Deep Learning

Automatic Differentiation

Logistics

- Homework 1 due today
- Homework 2 out today, due in 2 weeks
- Today: Backpropogation/autograd.
  - Should be useful for homework 2!

What's on the Menu today?

- Recap
- Recap of freshman calculus
- Dive into chain rule
- Computational Graph & Reverse-mode differentiation (i.e. chain rule on steroids)

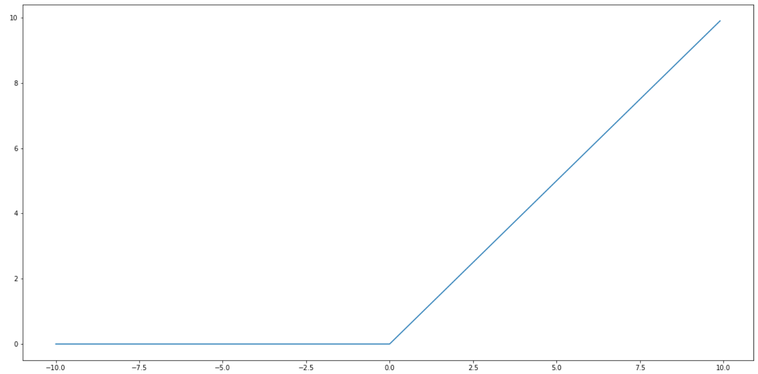
- DIY: Useful tricks

Recap

Last time: ReLU activation

- Modern deep networks usually use some variant of the *rectified linear unit* activation:

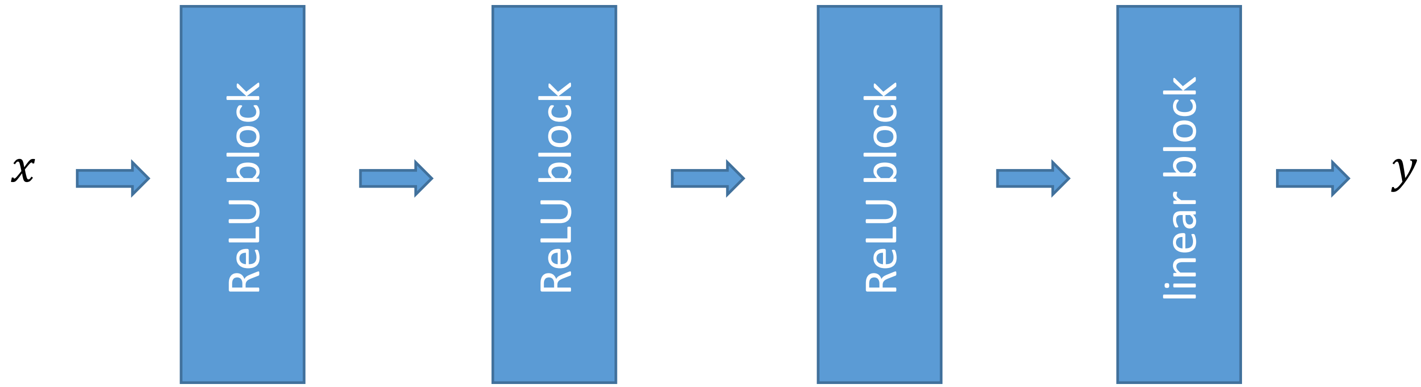
$$\sigma(x) = \max(x, 0)$$



- This still shares some inspiration with sigmoid: it is “off” when the input is negative.
- Since it does not saturate on the positive end, it has a much larger range of “learning”.

Last Time: ReLU activation MLP

- A more modern MLP looks like:



- ReLU networks are piecewise linear

Last Time: Cross-Entropy Loss

- Input 1: a *distribution* over the C possible output classes

$$p = (p_1, \dots, p_C), \qquad \sum_{i=1}^{C} p_i = 1$$

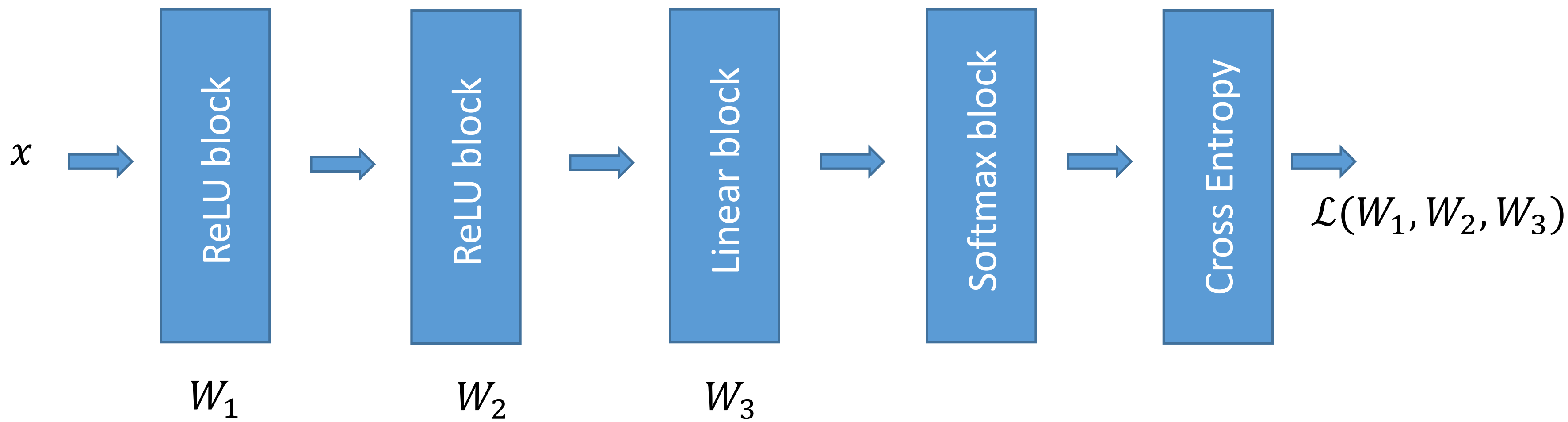
- Input 2: the true class value as a 1-hot vector:

$$y = (0, \dots, 1, \dots, 0)$$

- The cross-entropy loss is:

$$\ell(p, y) = \sum_i -1[y = i]\log(p_i)$$
$$= -\log(p_{correct\ class})$$

Today: Automatic Differentiation



- We need to compute gradients $\nabla_{W_i}\mathcal{L}(W_1, W_2, W_3)$
- You could code this up by hand for this network, but it would be a pain.
- Every time you change the network, you'd have to change the code!

Right matrix-multiplies

- In math class, you usually multiply matrices on the left:

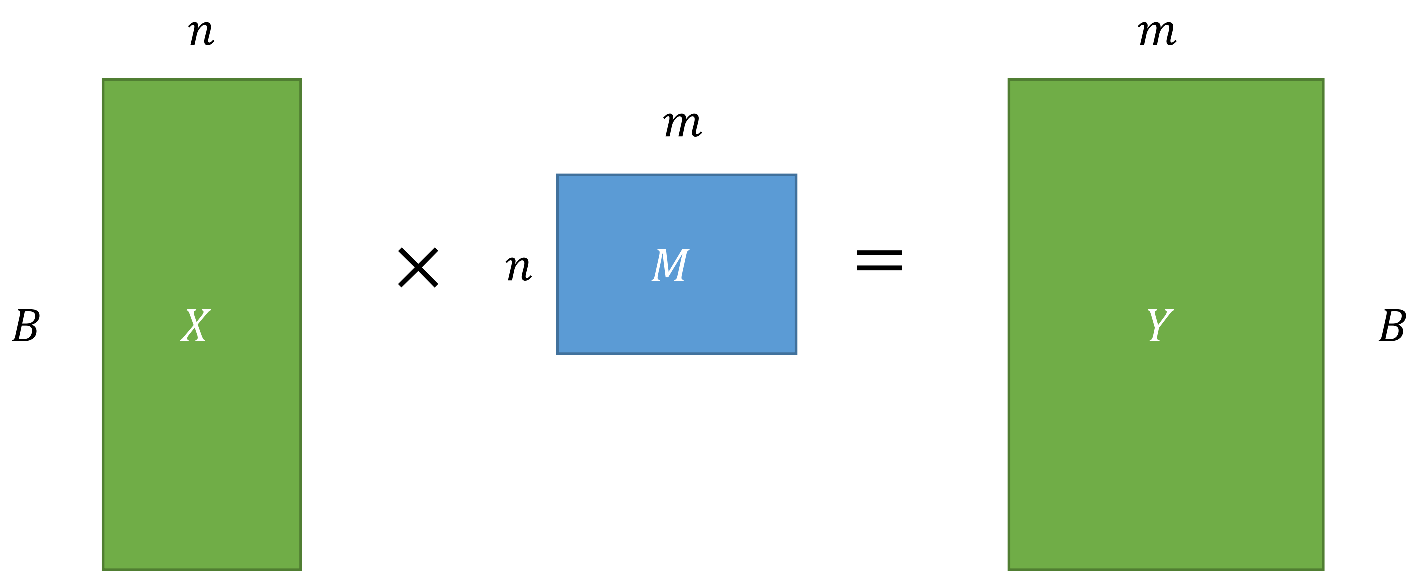
$$Mv$$

- In this lecture, we will multiply matrices on the right:

$$vM$$

- We do this to easily accommodate batch dimensions.

Right matrix-multiplies



A matrix $M \in \mathbb{R}^{n \times m}$ takes inputs in $\mathbb{R}^n$ and produces outputs in $\mathbb{R}^m$.

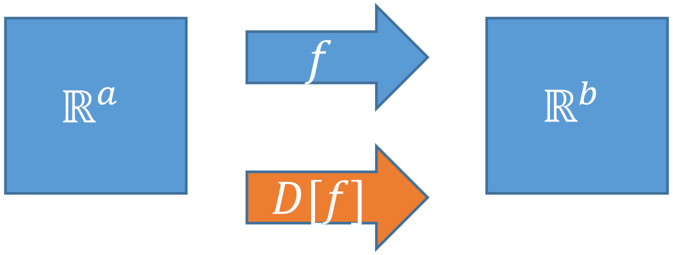
Recap of freshman calculus

What is a derivative, really?

- Let $f: \mathbb{R}^a \to \mathbb{R}^b$. Then the derivative is

$$D[f](x) \in \mathbb{R}^{a \times b}$$

- The derivative at x is a linear map (i.e. a matrix), whose inputs and outputs are the same dimension as f.



Special case: Gradients

- $f(x_1, x_2, x_3) = x_1 x_2 + x_3$
- $\nabla f(x_1, x_2, x_3) = (x_2, x_1, 1)$
- Technically, we should actually write:

$$\nabla f(x_1, x_2, x_3) = \begin{bmatrix} x_2 \\ x_1 \\ 1 \end{bmatrix}$$

- This is a 3×1 matrix, because f takes 3 dimensional inputs and has 1 dimensional outputs.

Derivative Formula

- The derivative has the formula:
$$D[f](x)_{ij} = \frac{df_j}{dx_i}(x)$$
- f_j is the j^{th} coordinate of f.
- What is the derivative of $f(x) = (x_1^2, x_1 x_2 x_3)$, which takes $\mathbb{R}^3$ to $\mathbb{R}^2$?
- Answer:
$$D[f](x) = \begin{bmatrix} 2x_1 & x_2 x_3 \\ 0 & x_1 x_3 \\ 0 & x_1 x_2 \end{bmatrix}$$

Another Example

- $f(x_1, x_2) = (x_2^2,\ x_1 + x_2,\ x_1 x_2)$
- $f_1(x_1, x_2) = x_2^2$
- $f_2(x_1, x_2) = x_1 + x_2$
- $f_3(x_1, x_2) = x_1 x_2$
- The derivative is 2×3:

$$D[f](x) = \begin{bmatrix} ? & ? & ? \\ ? & ? & ? \end{bmatrix}$$

- Answer:

$$D[f](x) = \begin{bmatrix} 0 & 1 & x_2 \\ 2x_2 & 1 & x_1 \end{bmatrix}$$

Chain Rule

The Chain Rule

- In calculus we all learned:

$$(g \circ f)'(x) = f'(x)g'\big(f(x)\big)$$

- In higher dimensions, we have a matrix statement:

$$D[g \circ f](x) = D[f](x)D[g]\big(f(x)\big)$$

- Let's check the dimensions match:

- $D[f] \in \mathbb{R}^{a\times b}$ and $D[g] \in \mathbb{R}^{b\times c}$. $D[g \circ f] \in \mathbb{R}^{a\times c}$.

Example

- $f(x) = x^4$
- $g(y) = \sqrt{y}$

- $D[f](x) = 4x^3$
- $D[g](y) = \frac{1}{2\sqrt{y}}$
- $D[g \circ f](x) = D[f](x)D[g]\big(f(x)\big) = 2x$

Multiple Inputs

- Suppose f has multiple, multi-dimensional inputs:
$$f(X, Y): \mathbb{R}^a \times \mathbb{R}^b \to \mathbb{R}^c$$
- The partial derivatives of f with respect to the two arguments are defined analogously:
$$D_X[f](x, y) \in \mathbb{R}^{a \times c}$$
- The equation is:
$$D_X[f](x, y)_{ij} = \frac{\partial f_j}{\partial X_i}(x, y)$$

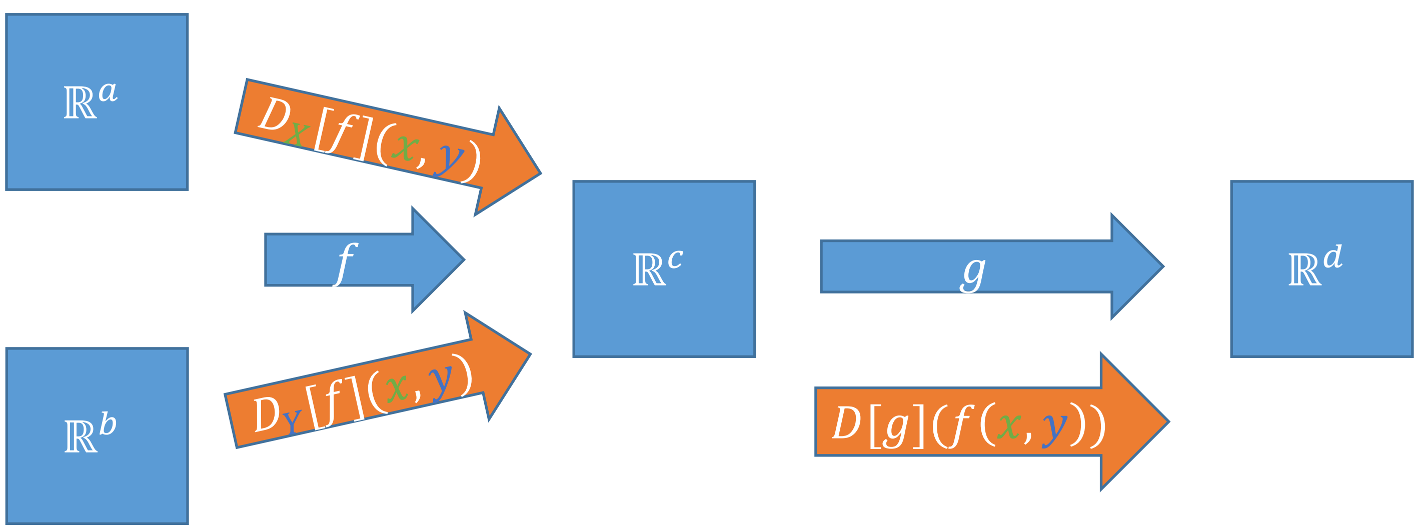
Chain rule with multiple inputs

- The chain rule works the same.
- Let $g: \mathbb{R}^c \to \mathbb{R}^d$ and

$$f(X, Y): \mathbb{R}^a \times \mathbb{R}^b \to \mathbb{R}^c$$

- The partial derivative is:

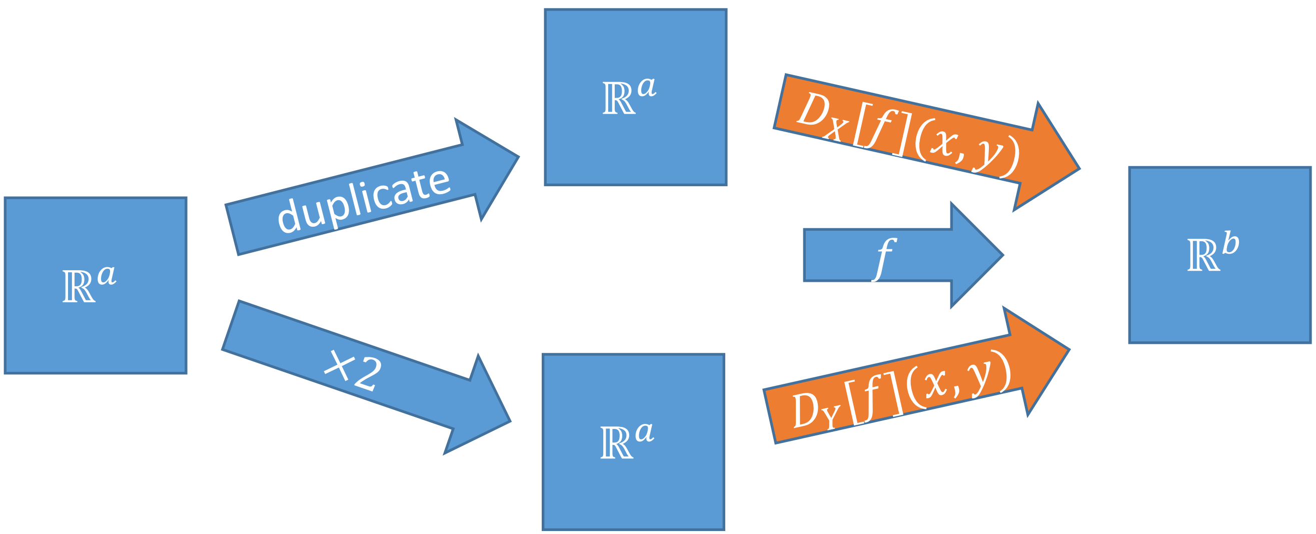
$$D_X[g \circ f](x, y) = D_X[f](x, y) D[g]\big(f(x, y)\big)$$



Re-Using Inputs

$$f(X, Y): \mathbb{R}^a \times \mathbb{R}^a \rightarrow \mathbb{R}^b$$
$$g(X) = f(X, 2X)$$

- What is $D[g]$?



