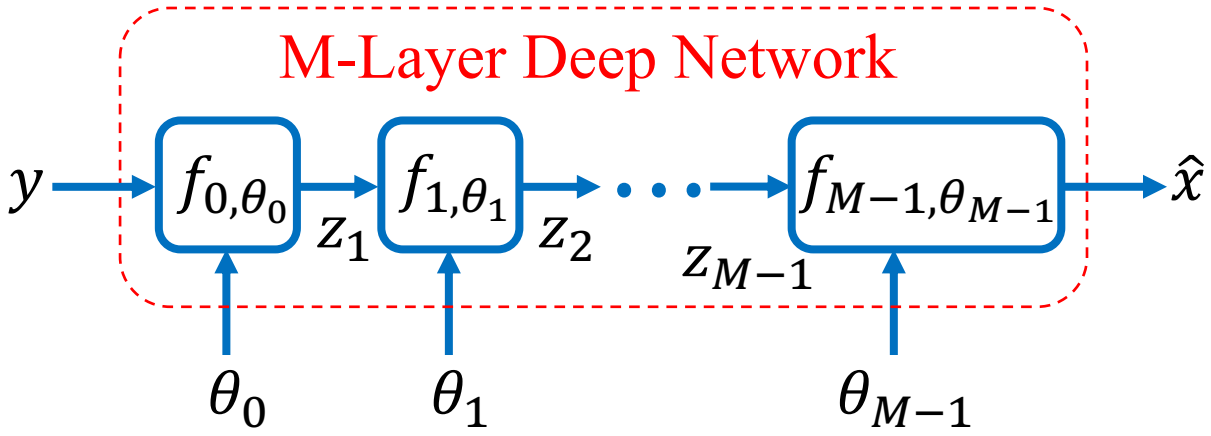
Optimization of Deep Functions

- 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 ⇒ 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

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

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

ϵ_k^t *error vector*

adjoint gradient

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

- 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

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

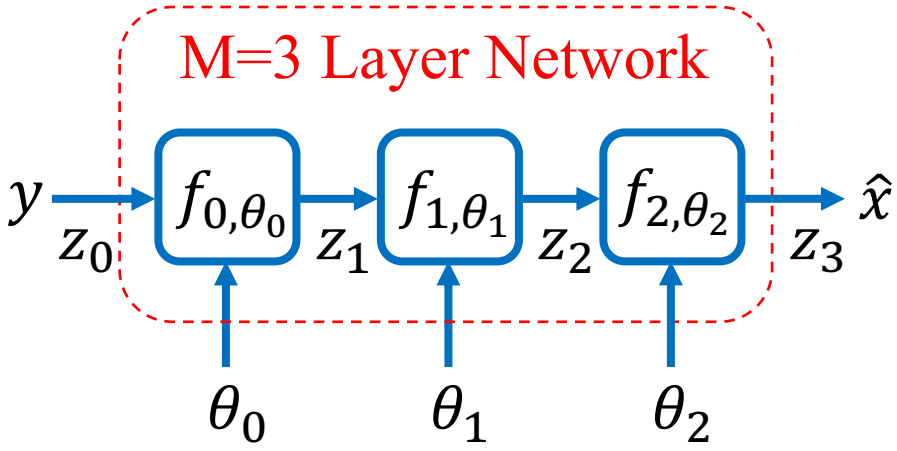
adjoint gradient — $[\nabla f_\theta(y_k)]^t$

ϵ_k error vector — $\left(x_k - f_\theta(y_k)\right)$

$$\underbrace{\quad}_{P\times 1 \text{ Loss gradient}} = \frac{-2}{K}\sum_{k=0}^{K-1} \underbrace{\frac{\partial [f_\theta(y_k)]_j}{\partial \theta_i}}_{\substack{P\times N_x \\ \text{adjoint function} \\ \text{gradient}}} \underbrace{\quad}_{N_x\times 1 \text{ error vector}}$$

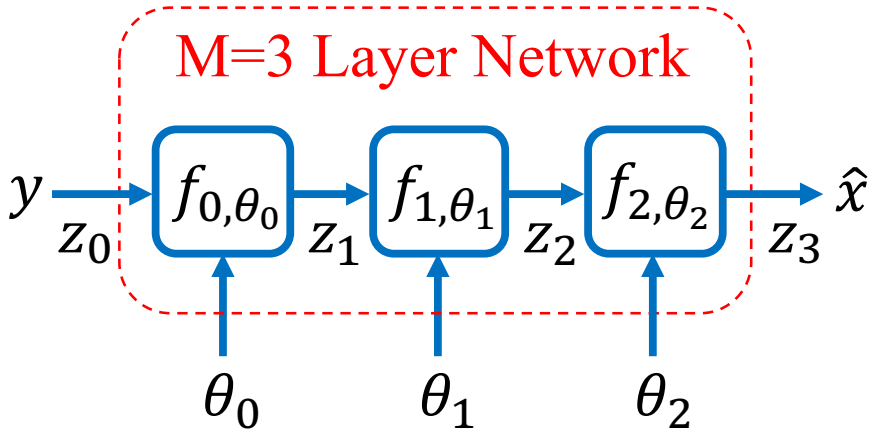
- The adjoint gradient of the loss function:
  - Input and output are exchanged
  - Reverses flow of network

