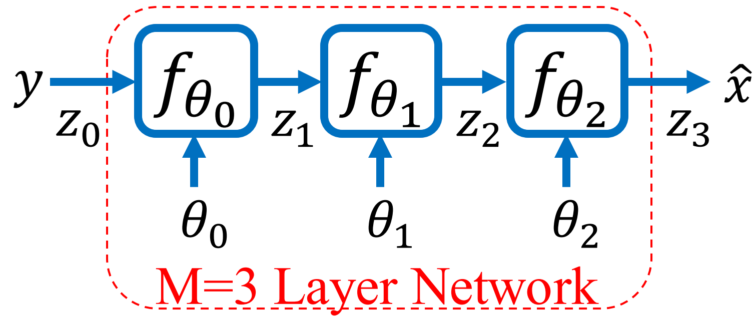
- Compute loss gradient by reversing network flow:
  - For each training vector,

$$g_{m,k} = \nabla_{\theta_m} \|x_k - f_\theta(y_k)\|^2 = -2\big(x_k - f_\theta(y_k)\big)^t \ \nabla f_\theta(y_k)$$

  - So then the gradient of the loss function is given by

$$\nabla_{\theta_m} L(\theta) = g_m = \frac{1}{K} \sum_{k=0}^{K-1} g_{m,k}$$

BP Step 1: Forward Propagate States



- Forward propagation pseudo code:

$$
\begin{aligned}
& z_0 \leftarrow y \\
& \text{For } (m = 0\ to\ M-1)\ \{ \\
& \quad z_{m+1} \leftarrow f_{\theta_m} z_m \\
& \quad \} \\
& \hat{x} \leftarrow z_M
\end{aligned}
$$

Forward Propagation

BP Step 2: Back Propagation

- Backpropagation pseudo code

For$(m = 0 \text{ to } M-1)\ \ g_m \leftarrow 0$

For $(k = 0 \text{ to } K-1)$ {

  $\epsilon_M \leftarrow -2\big(x_k - f_\theta(y_k)\big)$

  For$(m = M-1 \text{ to } 0)$ {

    $A \leftarrow \nabla_z f_{\theta_m}(z_m)$

    $B \leftarrow \nabla_\theta f_{\theta_m}(z_m)$

    $\epsilon_m \leftarrow A^t\, \epsilon_{m+1}$

    $g_m \leftarrow g_m + B^t\, \epsilon_{m+1}$

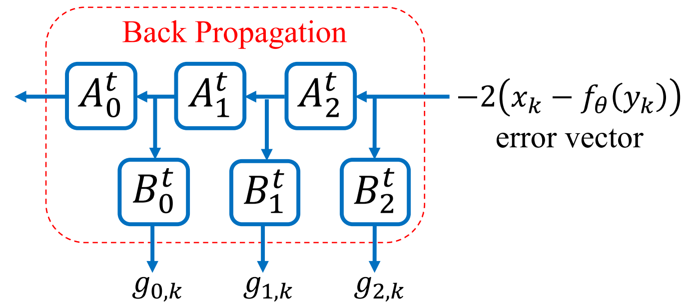
    }

  }

For$(m = 0\ to\ M-1)\ \ g_m \leftarrow g_m/K$

Return(g_m)

Back Propagation



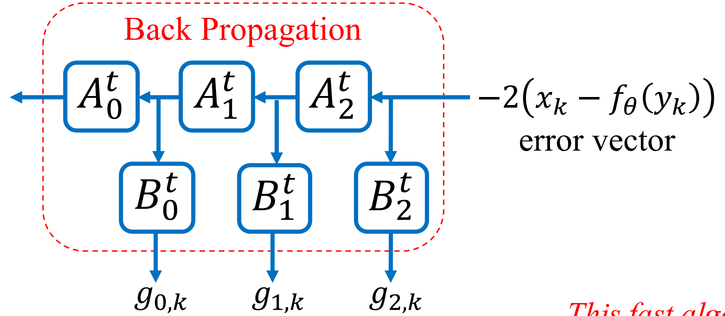
Results in

$$g_m = \nabla_{\theta_m} L(\theta)$$

where

$$L(\theta) = \frac{1}{K}\sum_{k=0}^{K-1} \|x_k - f_\theta(y_k)\|^2$$

Back Propogation: Computational Efficiency



This fast algorithm is sometimes referred to as adjoint differentiation.