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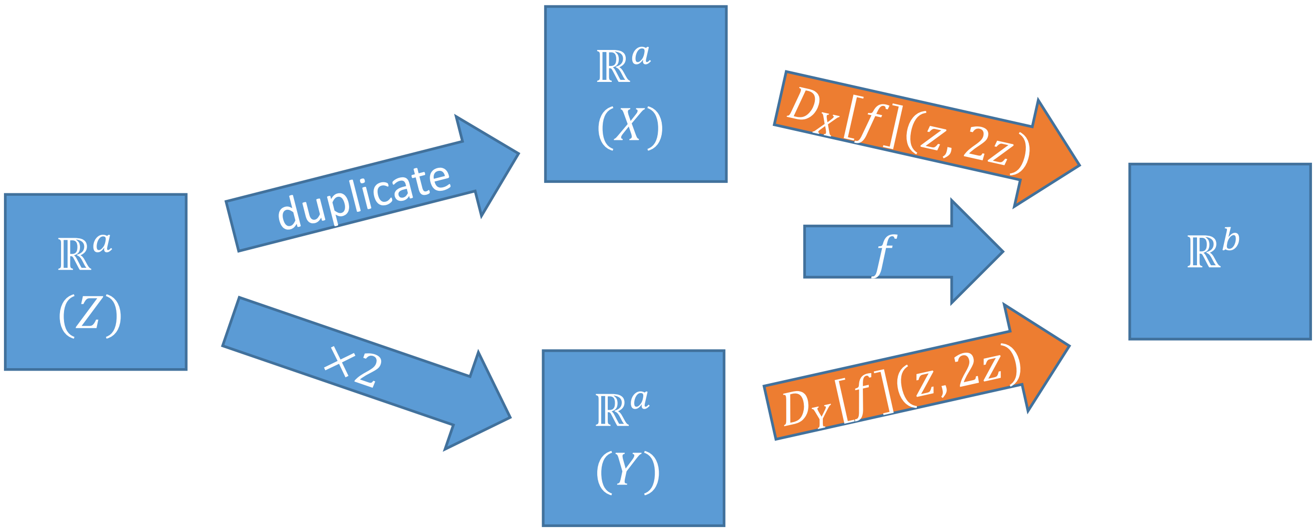


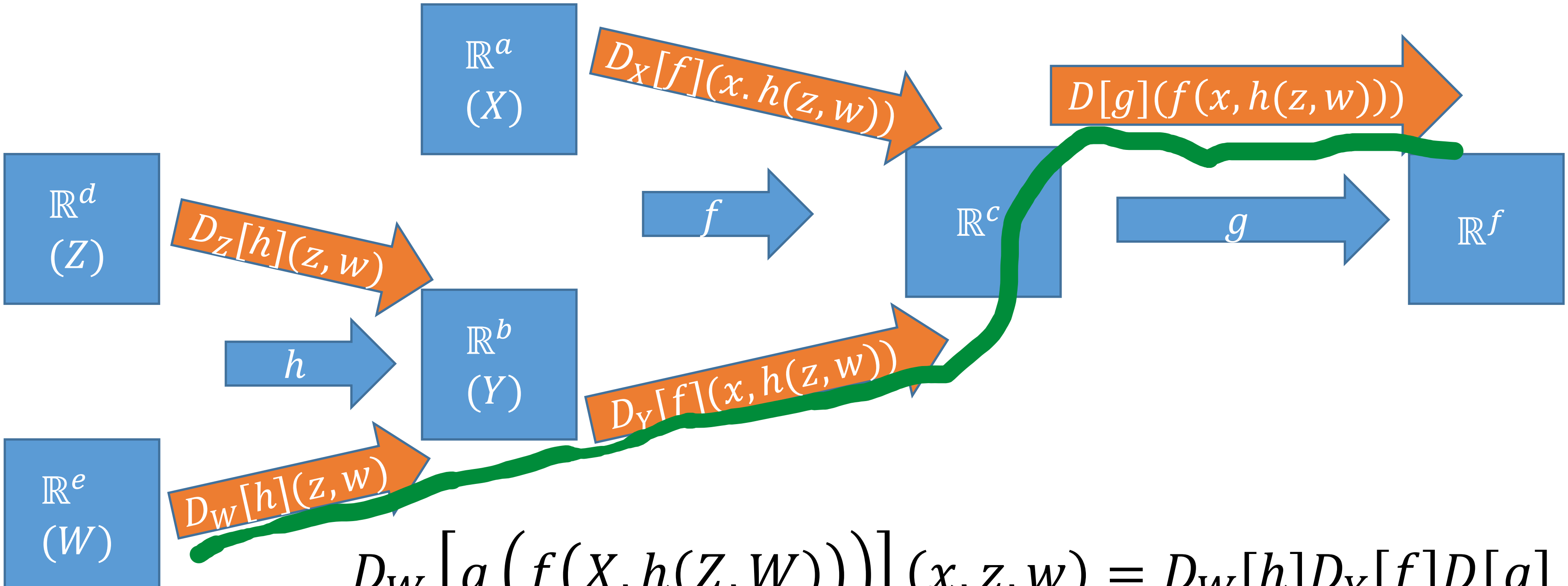
$$D_Z[f(Z, 2Z)] = D_X[f](z, z) + 2D_Y[f](z, 2z)$$

- When the inputs split, we need to sum the individual derivatives.

More complicated functions

$$g\colon \mathbb{R}^c \to \mathbb{R}^f$$
$$f(X,Y)\colon \mathbb{R}^a \times \mathbb{R}^b \to \mathbb{R}^c$$
$$h(Z,W)\colon \mathbb{R}^d \times \mathbb{R}^e \to \mathbb{R}^b$$

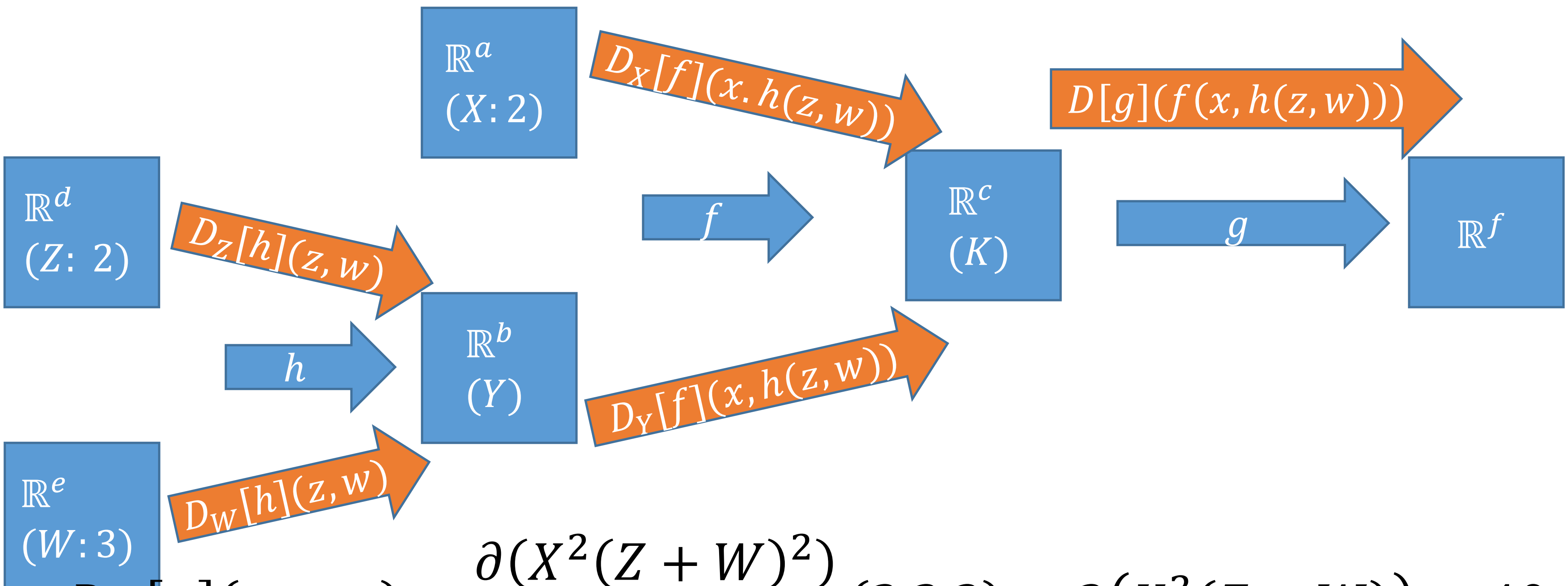
The function : $g\Big(f\big(X, h(Z,W)\big)\Big)$



$$D_W\Big[g\Big(f\big(X,h(Z,W)\big)\Big)\Big](x,z,w) = D_W[h]D_Y[f]D[g]$$

Example

$$g(K) = K^2$$
$$f(X, Y) = XY$$
$$h(Z, W) = Z + W$$



$$D_W[g](x, z, w) = \frac{\partial(X^2(Z+W)^2)}{\partial W}(2,2,3) = 2\big(X^2(Z+W)\big) = 40$$

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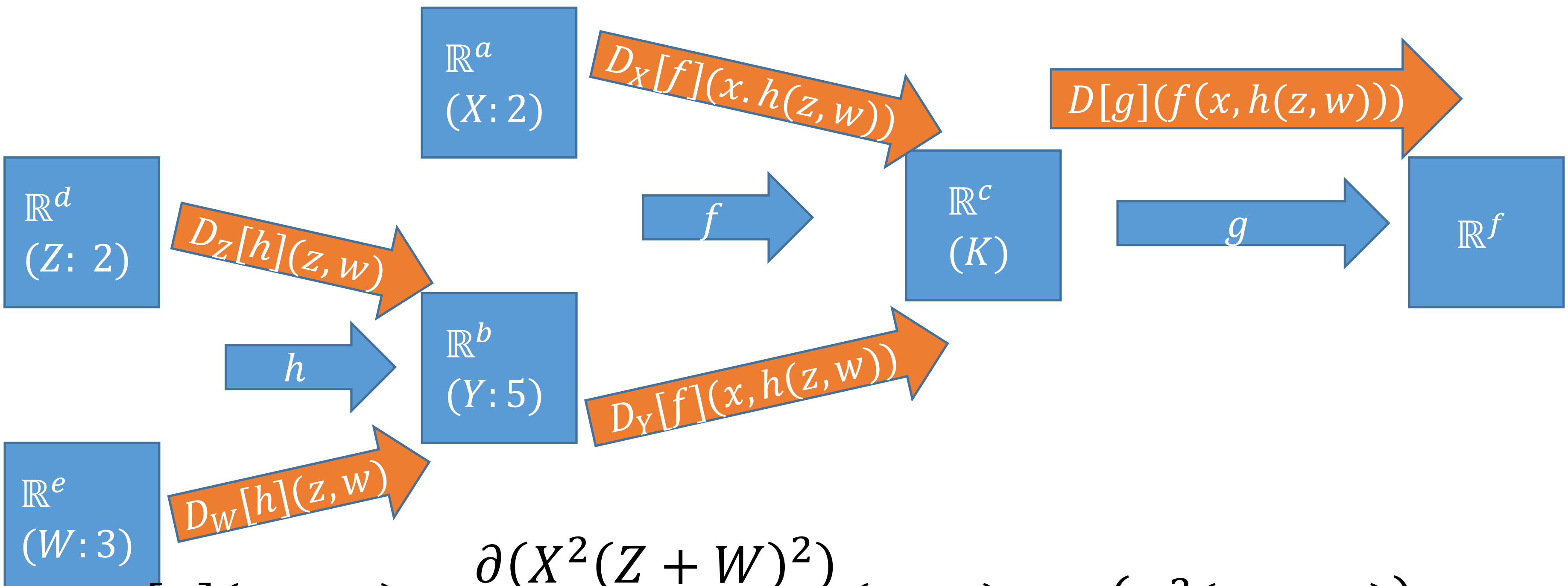

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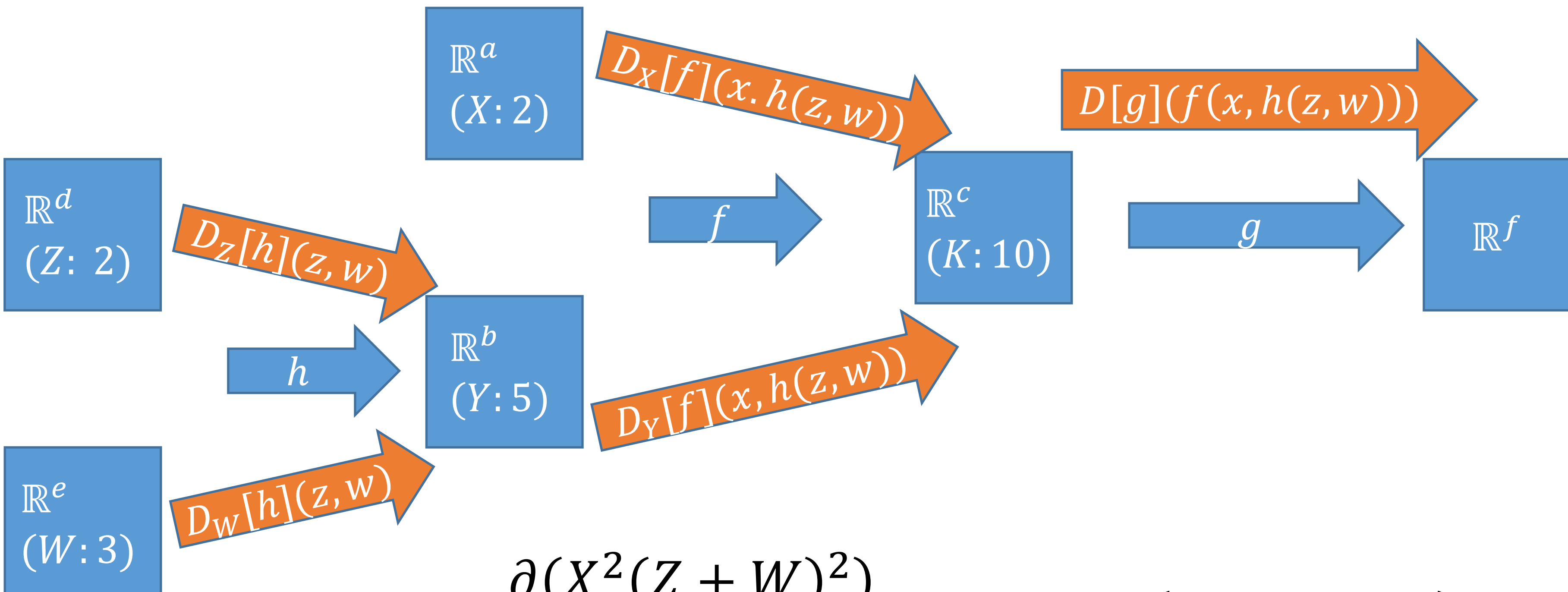