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

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

  - Adjoint gradient with respect to z_0

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

  - Gradient with respect to θ_0

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

  - Gradient with respect to θ_0

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

Gradients for Each Node

- Input gradient of layer:

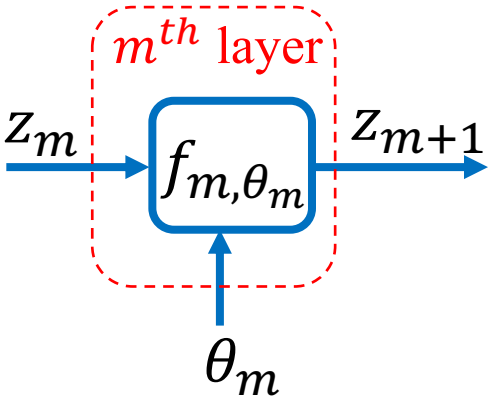
$$A_m \leftarrow \nabla_z f_{\theta_m}(z_m) =$$

j index

i index

$N_{m+1} \times N_m$ input gradient

$$\frac{\partial [f_{\theta_m}]_i}{\partial [z_m]_j}$$



- Parameter gradient of layer:

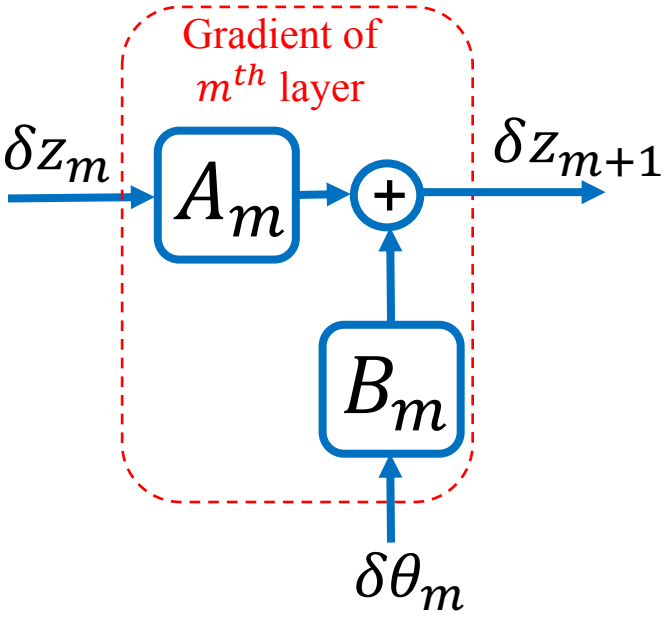
$$B_m \leftarrow \nabla_\theta f_{\theta_m}(z_m) =$$

j index

i index

$N_{m+1} \times P_m$ parameter gradient

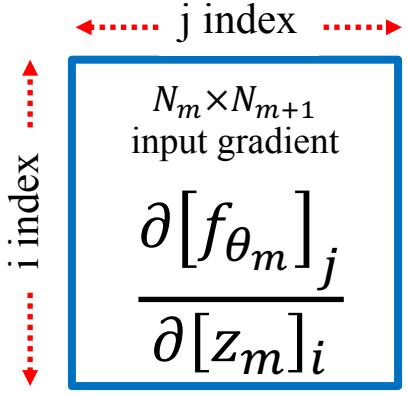
$$\frac{\partial [f_{\theta_m}]_i}{\partial [\theta_m]_j}$$

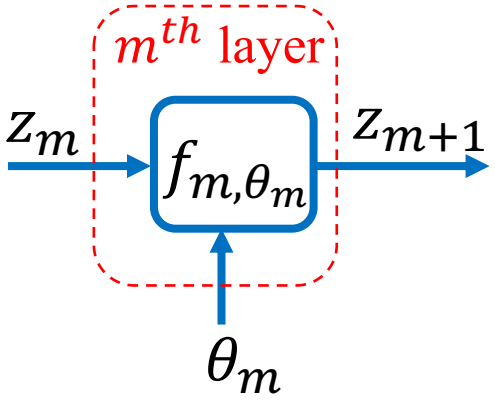


Adjoint Gradients for Each Node

- Input gradient of layer:

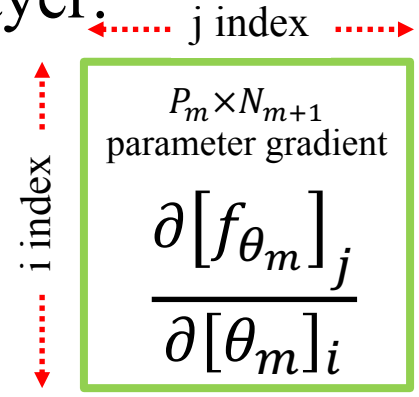
$$A_m^t \leftarrow \left[\nabla_z f_{\theta_m}(z_m)\right]^t =$$