- Order of computation matters!!
  - Left to Right: Dense matrix products $\Rightarrow \mathcal{O}(N^3K)$
  - Right to Left: Vector matrix products $\Rightarrow \mathcal{O}(N^2K)$

$$g_o = \boxed{\begin{matrix} P_0 \times 1 \\ \text{Loss gradient} \end{matrix}} = \frac{1}{K}\sum_{k=0}^{K-1} \boxed{\begin{matrix} P_0 \times N_1 \\ \text{parameter} \\ \text{gradient} \\ B_0^t \end{matrix}} \boxed{\begin{matrix} N_1 \times N_2 \\ \text{input} \\ \text{gradient} \\ A_1^t \end{matrix}} \boxed{\begin{matrix} N_2 \times N_3 \\ \text{input} \\ \text{gradient} \\ A_2^t \end{matrix}} \boxed{\begin{matrix} N_3 \times 1 \\ \text{error vector} \end{matrix}}$$

left to right $\Longrightarrow$

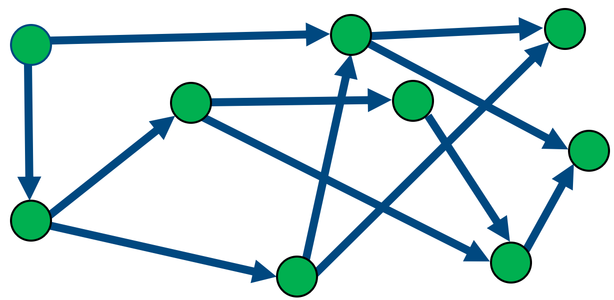
$\Longleftarrow$ *right to left*

GD on Acyclic Graph Structures

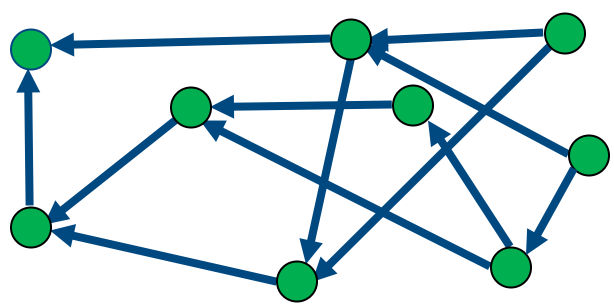
- Definition of DAG
- General Node Structure
- Back Propagation on Graphs

Define DAG

- Directed Acyclic Graph (DAG)
  - A directed graph with no loops.
  - Starting at any node, you will eventually hit a termination

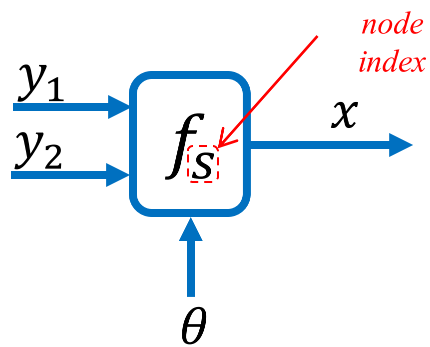


  - If you reverse the arrows (i.e., flow), it's still a DAG



Define DL Node

- Assume that DL network is a DAG.
  - Then w.o.l.o.g for a fan-in of 2, each nodes is