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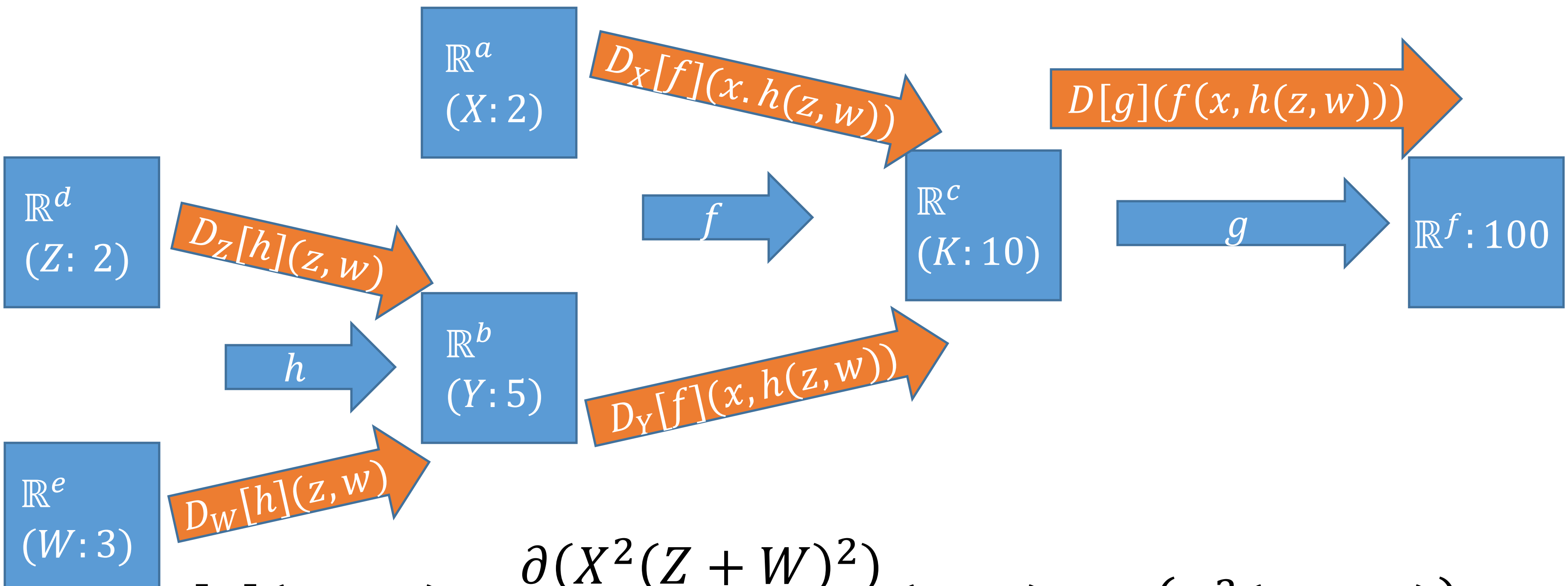

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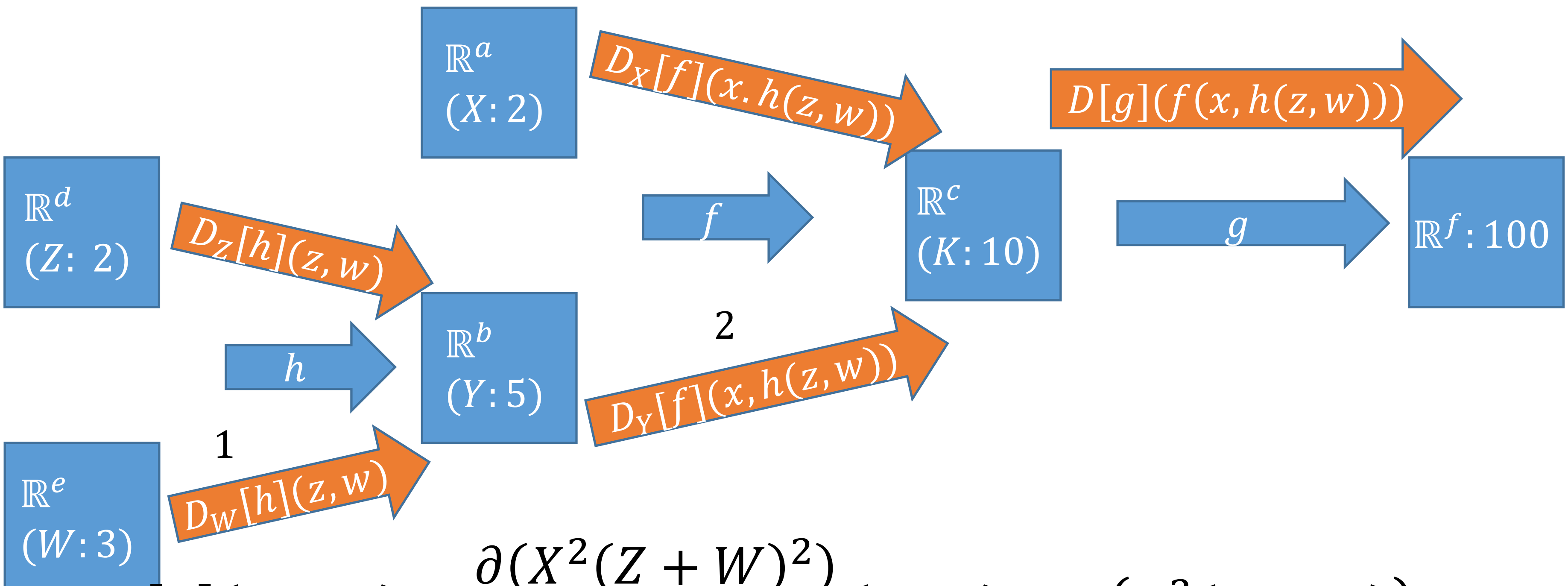

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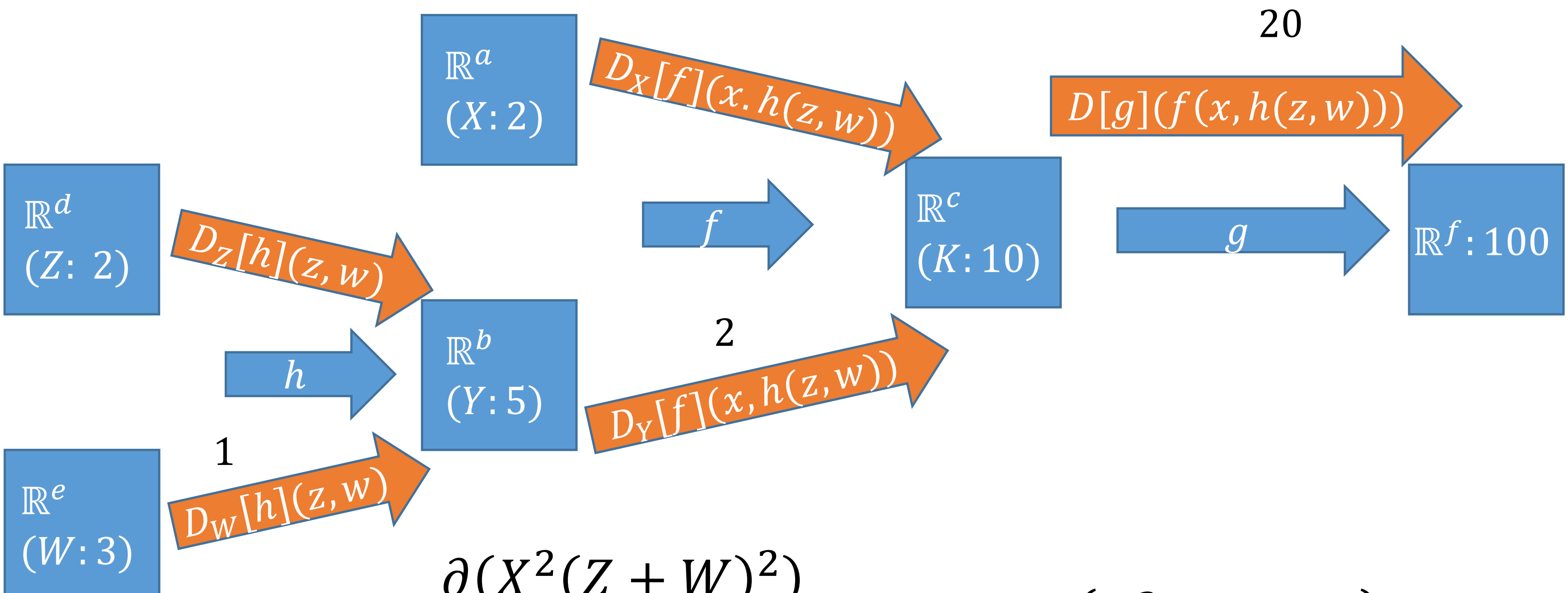
Example

$$g(K) = K^2$$
$$f(X,Y): XY$$
$$h(Z,W): Z + W$$



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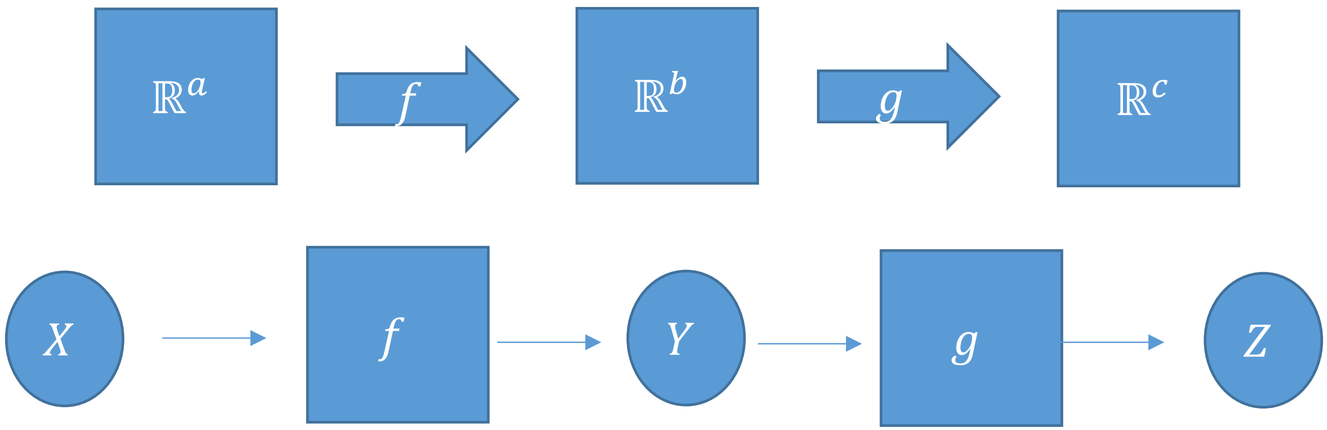
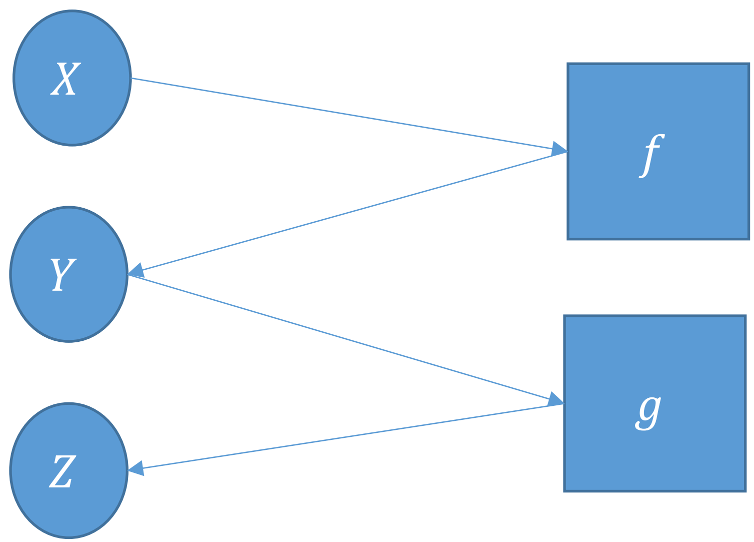
Computational Graph

Computational Graph

- Directed Acyclic graph with two kinds of nodes.
- Two kinds of nodes: "operation" nodes and "variable" nodes.
- Each "operation" node represents a function
- Each "variable" node represents either function inputs or outputs (or both)
- The graph is bipartite: variable nodes are only connected to operation nodes, and operation nodes are only connected to variable nodes.
- All source and sink nodes are variable nodes.

Computational Graph

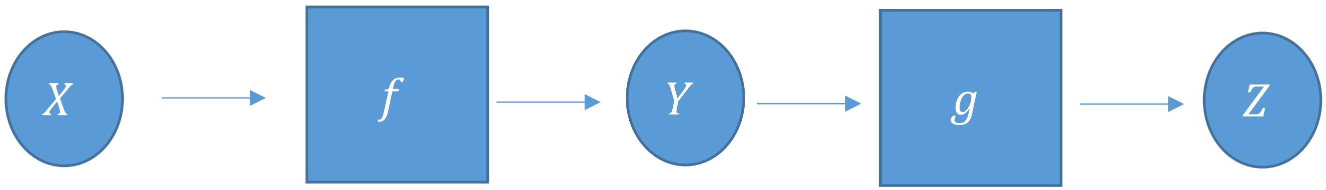




Variable nodes

Operation nodes

Data held by nodes

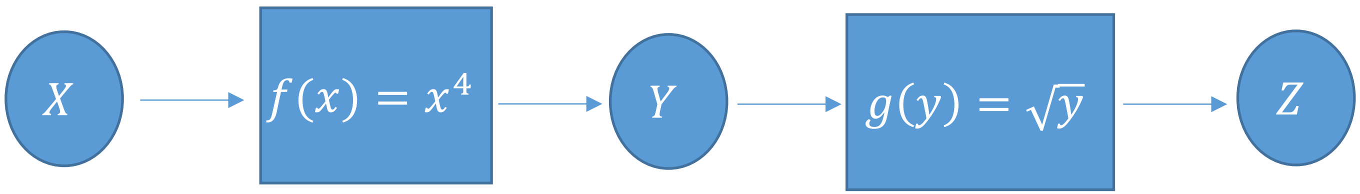


- Variable nodes will hold real numbers/vectors/matrices representing the "value" of the variable they represent.
- Operation nodes may hold various arbitrary state needed to implement either the forward or backward passes.