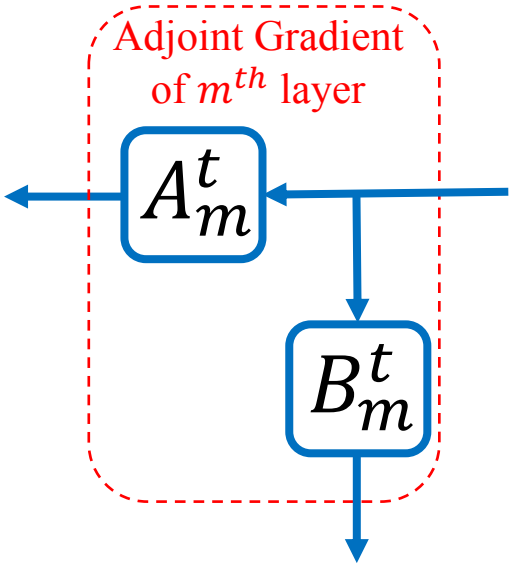




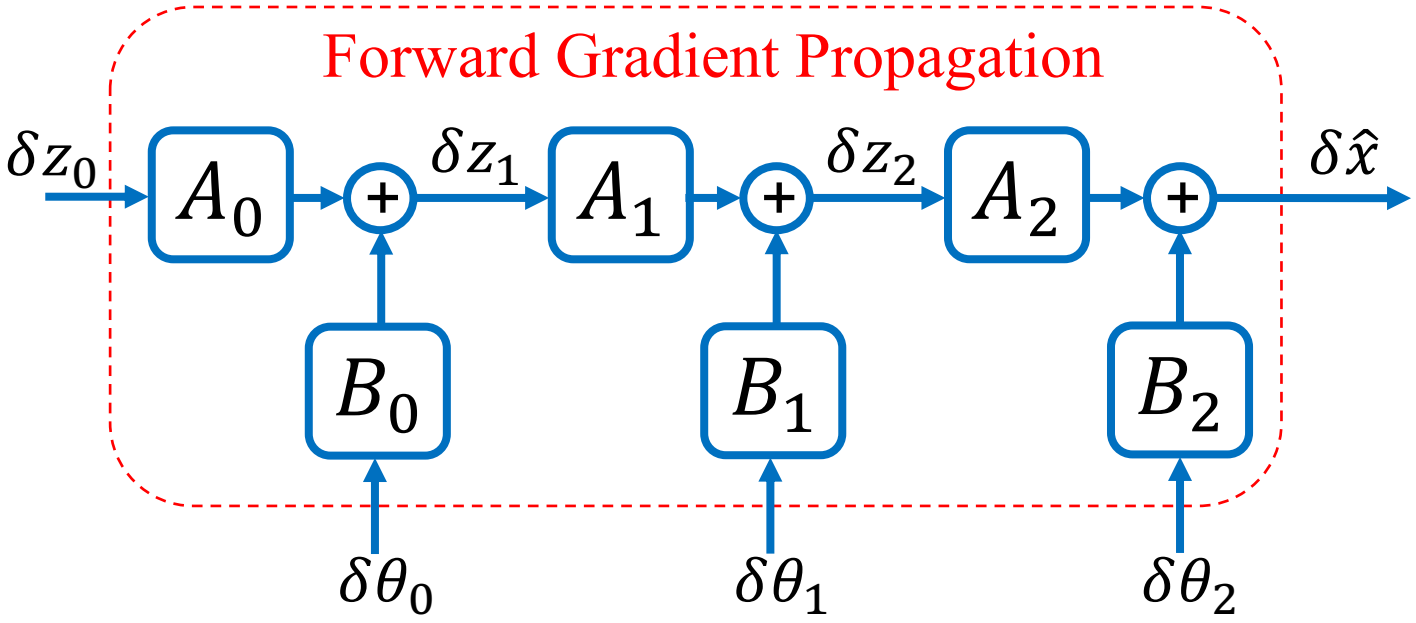
- Parameter gradient of layer:

$$B_m^t \leftarrow \left[\nabla_\theta f_{\theta_m}(z_m)\right]^t =$$





Forward Propagation of Gradient



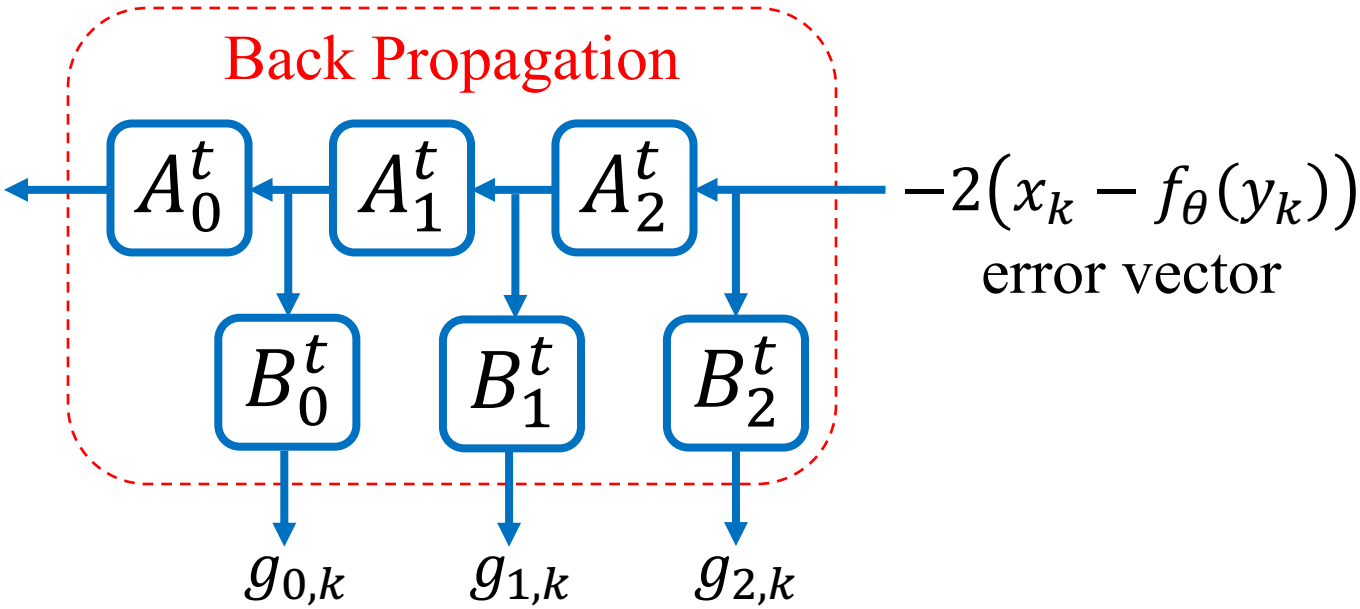
- By the chain rule, the gradients with respect to inputs are