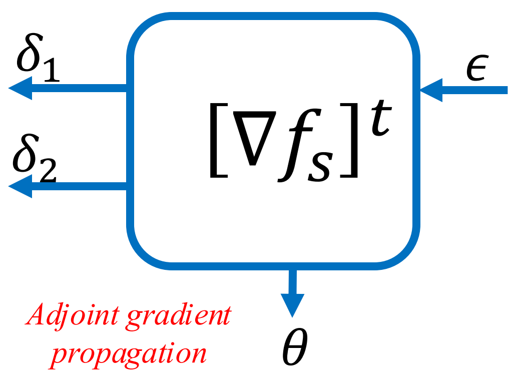
$$x = f_{s,\theta}(y_1, y_2)$$

$$A_{s,1} = \nabla_{y_1} f_s$$

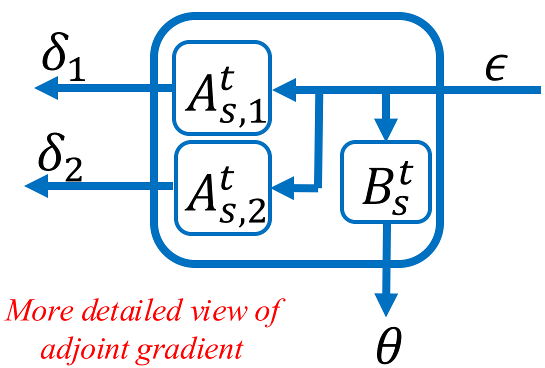
$$A_{s,2} = \nabla_{y_2} f_s$$

$$B_s = \nabla_\theta f_s$$

  - And the back propagation is



Adjoint gradient propagation

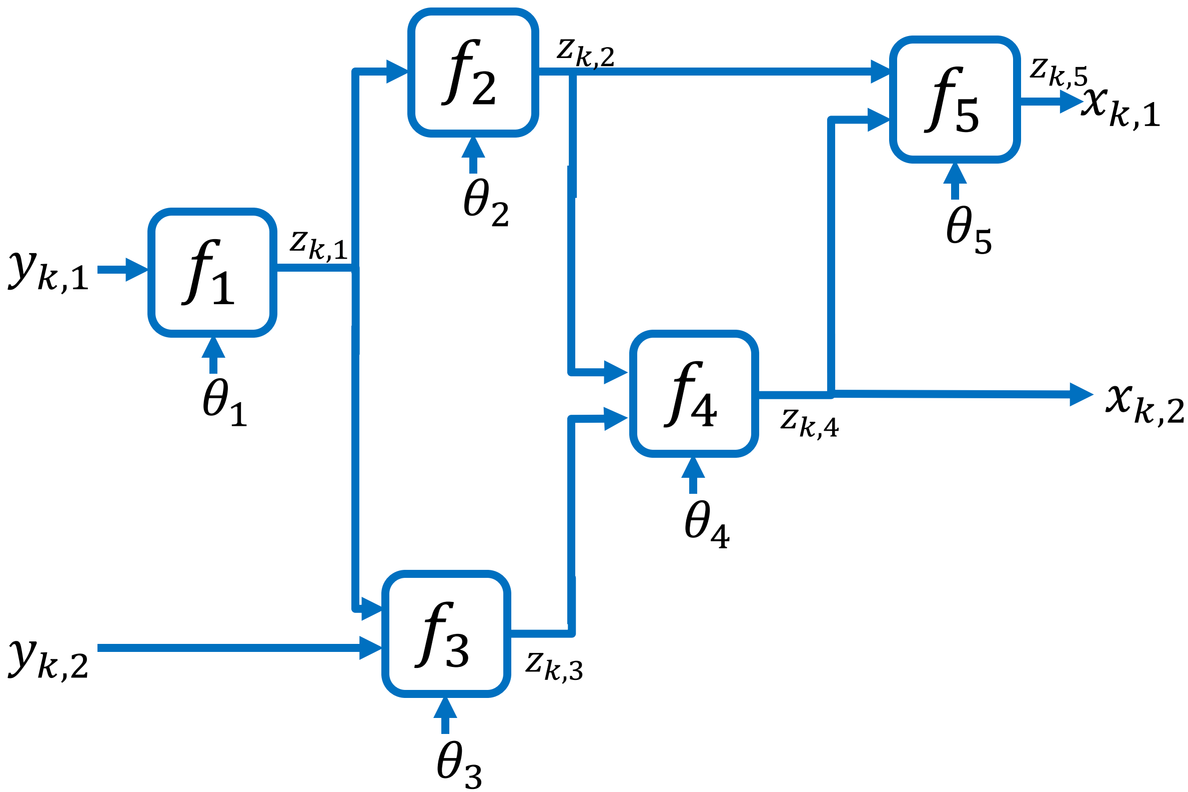


More detailed view of adjoint gradient propagation

Step 1: Forward Propagation for DAG

- Forward propagation.