Backprop: “reverse-mode differentiation”

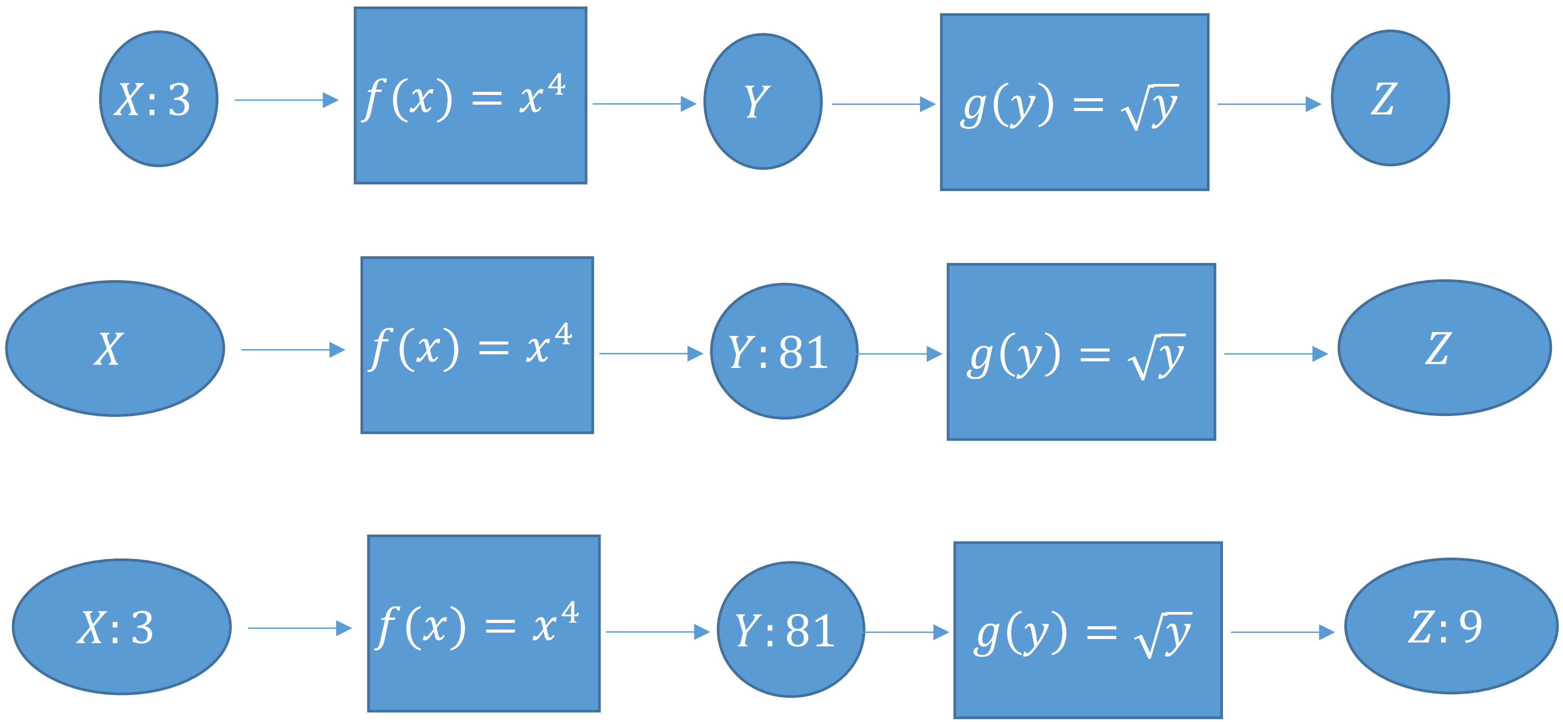
- Backpropagation is an algorithm for automatically computing the gradient of a function specified by a computation graph.
- It has two phases, the “forward pass” and the “backward pass”

Forward pass

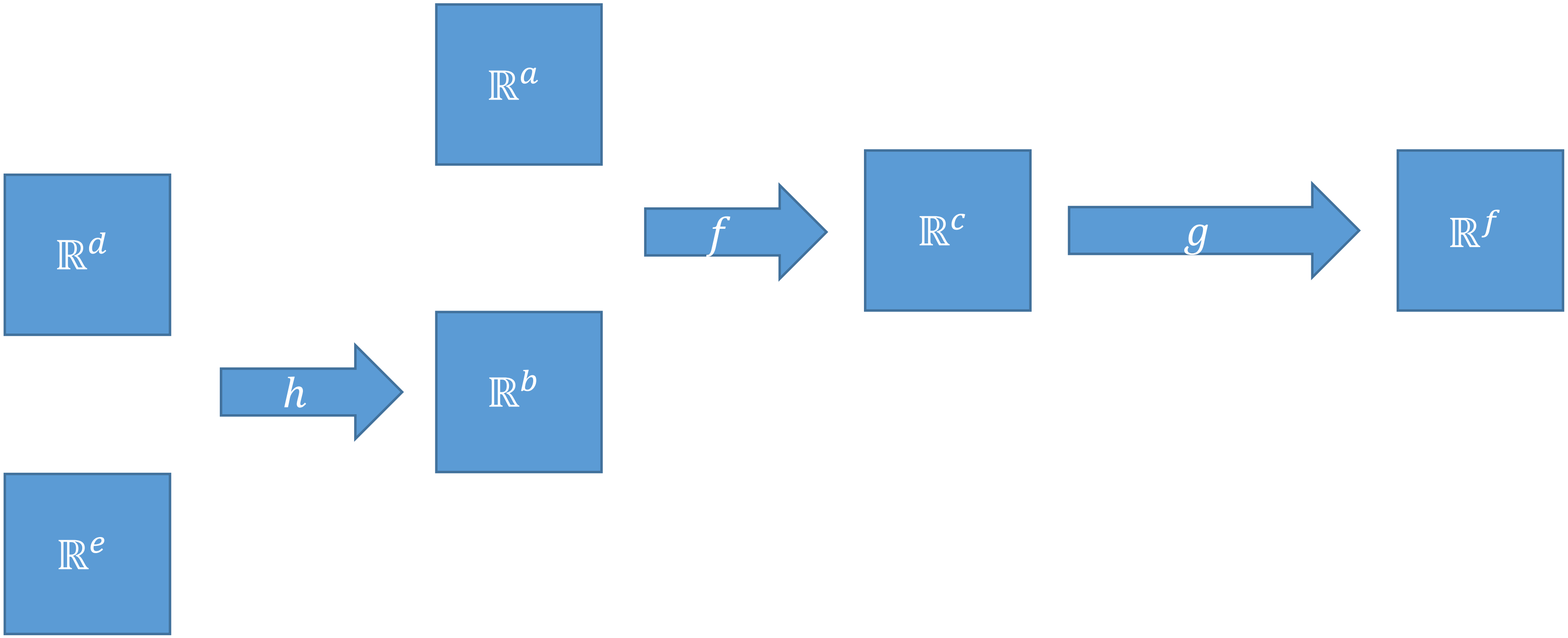


- **Step 1**: Start with seeding the source variable node with some value, say $X = 3$
- **Step 2**: Look at all the operation nodes for which all inputs have values assigned.
- **Step 3**: Compute these operations, and assign the output to the output variable nodes. Potentially save some state in the operation node.
- **Step 4**: Repeat

Forward Pass



More Complicated Forward Pass



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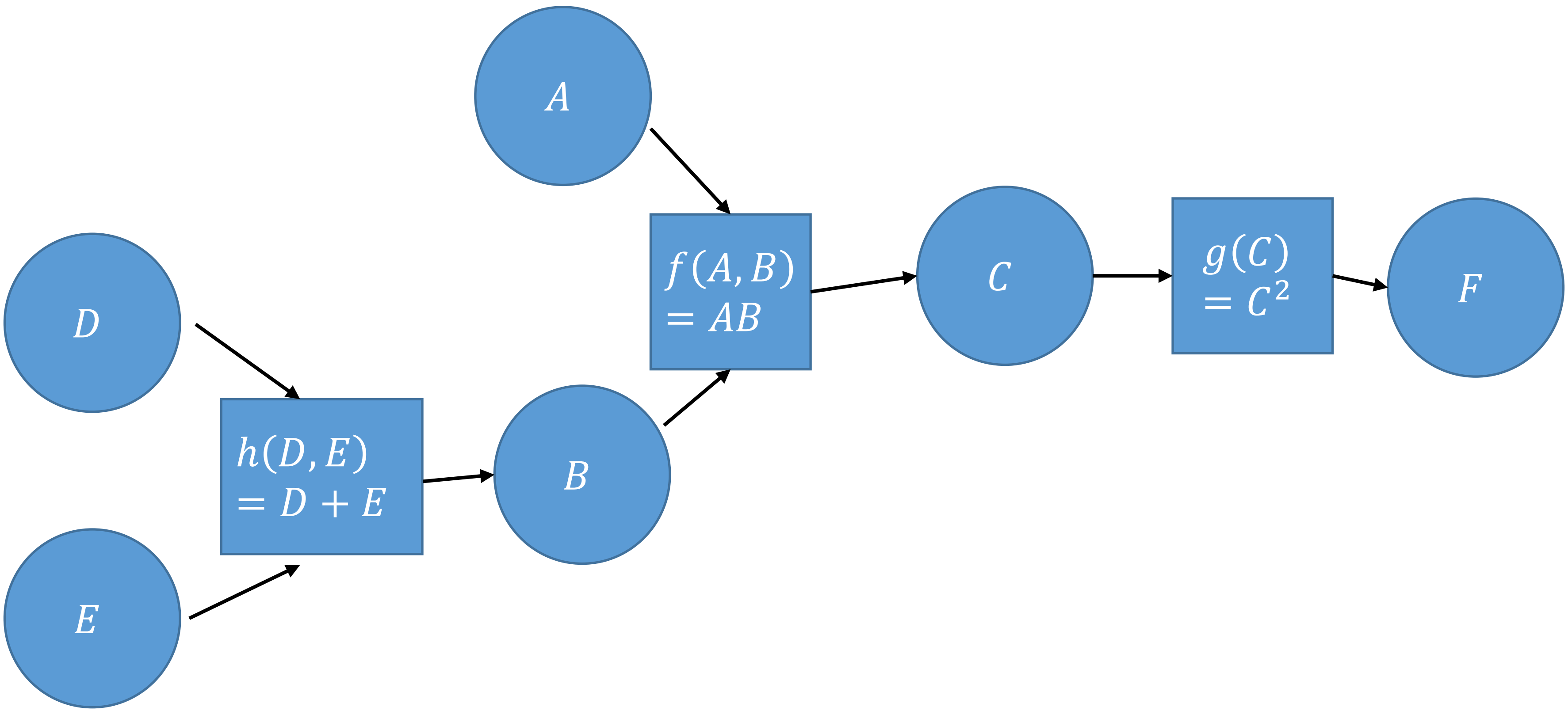

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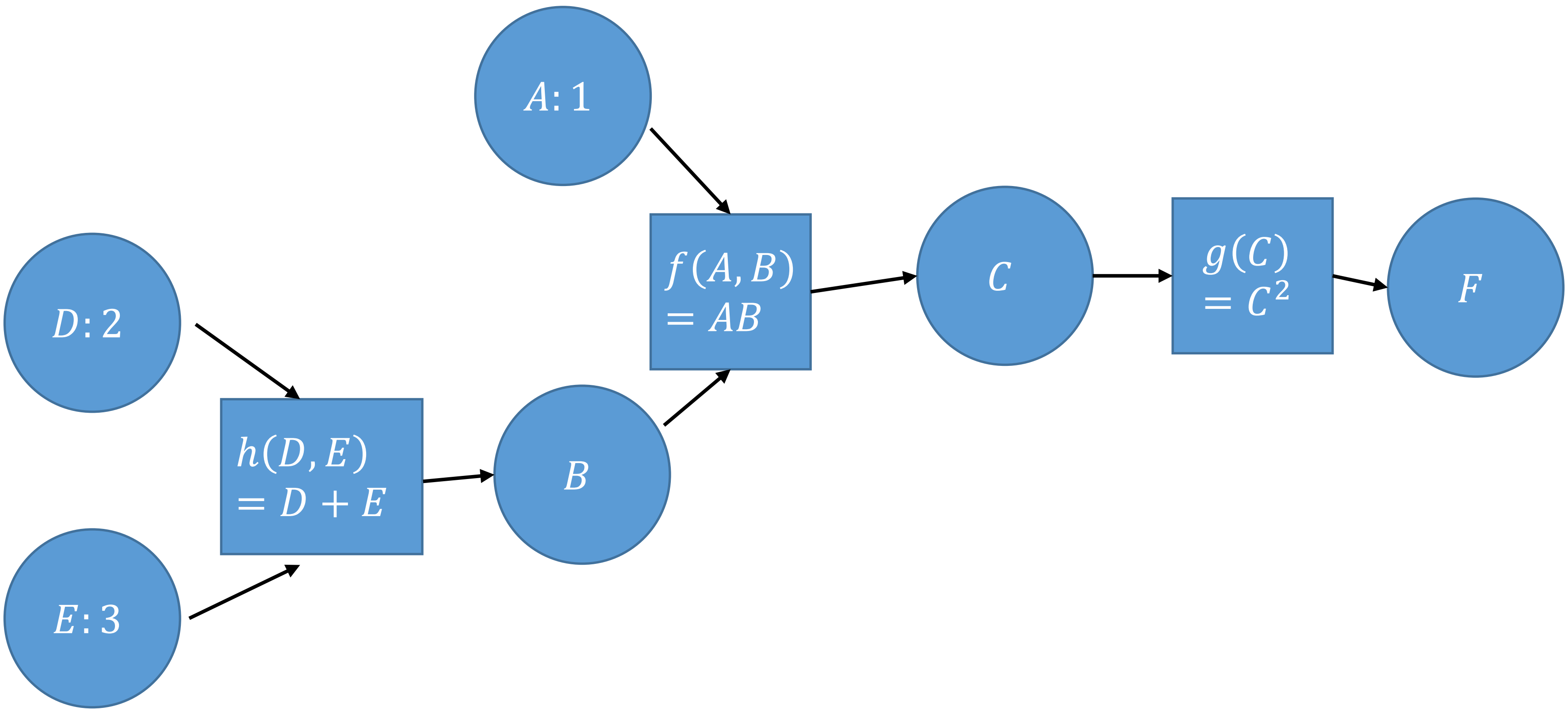

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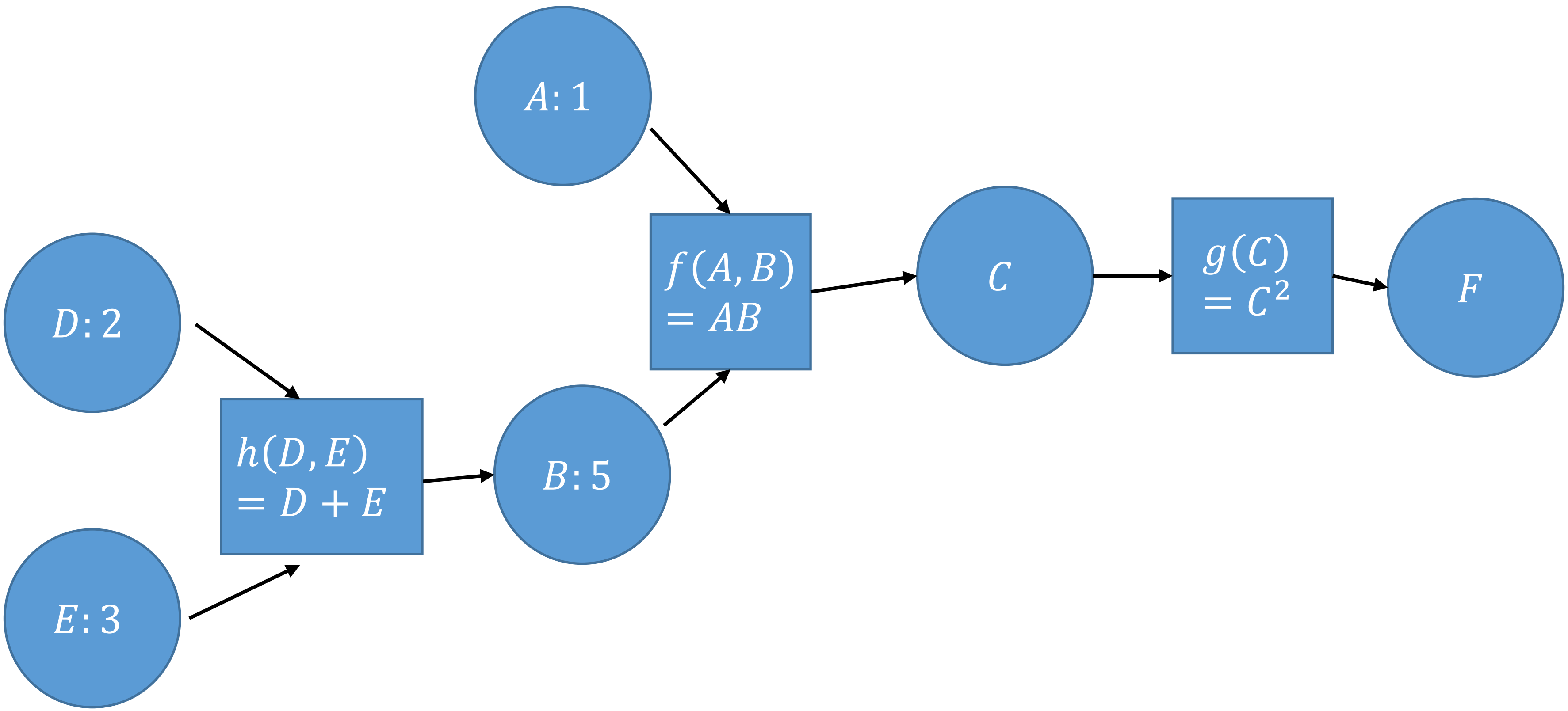