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

- 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



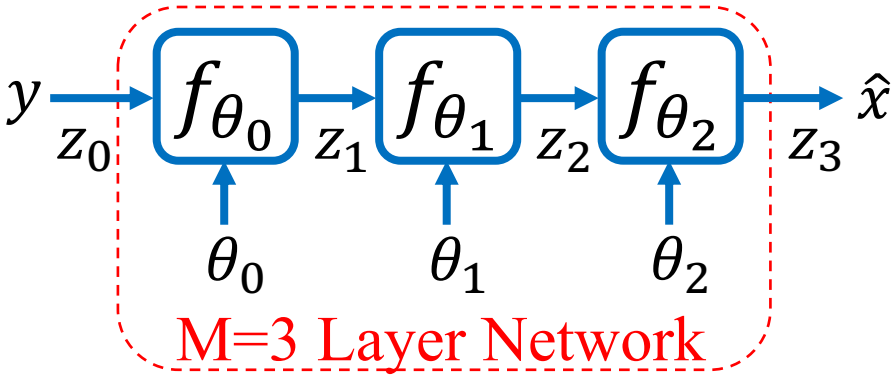
- Compute loss gradient by reversing network flow:
  - For each training vector,

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

  - 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:

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

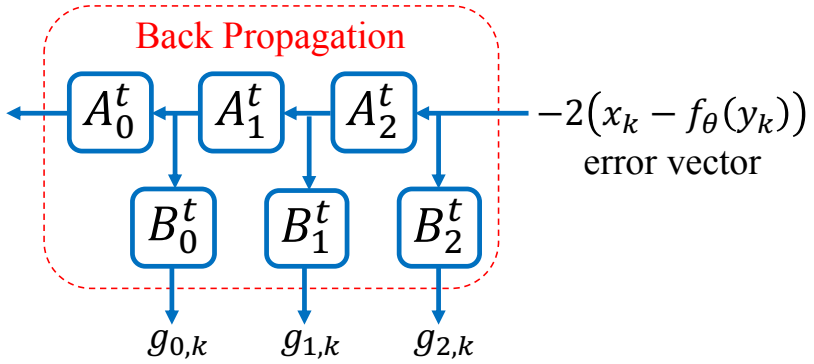
Forward Propagation

BP Step 2: Back Propagation

- Backpropagation pseudo code

For$(m = 0$ to $M-1)$ $g_m \leftarrow 0$
For $(k = 0$ to $K-1)$ {
  $\epsilon_M \leftarrow -2\left(x_k - f_\theta(y_k)\right)$
  For$(m = M-1$ 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



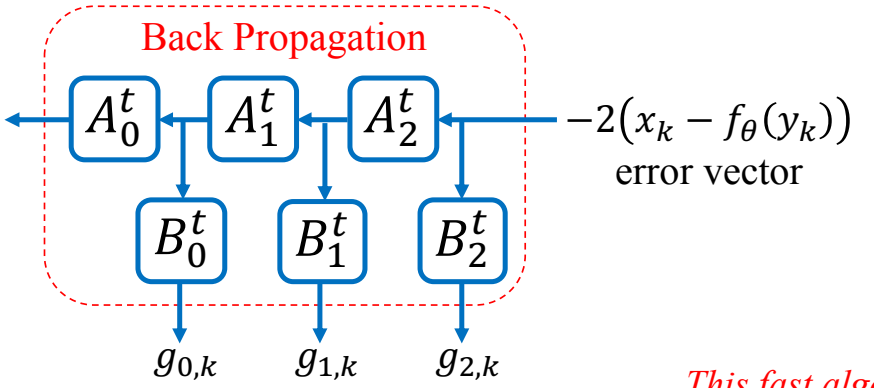
Results in

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

where

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

Back Propogation: Computational Efficiency



This fast algorithm is sometimes referred to as adjoint differentiation.