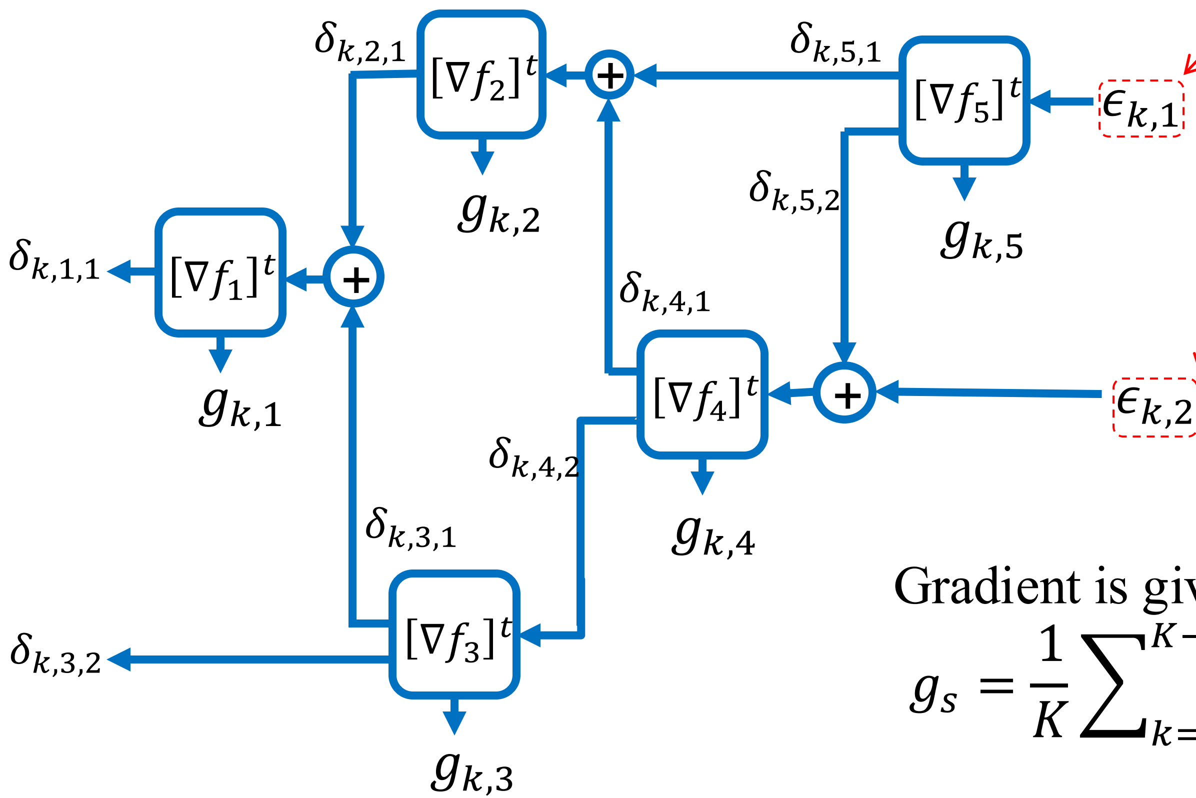
$$\begin{bmatrix} x_{k,1} \\ x_{k,2} \end{bmatrix} = f_\theta\left(\begin{bmatrix} y_{k,1} \\ y_{k,2} \end{bmatrix}\right)$$



Step 2: Back Propagation for DAG

- Back propagation using adjoint gradients.

$$\begin{bmatrix}\epsilon_{k,1}\\ \epsilon_{k,2}\end{bmatrix} = -2\left(x_k - f_\theta(y_k)\right)$$

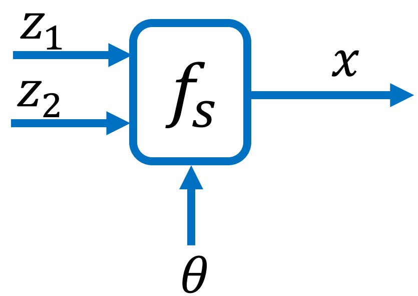


Gradient is given by

$$g_s = \frac{1}{K}\sum_{k=0}^{K-1} g_{k,s}$$

Implementation of Each Node

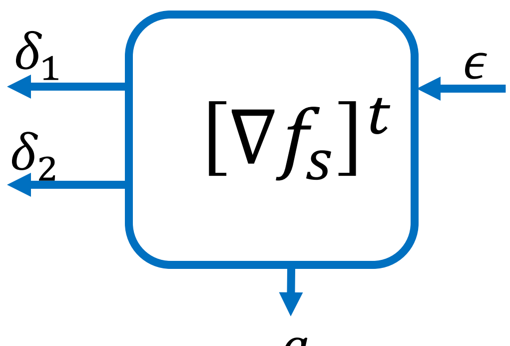
- For each node you need two functions:
  - Function for forward propagation



$$x \leftarrow f(z_1, z_2, \theta)$$

You need a software implementation of this forward function.