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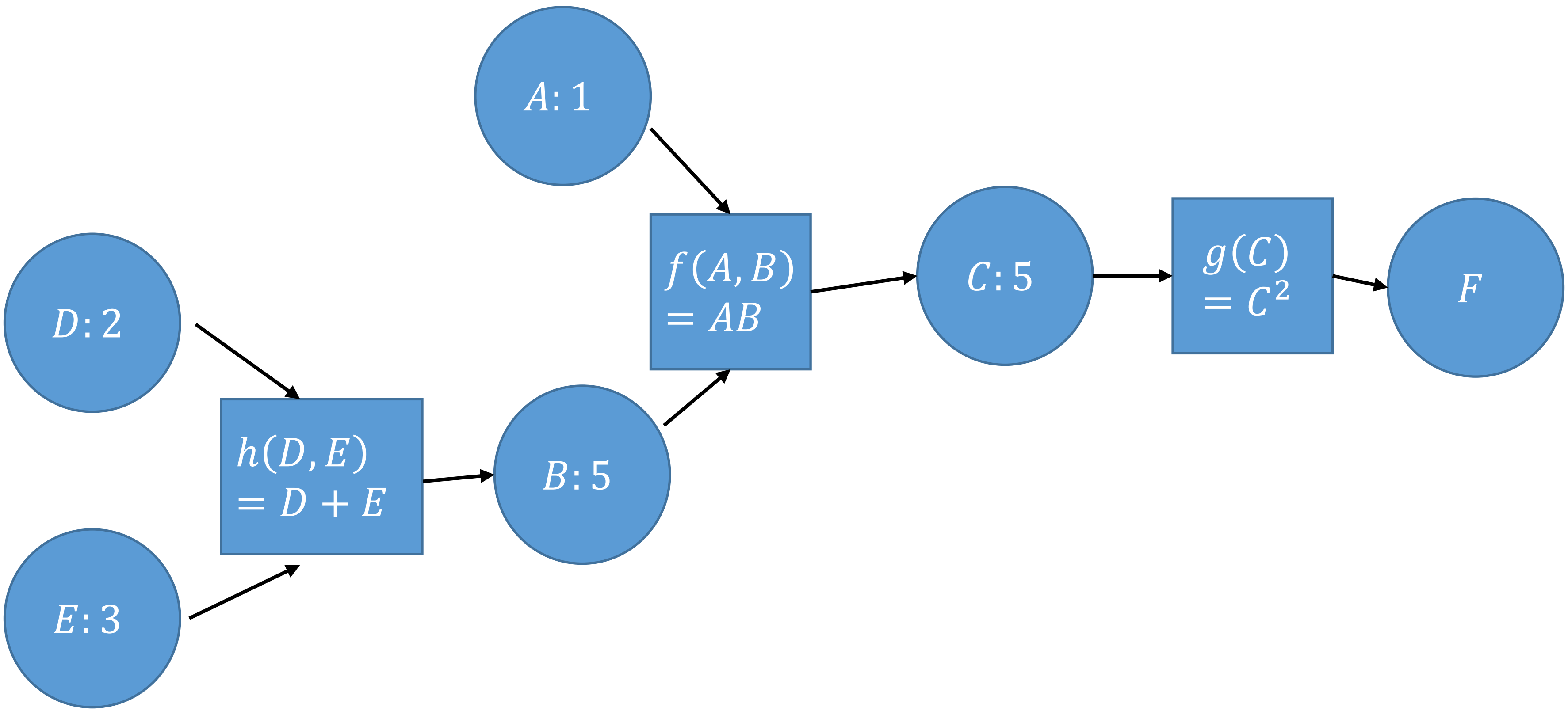

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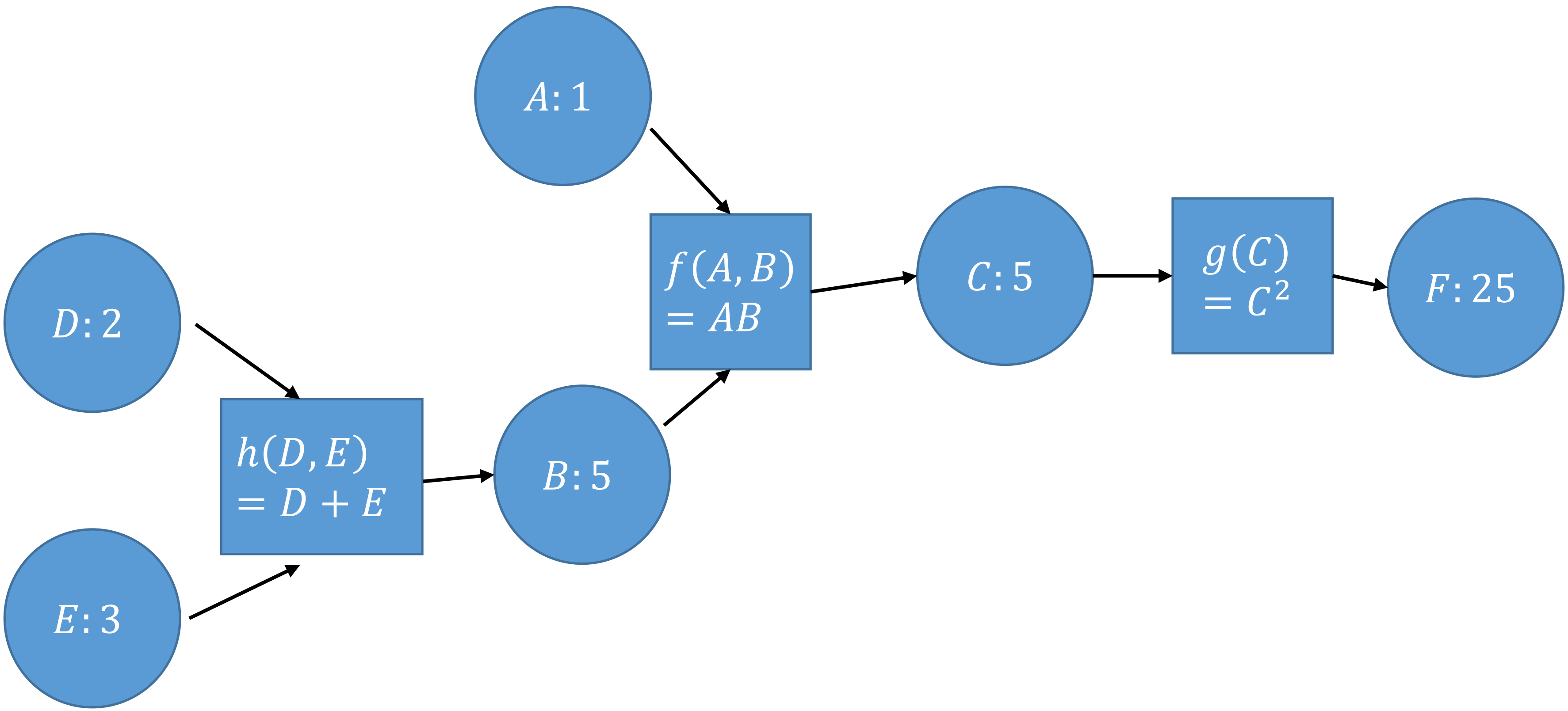
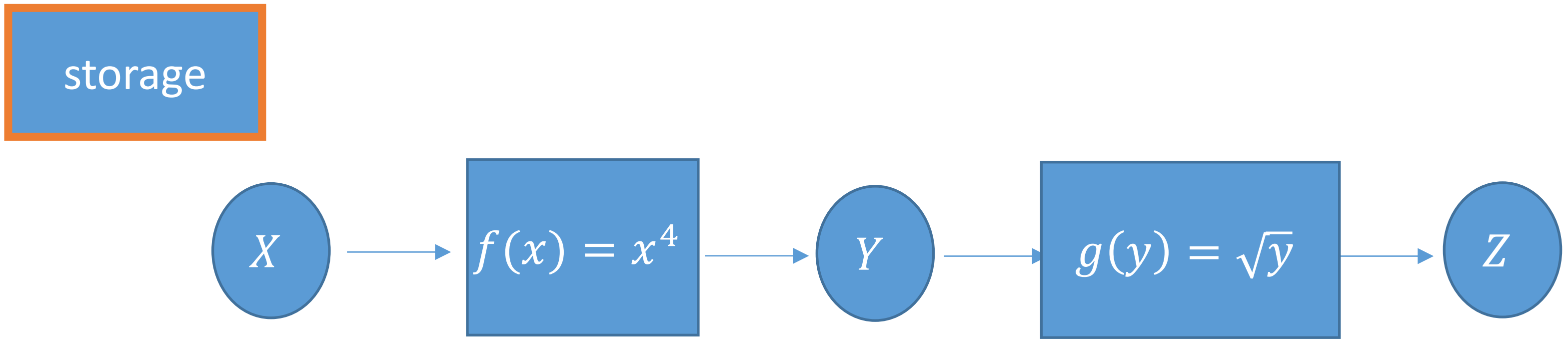


Compute Derivatives in Forward Pass



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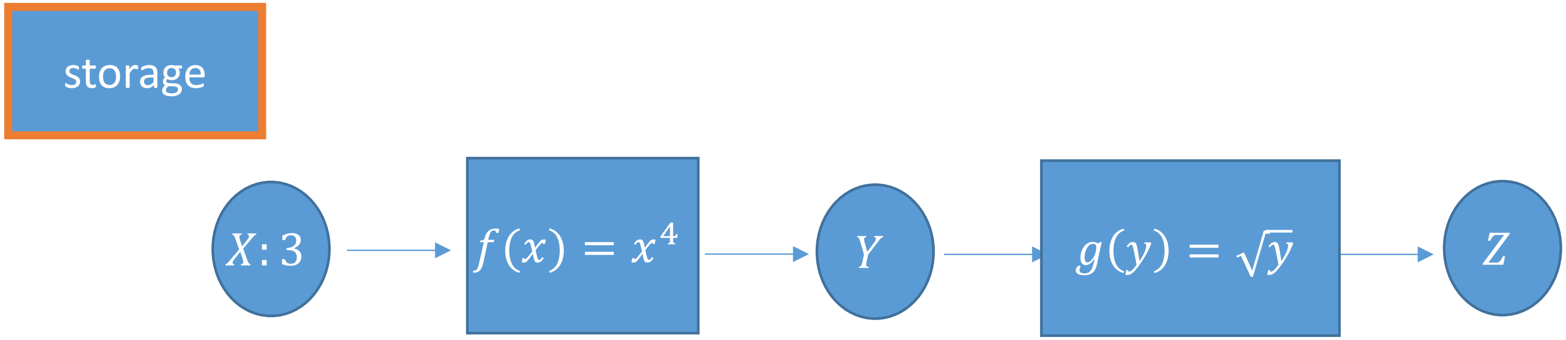

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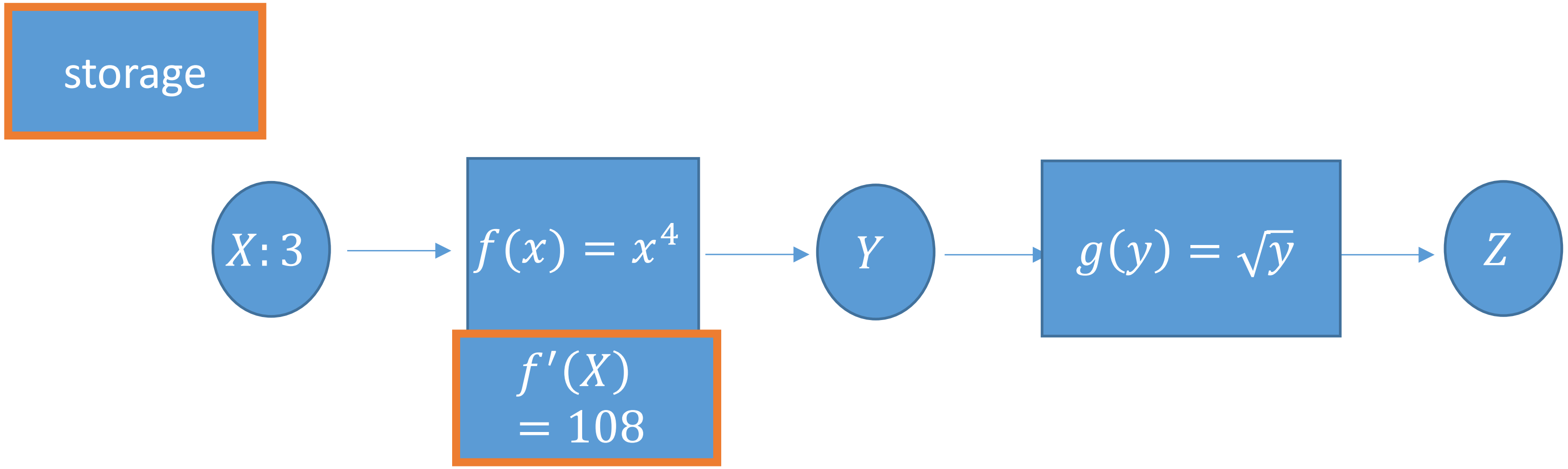

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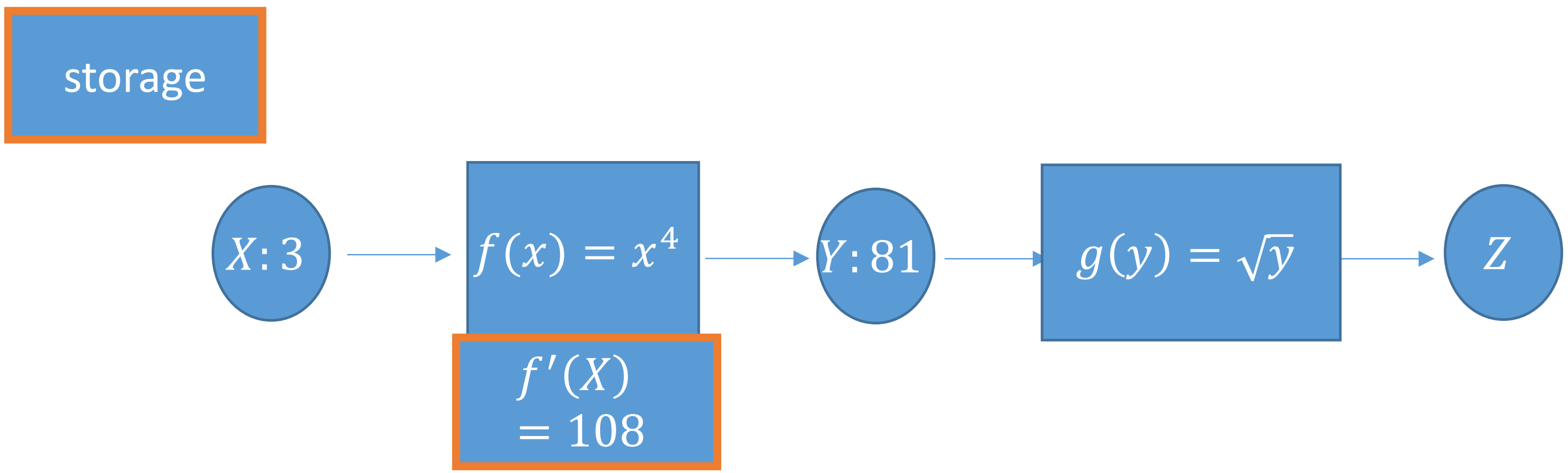

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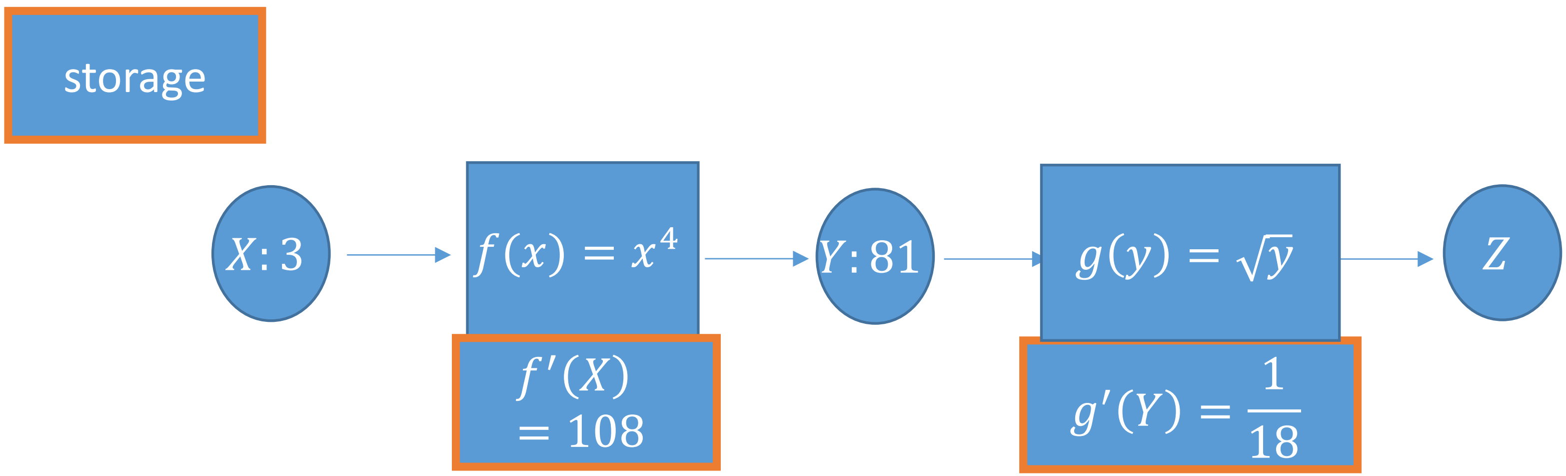