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

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

left to right

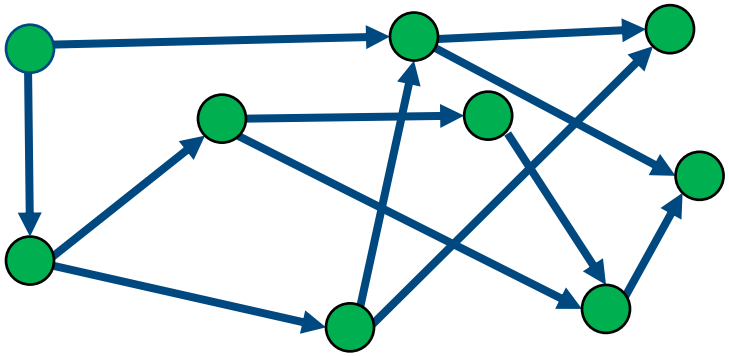
right to left

GD on Acyclic Graph Structures

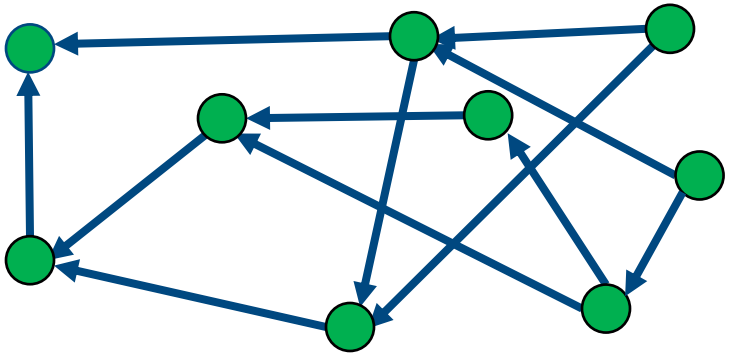
- Definition of DAG
- General Node Structure
- Back Propagation on Graphs