  - Function for adjoint gradient (i.e., back propagation)



$$[\delta_1, \delta_2, g] \leftarrow G(\epsilon, z_1, z_2, \theta)$$

You need a software implementation of this function that multiplies ϵ by the adjoint gradient.

<u>Very important</u>: You don't need to ever compute $[\nabla f_s]^t$!!

General Loss Functions

- The Weakness of MSE Loss Functions
- MAE and Cross Correlation Loss Functions
- Back Propagating General Loss Functions

Weakness of MSE Loss

- MSE loss is given by

$$L_{MSE}(\theta) = \frac{1}{K}\sum_{k=0}^{K-1}\|x_k - f_\theta(y_k)\|^2$$

- Excessively weights outliers
  - If training sample is wrong, then prediction error can be very large.
  - If a few bad training samples can dramatically degrade results.

$$[\nabla L_{MSE}(\theta)]^t = \frac{-2}{K}\sum_{k=0}^{K-1} \overbrace{[\nabla f_\theta(y_k)]^t}^{\text{adjoint gradient of function}} \overbrace{\left(x_k - f_\theta(y_k)\right)}^{\text{prediction error}}$$

A General Class of Loss Functions

- General loss functions

$$L(\theta) = \frac{1}{K} \sum_{k=0}^{K-1} \rho\big(x_k, f_\theta(y_k)\big)$$

  - where ρ is a <u>distortion</u> function s.t. $\forall a, b,\ \rho(a, b) \geq \rho(a, a)$.

- Typical choices include
  - Mean Squared Error (MSE)
    - $\rho(\mathrm{a}, \mathrm{b}) = \|\mathrm{a} - \mathrm{b}\|^2 = \sum_i (a_i - b_i)^2$ for $\forall a, b \in \Re^{N_x}$
  - Mean Absolute Error (MAE)
    - $\rho(\mathrm{a}, \mathrm{b}) = \|\mathrm{a} - \mathrm{b}\|_1^1 = \sum_i |a_i - b_i|$ for $\forall a, b \in \Re^{N_x}$
  - Multicategory Cross Entropy (assumes $b_i > 0$, $\sum_i b_i = 1$, and $a_i \geq 0$)
    - $\rho(\mathrm{a}, \mathrm{b}) = -\sum_i \mathrm{a}_i \log b_i$ for $\forall a, b \in \mathcal{S}^{N_x}$

Gradient for General for Loss

- Alternative loss functions

$$L(\theta) = \frac{1}{K}\sum_{k=0}^{K-1} \rho\big(x_k, f_\theta(y_k)\big)$$

Results in gradient

$$[\nabla L(\theta)]^t = \frac{1}{K}\sum_{k=0}^{K-1} [\nabla_\theta f_\theta(y_k)]^t \, \epsilon_k$$

$$\epsilon_k = \nabla_b \rho(a,b)\Big|_{\substack{a=x_k \\ b=f_\theta(y_k)}}$$

$$\boxed{\begin{array}{c} P \times 1 \\ \text{Loss gradient} \end{array}} = \frac{1}{K}\sum_{k=0}^{K-1} \boxed{\begin{array}{c} P \times N_x \\ \text{function gradient} \\ [\nabla_\theta f_\theta(y_k)]^t \end{array}} \boxed{\begin{array}{c} N_x \times 1 \\ \epsilon_k \text{ error vector} \end{array}}$$

Error Vector for General Loss Functions

$$L(\theta) = \frac{1}{K}\sum_{k=0}^{K-1} \rho\big(x_k, f_\theta(y_k)\big)$$

General loss functions

$$\epsilon_k = \nabla_b \rho(a, b)\Big|_{\substack{a = x_k \\ b = f_\theta(y_k)}}$$