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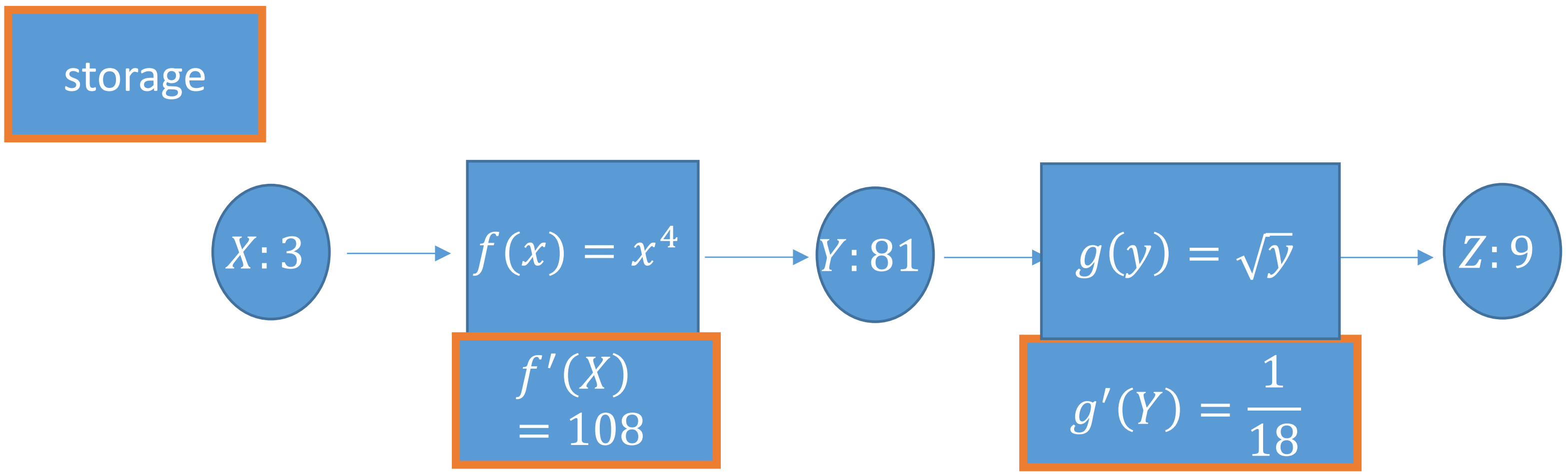
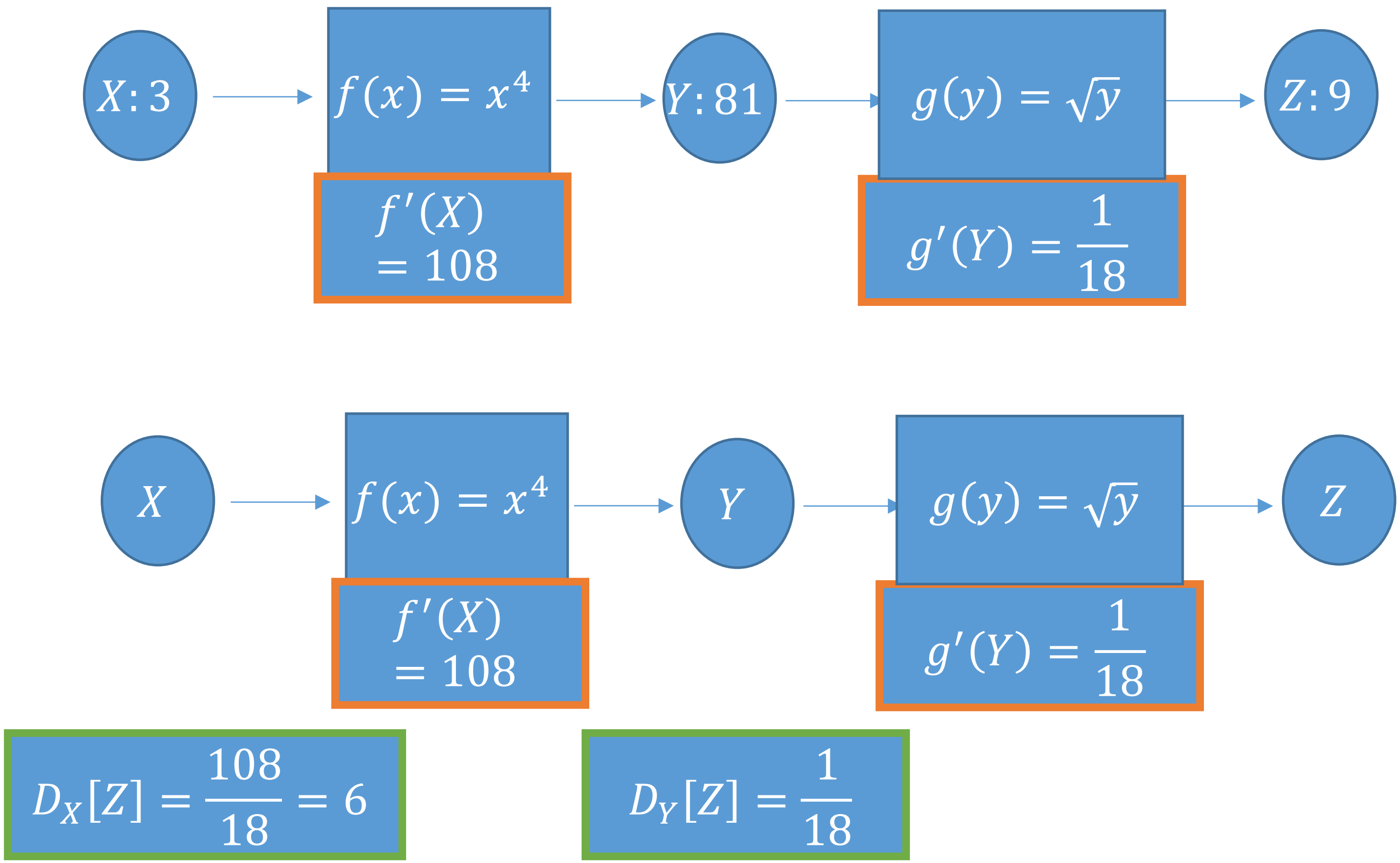


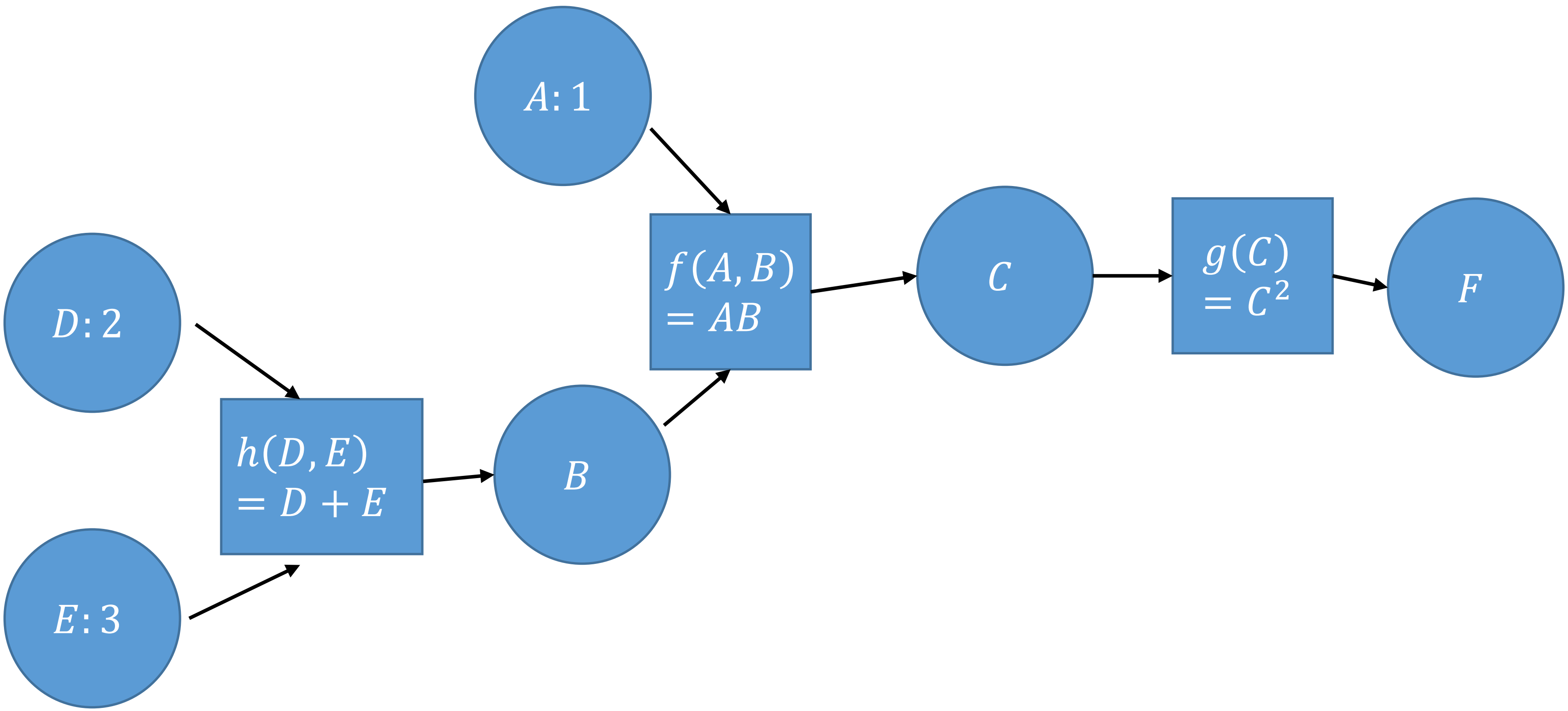
Backward Pass

- The backward pass uses the data in the forward pass to compute the gradient of the sink node with respect to every variable node.
- Forward pass propagates from the source variable nodes to the sink variable.
- Backward pass propagates backwards from sink node to source.
- You MUST do a forward pass before the backward pass.

Backward Pass



More Complicated Forward Pass



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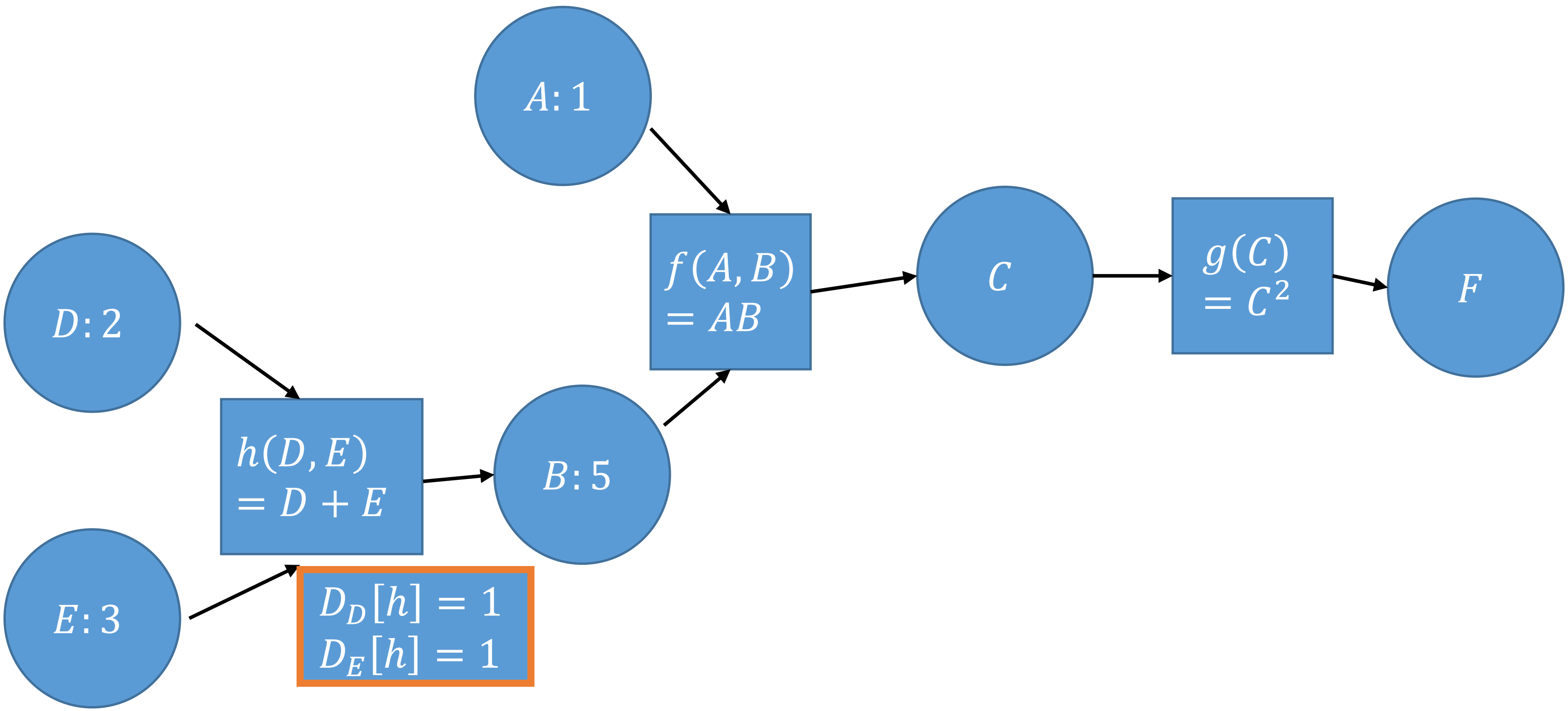

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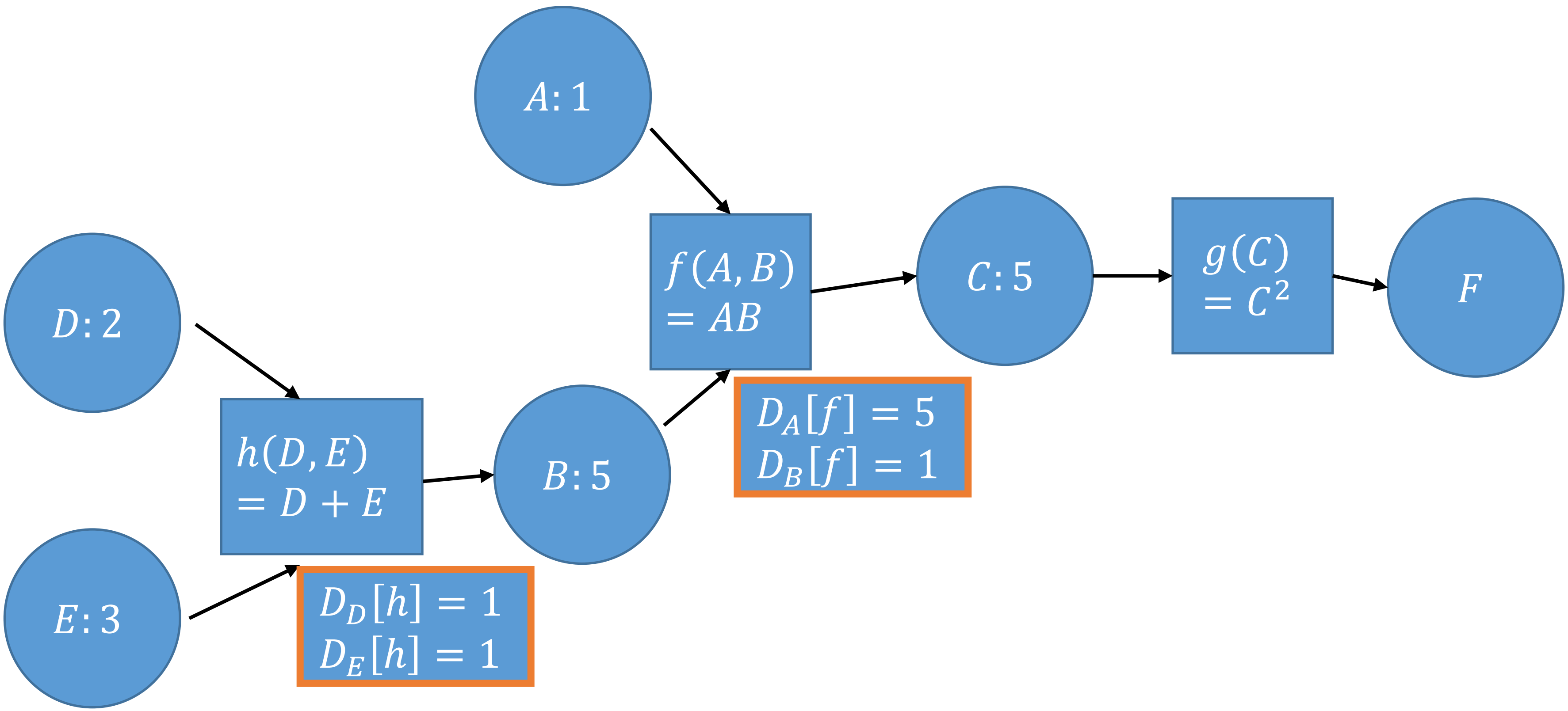