Define DAG

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

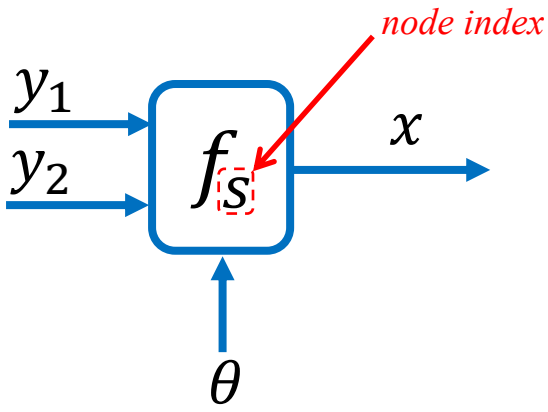


  - If you reverse the arrows (i.e., flow), it's still a DAG



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



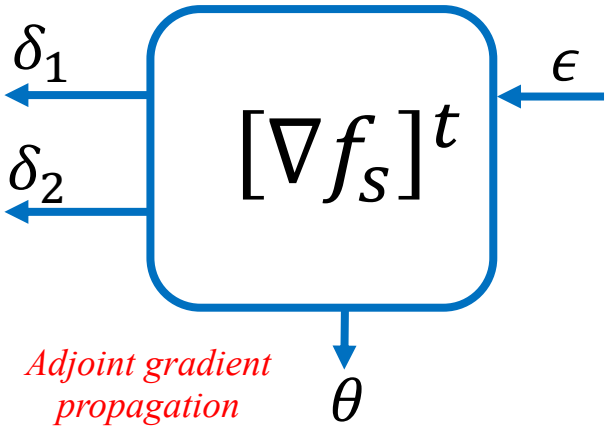
$$x = f_{s,\theta}(y_1, y_2)$$

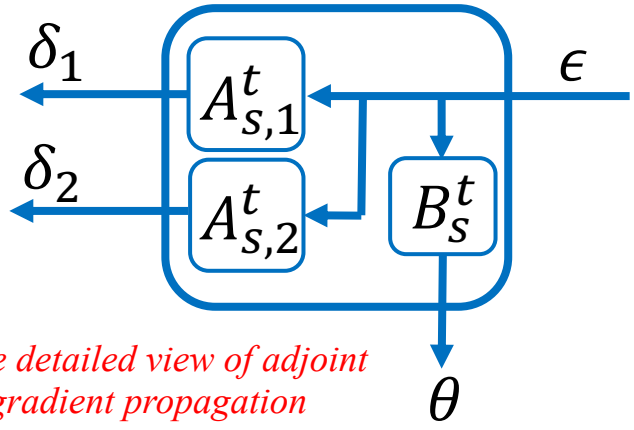
$$A_{s,1} = \nabla_{y_1} f_s$$

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

$$B_s = \nabla_{\theta} f_s$$

  - And the back propagation is

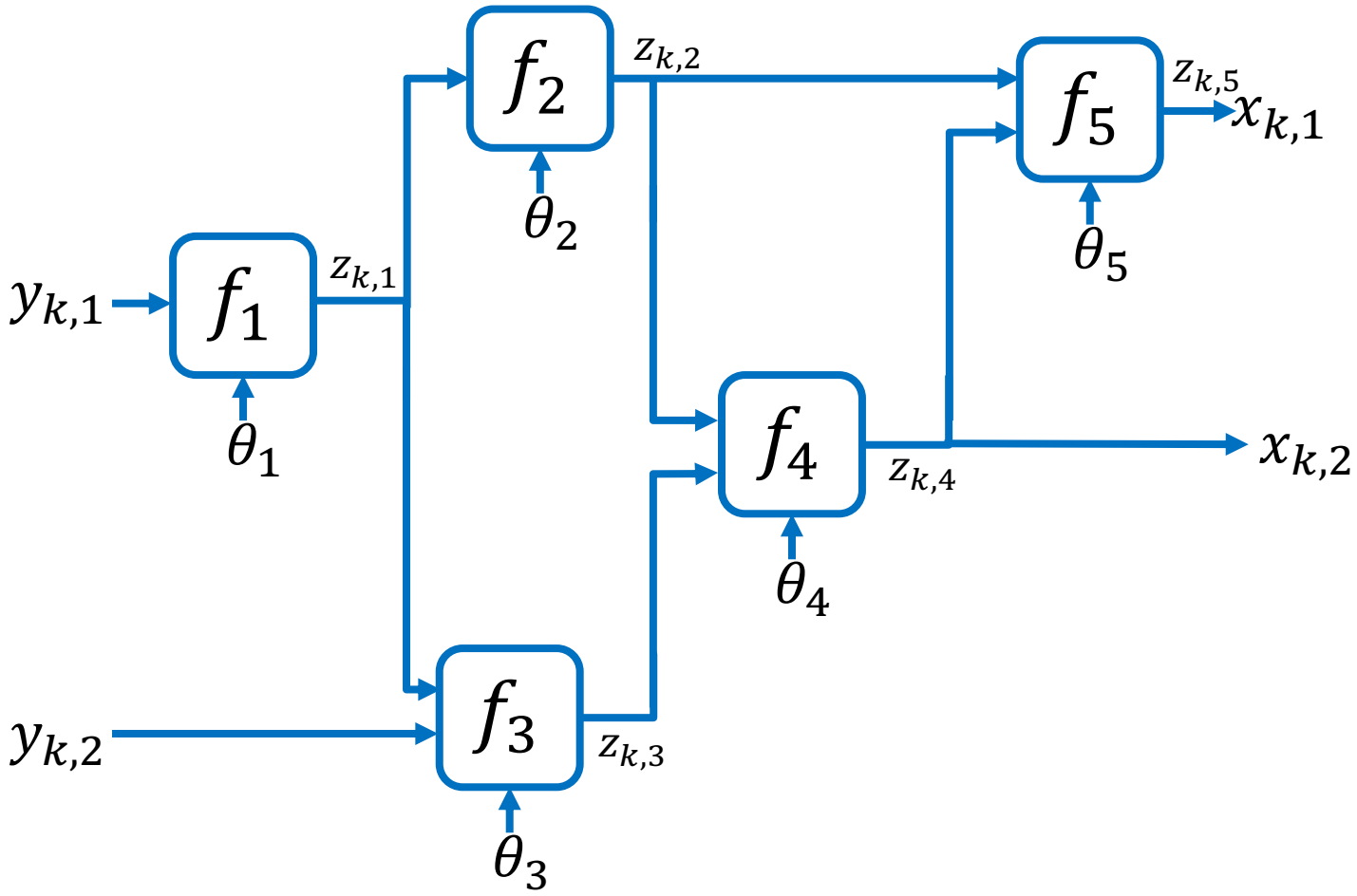




Step 1: Forward Propagation for DAG

- Forward propagation.

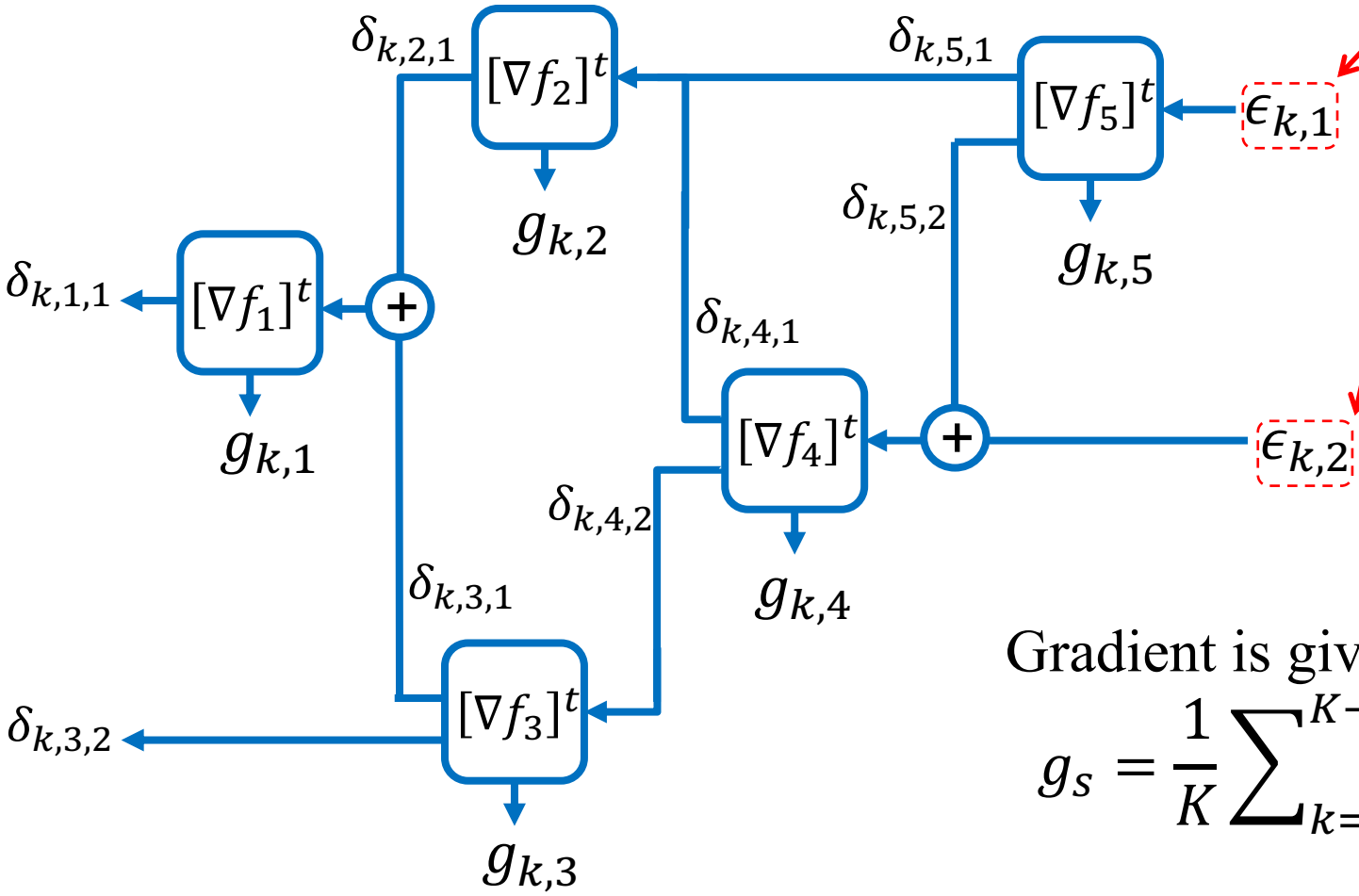
$$\begin{bmatrix} x_{k,1} \\ x_{k,2} \end{bmatrix} = f_\theta\left(\begin{bmatrix} y_{k,1} \\ y_{k,2} \end{bmatrix}\right)$$