General error function

- MSE

  Loss: $\rho(\mathrm{a}, \mathrm{b}) = \|\mathrm{a} - \mathrm{b}\|^2$ Error: $\epsilon_k^t = -2\big(x_k - f_\theta(y_k)\big)$

- MAE

  Loss: $\rho(\mathrm{a}, \mathrm{b}) = \|\mathrm{a} - \mathrm{b}\|_1^1$ Error: $\epsilon_k^t = -sign\,\big(x_k - f_\theta(y_k)\big)$

- Cross entropy*

  Loss: $\rho(\mathrm{a}, \mathrm{b}) = -\sum_i \mathrm{a}_i \log b_i$ Error: $\epsilon_k^t = -\boxed{\frac{x_k}{f_\theta(y_k)}}$

  (Assumes $b_i > 0$, $\sum_i b_i = 1$, and $a_i \geq 0$)

  Point-wise division

*The software utility includes softmax preprocessing: https://pytorch.org/docs/stable/generated/torch.nn.CrossEntropyLoss.html

Gradient for Cross Entropy Loss

- Paradox:
  - Let $f_\theta(y) = \theta$ for $\sum_i \theta_i = 1$, and for all i let $x_i = a$, then for cross-entropy we have that:

$$L(\theta) = -\sum_i x_i \log \theta_i = -\sum_i a \log \theta_i \qquad \text{for } \sum_i \theta_i = 1$$

So that

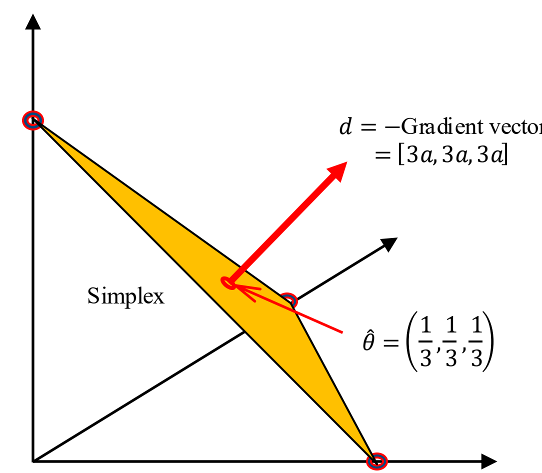
$$[\nabla_\theta L(\theta)]_i = [\nabla_\theta \rho(x, \theta)]_i = -\frac{x_i}{\theta_i} = -\frac{a}{\theta_i}$$

  - Paradox: Even when $\hat{\theta}_i = \frac{x_i}{\sum_i x_i} = \frac{1}{3}$, the gradient is not zero!

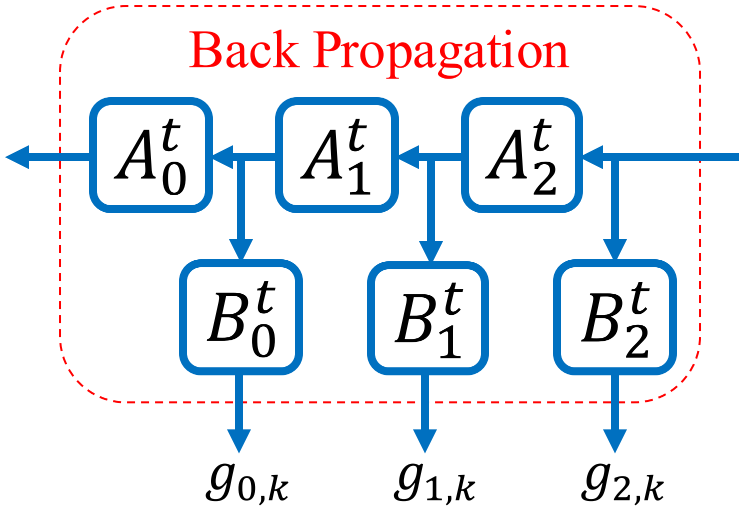
$$d = -\nabla_\theta L(\hat{\theta}) = [3a, 3a, 3a]$$

  - How can this be??

3D Example:
Gradient is perpendicular
to constraint space!