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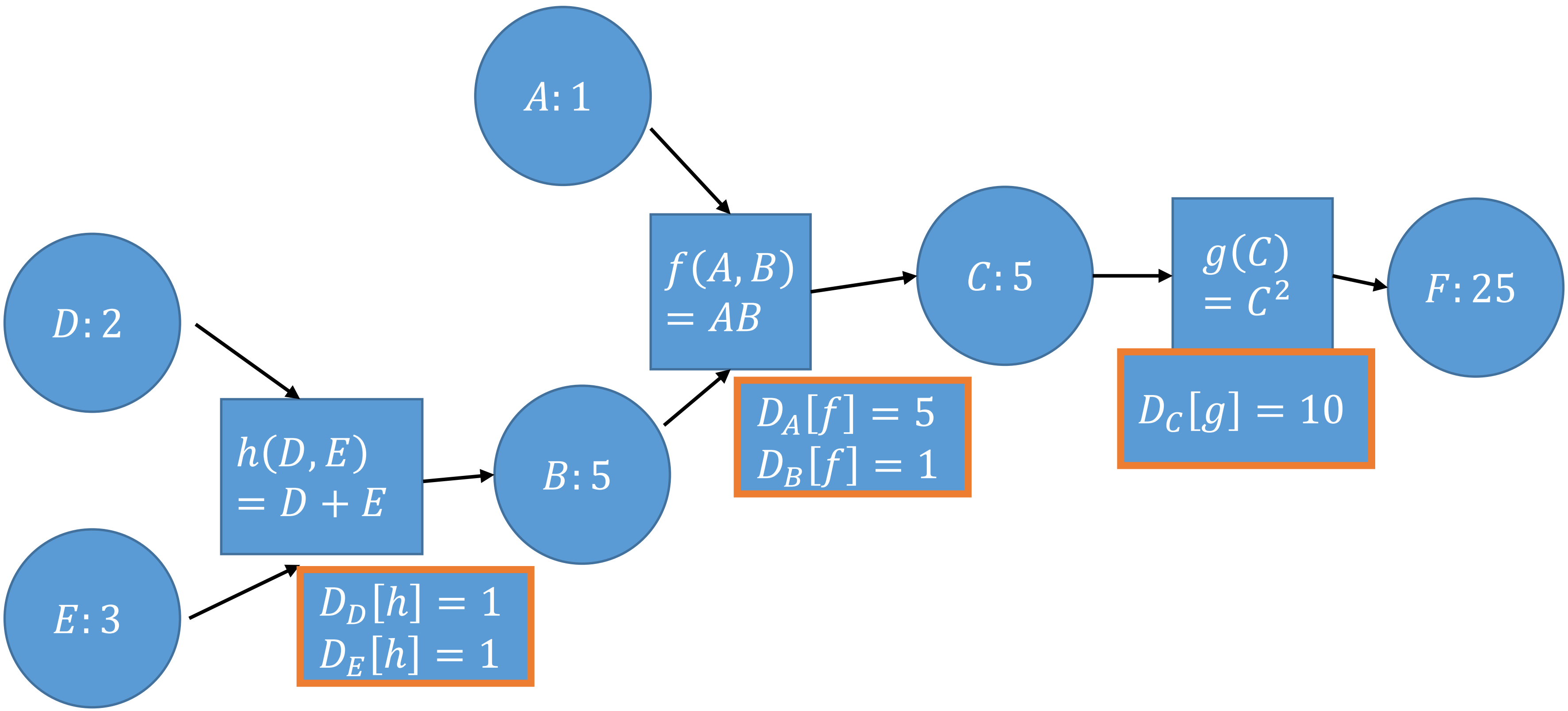

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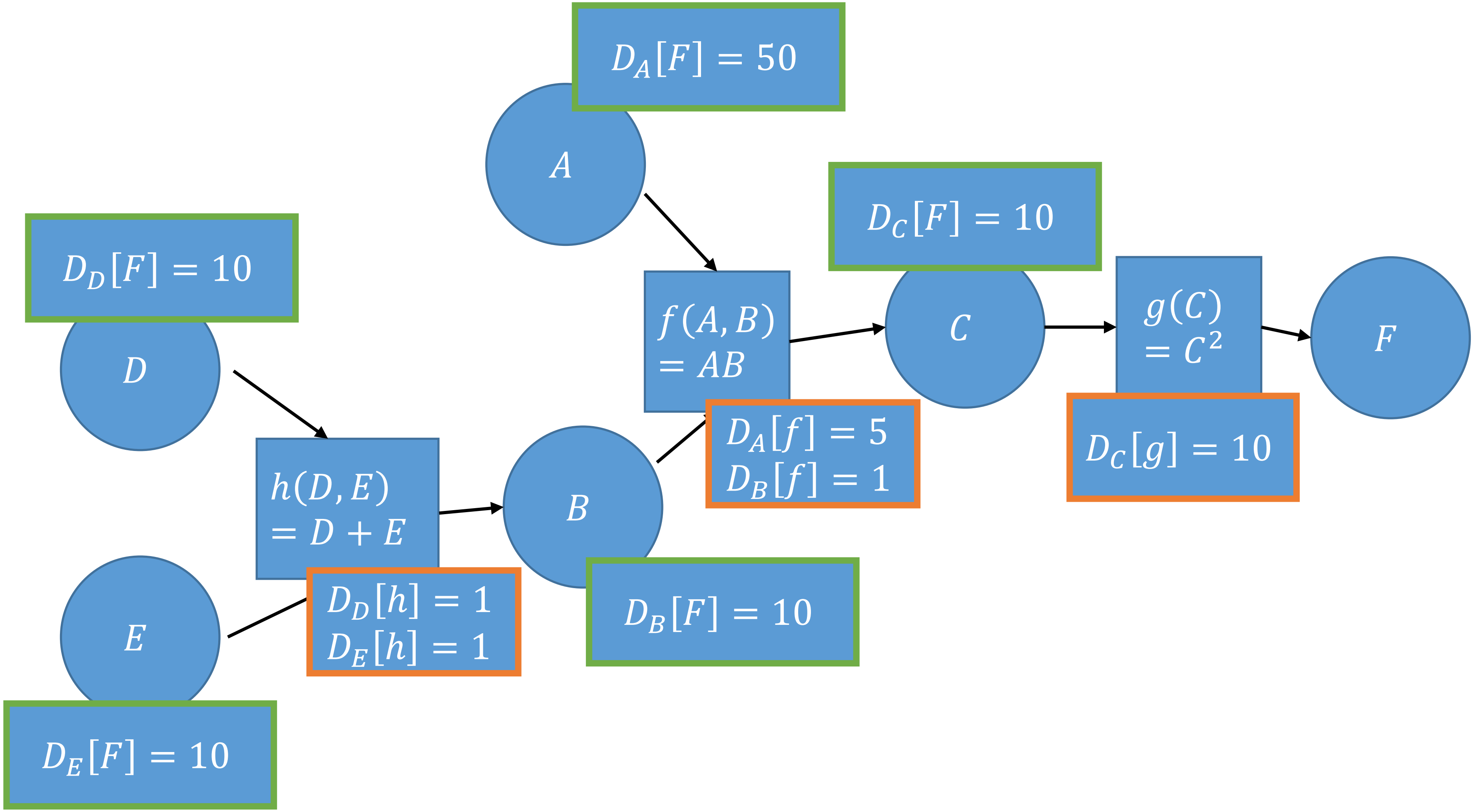
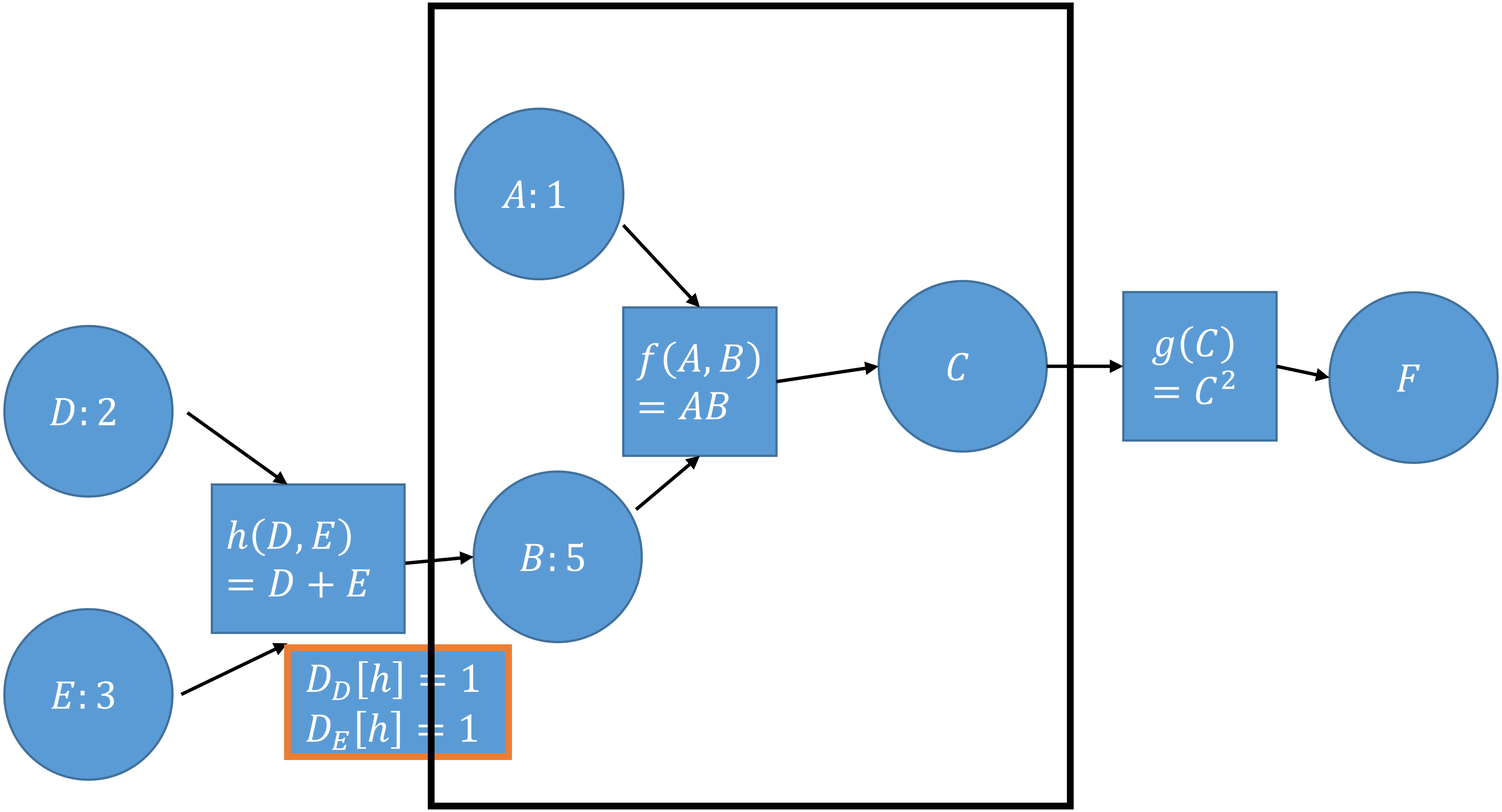


Backprop is "local"

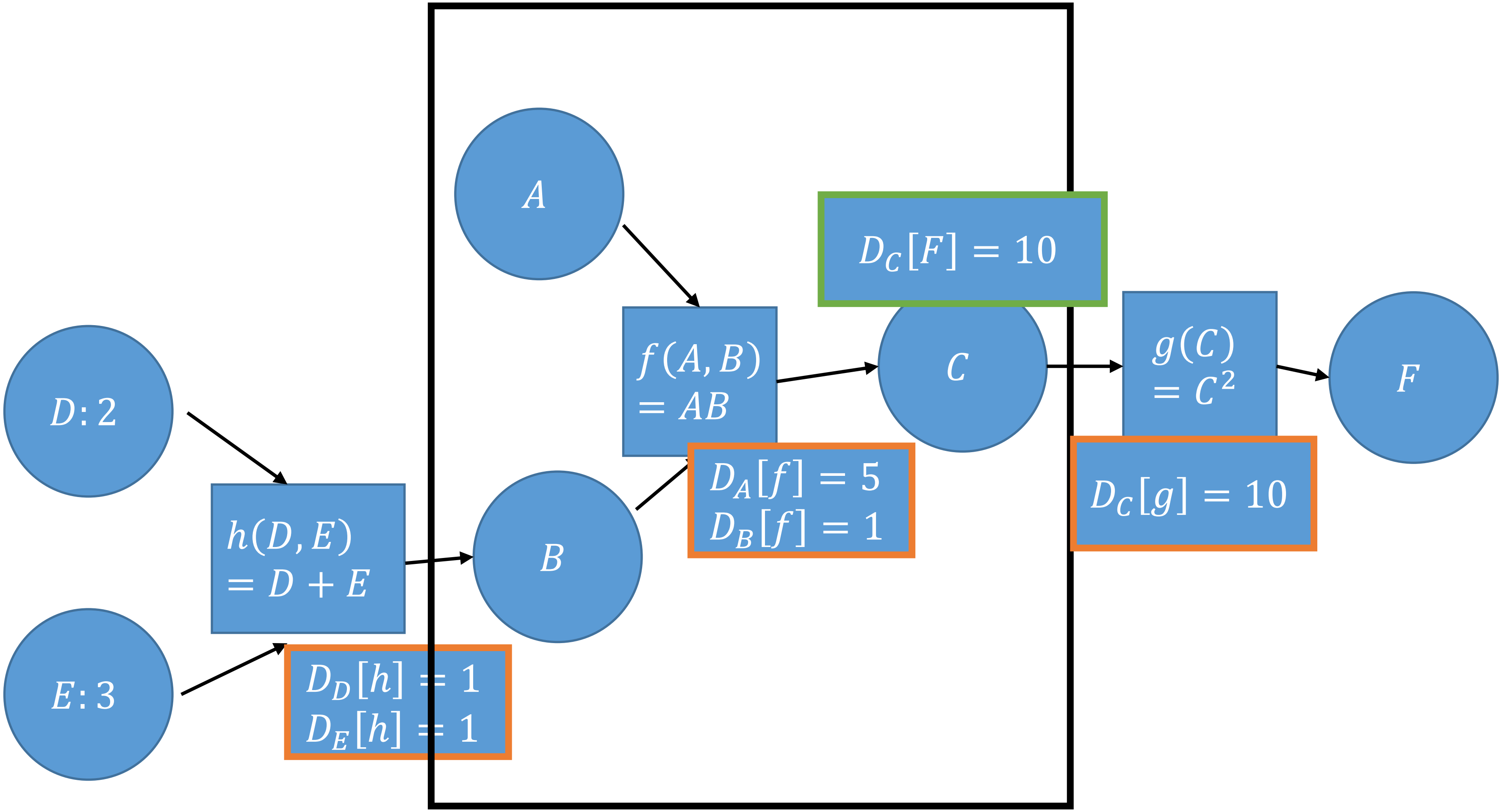
- Each "operator" node only needs to see its immediate neighbors in order to compute the both the forward and backward passes.

Forward pass is "local"



The f node doesn't need to know anything
Outside this box

Backward pass is "local"



The f node doesn't need to know anything
Outside this box

In Code

- Operation nodes have pointers to the input variable nodes and the output variable nodes.