Step 2: Back Propagation for DAG

- Back propagation using adjoint gradients.

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

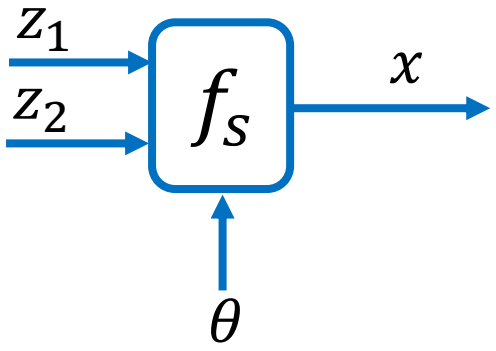


Gradient is given by

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

Implementation of Each Node

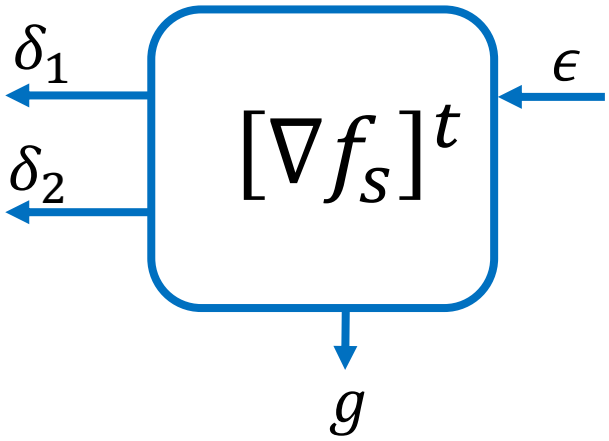
- For each node you need two functions:
  - Function for forward propagation



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

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

$$L_{MSE}(\theta) = \frac{1}{K}\sum_{k=0}^{K-1}\rho\left(x_k, f_\theta(y_k)\right)$$

  - where ρ is a function s.t. $\rho(a,b) \geq \rho(a,a)$.

- 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
    - $\rho(\mathrm{a},\mathrm{b}) = -\sum_i \mathrm{a}_i \log b_i$ for $\forall a, b \in \mathcal{S}^{N_x}$

Gradient for General for Loss

- Alternative loss functions

$$L_{MSE}(\theta) = \frac{1}{K}\sum_{k=0}^{K-1} \rho\left(x_k, f_\theta(y_k)\right)$$

Results in gradient

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

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

$$\underbrace{\quad}_{P\times 1 \text{ Loss gradient}} = \frac{1}{K}\sum_{k=0}^{K-1} \underbrace{\nabla_\theta f_\theta(y_k)}_{P\times N_x \text{ function gradient}} \underbrace{\epsilon_k^t}_{N_x\times 1 \text{ error vector}}$$