Back Propagation for Typical Loss Functions



General: $\epsilon_k = \nabla_b \rho(a,b)\big|_{\substack{a=x_k \\ b=f_\theta(y_k)}}$

MSE: $\epsilon_k^t = -2\big(x_k - f_\theta(y_k)\big)$

MAE: $\epsilon_k^t = -sign\big(x_k - f_\theta(y_k)\big)$

CE: $\epsilon_k^t = -\frac{x_k}{f_\theta(y_k)}$

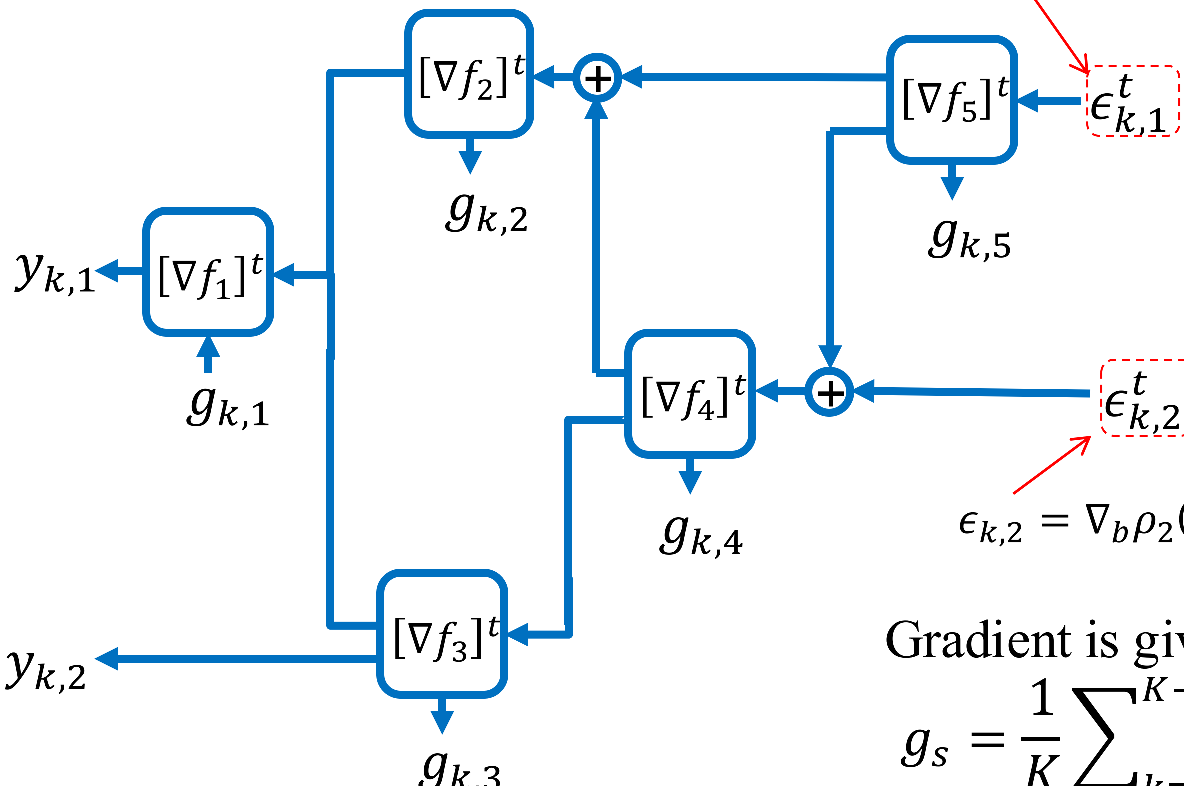
- Loss gradient given by

$$\nabla_{\theta_m} L(\theta) = \frac{1}{K}\sum_{k=0}^{K-1} g_{m,k}$$

DAG Back Propagation for General Loss

- Back propagation using adjoint gradients.

$$\epsilon_{k,1} = \nabla_b \rho_1(a,b)\Big|_{\substack{a=x_k \\ b=f_\theta(y_k)}}$$



$$\epsilon_{k,2} = \nabla_b \rho_2(a,b)\Big|_{\substack{a=x_k \\ b=f_\theta(y_k)}}$$

Gradient is given by

$$g_s = \frac{1}{K}\sum_{k=0}^{K-1} g_{k,s}$$