Error Vector for General Loss Functions

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

General loss functions

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

General error function

- MSE

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

- MAE

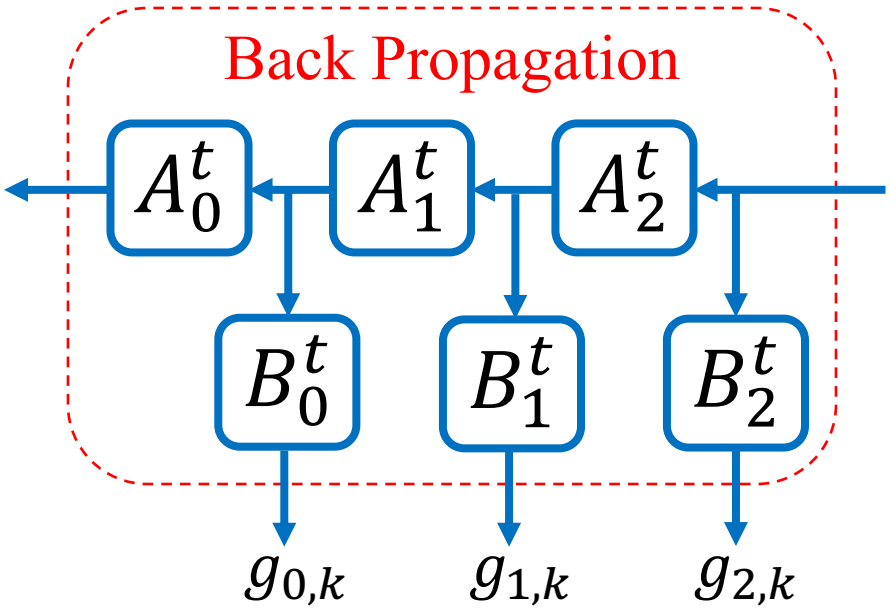
  Loss: $\rho(\mathrm{a},\mathrm{b}) = \|\mathrm{a}-\mathrm{b}\|_1^1$ Error: $\epsilon_k = -sign\left(x_k - f_\theta(y_k)\right)$

- Cross entropy

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

Point-wise division

Back Propagation for Typical Loss Functions



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

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

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

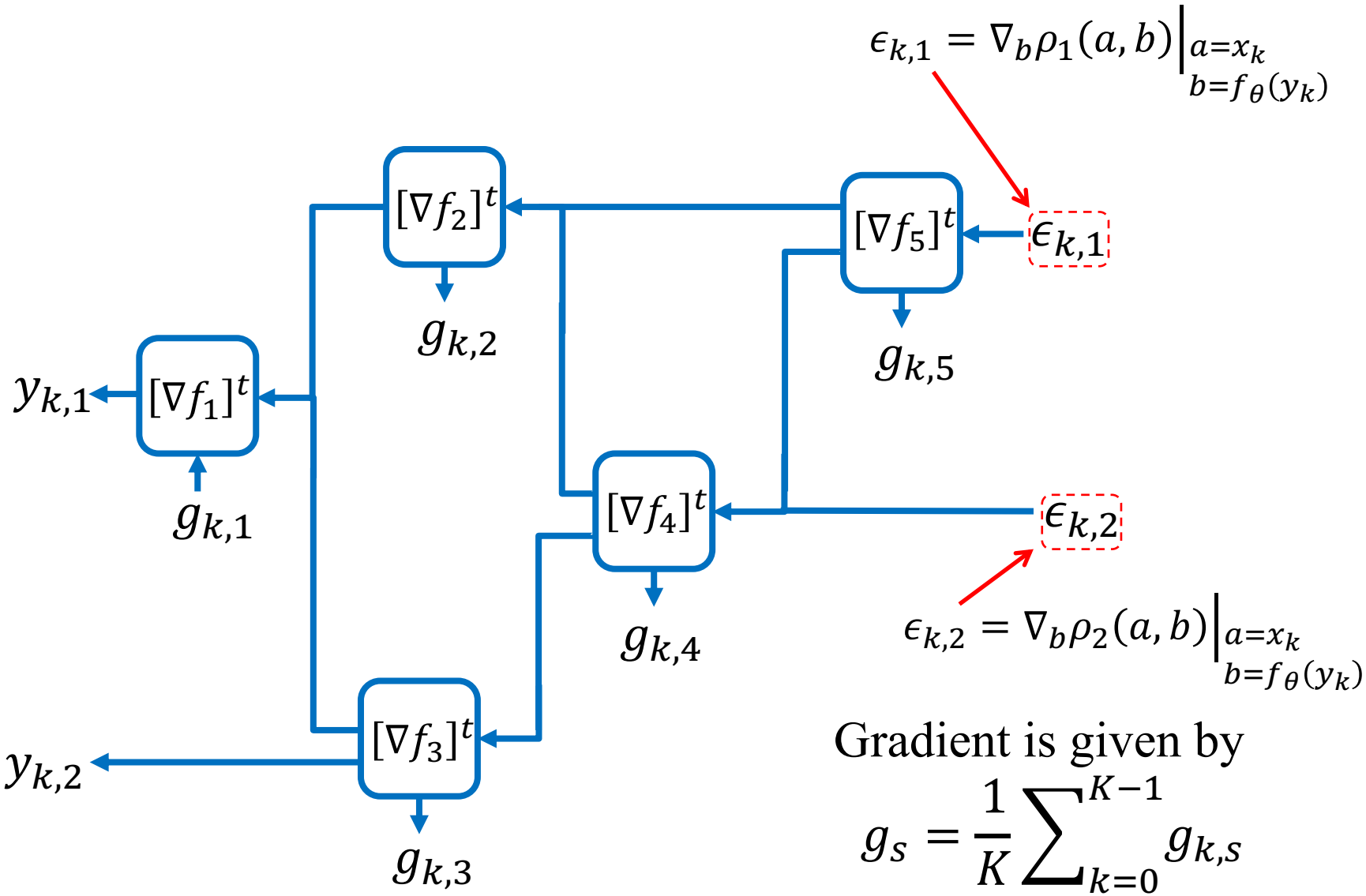
CE: $\epsilon_k = -\dfrac{x_k}{f_\theta(y_k)}$

- 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.



Gradient is given by

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