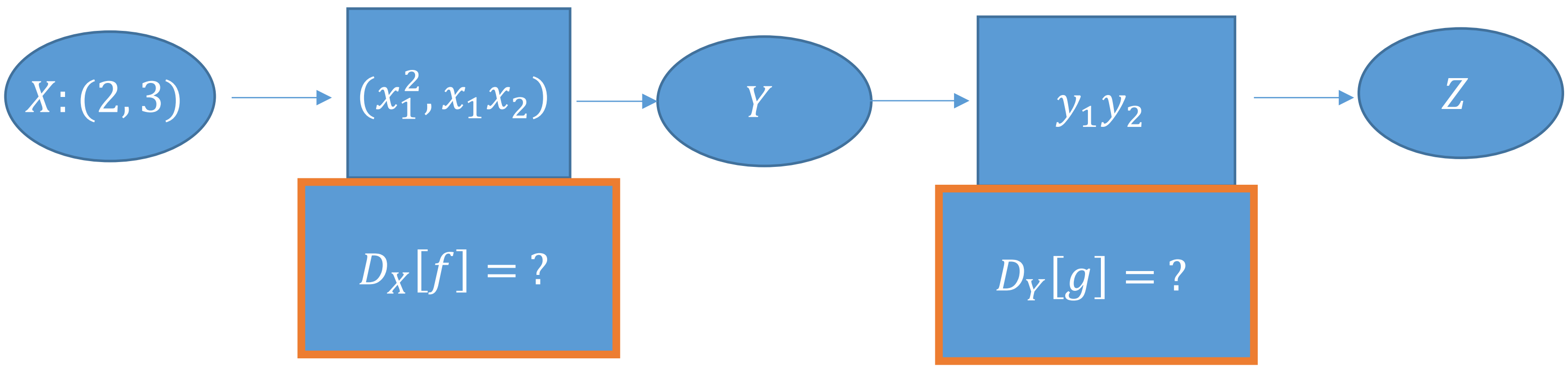
def forward(self, x):

1. Computes the output of the operation given the input, and assigns this output to all the output nodes.
2. Computes and stores relevant state (like the derivative).

def backward(self, x):

1. Takes input equal to the derivative with respect to the output.
2. Multiplies by stored derivatives to compute derivatives with respect to the inputs.

Forward Pass: Beyond Scalars



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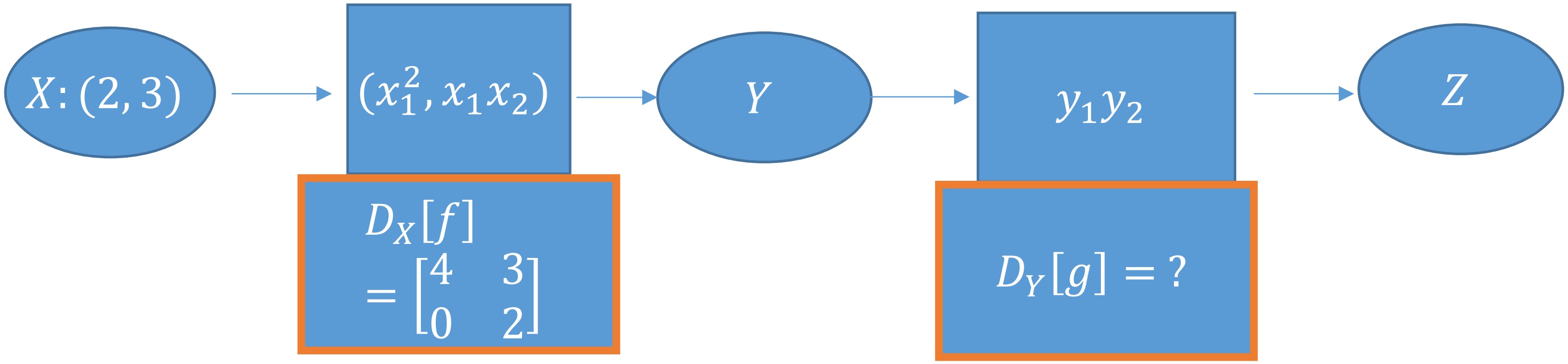

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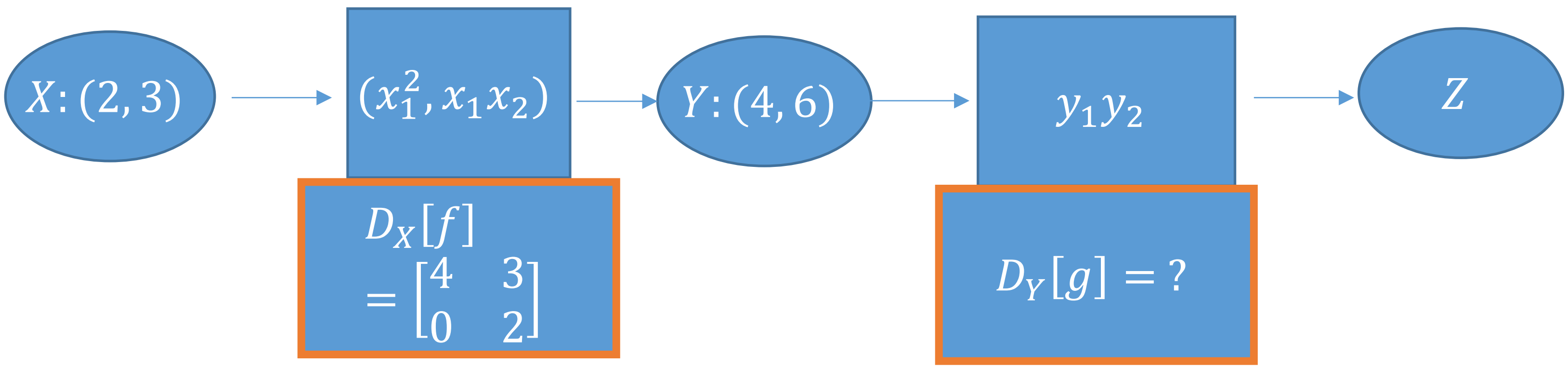

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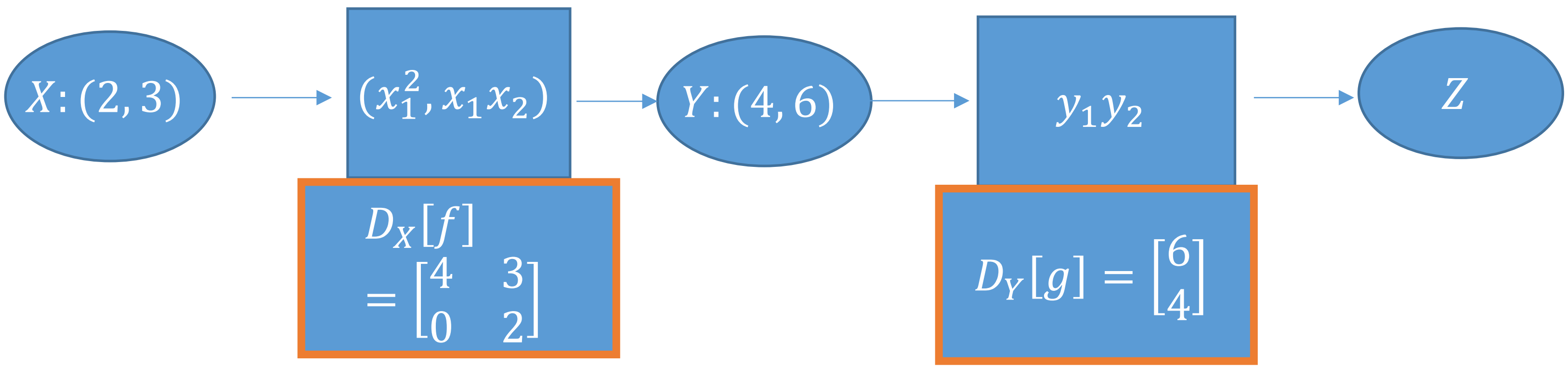
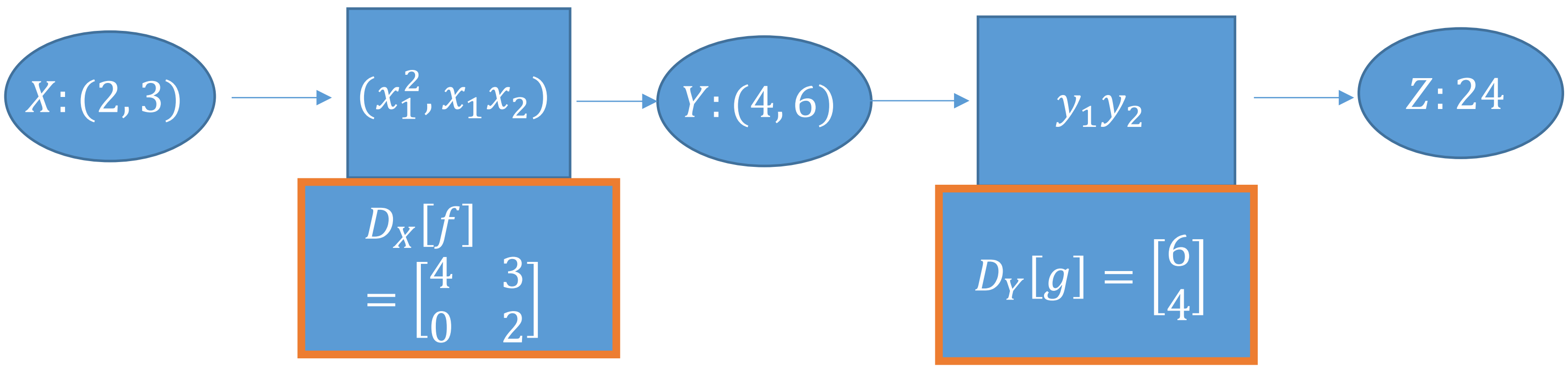
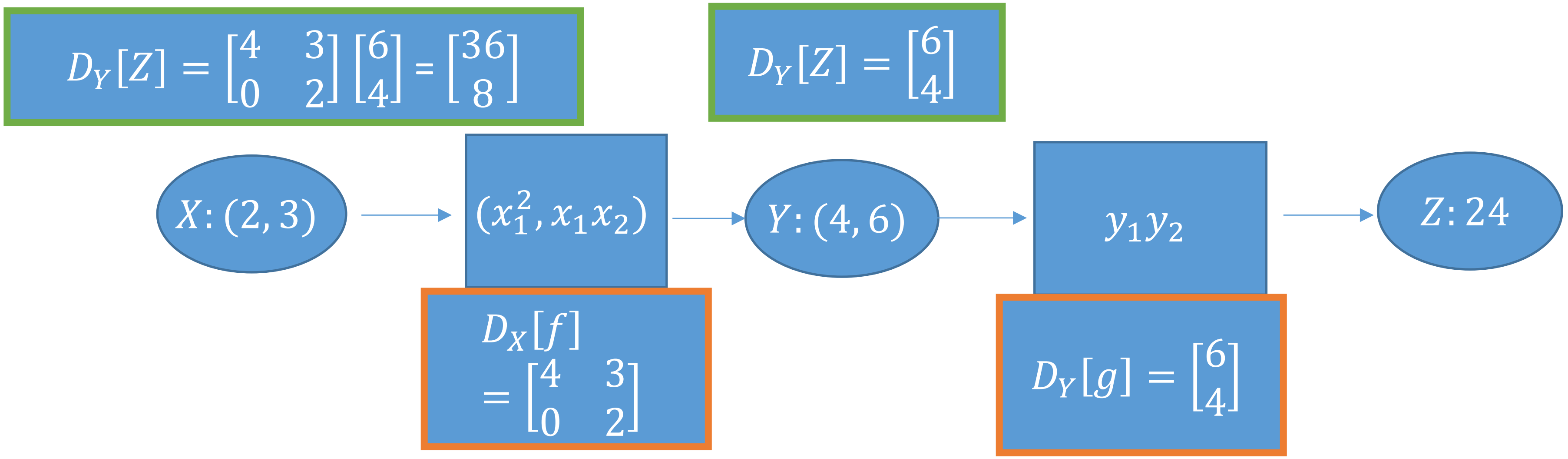


- What should the $D_X[Z]$ be?
- $Z = x_1^3 x_2$
- $D_X[Z] = \begin{bmatrix} 3x_1^2 x_2 \\ x_1^3 \end{bmatrix} = \begin{bmatrix} 36 \\ 8 \end{bmatrix}$

Backward Pass: Beyond Scalars

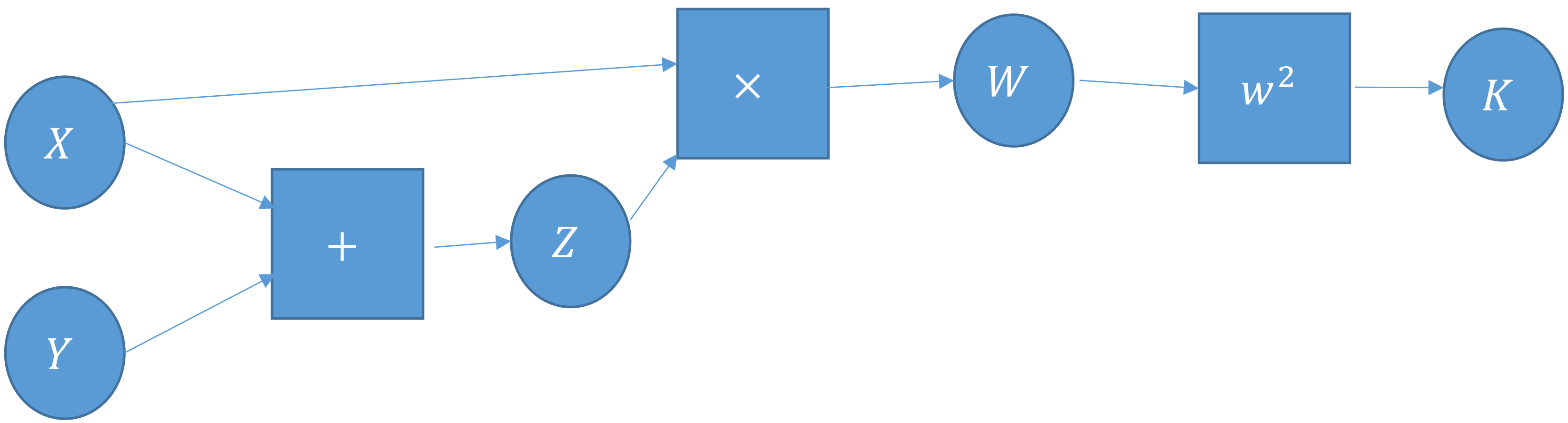


Backward Pass: Beyond Scalars



Even simple functions are operations

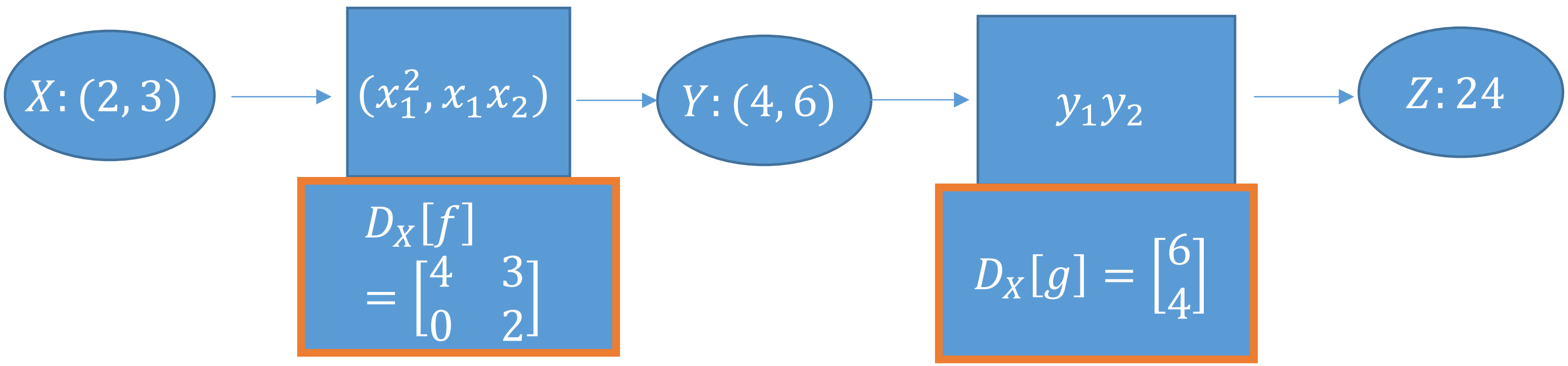
- $f(x, y) = x(x + y)^2$



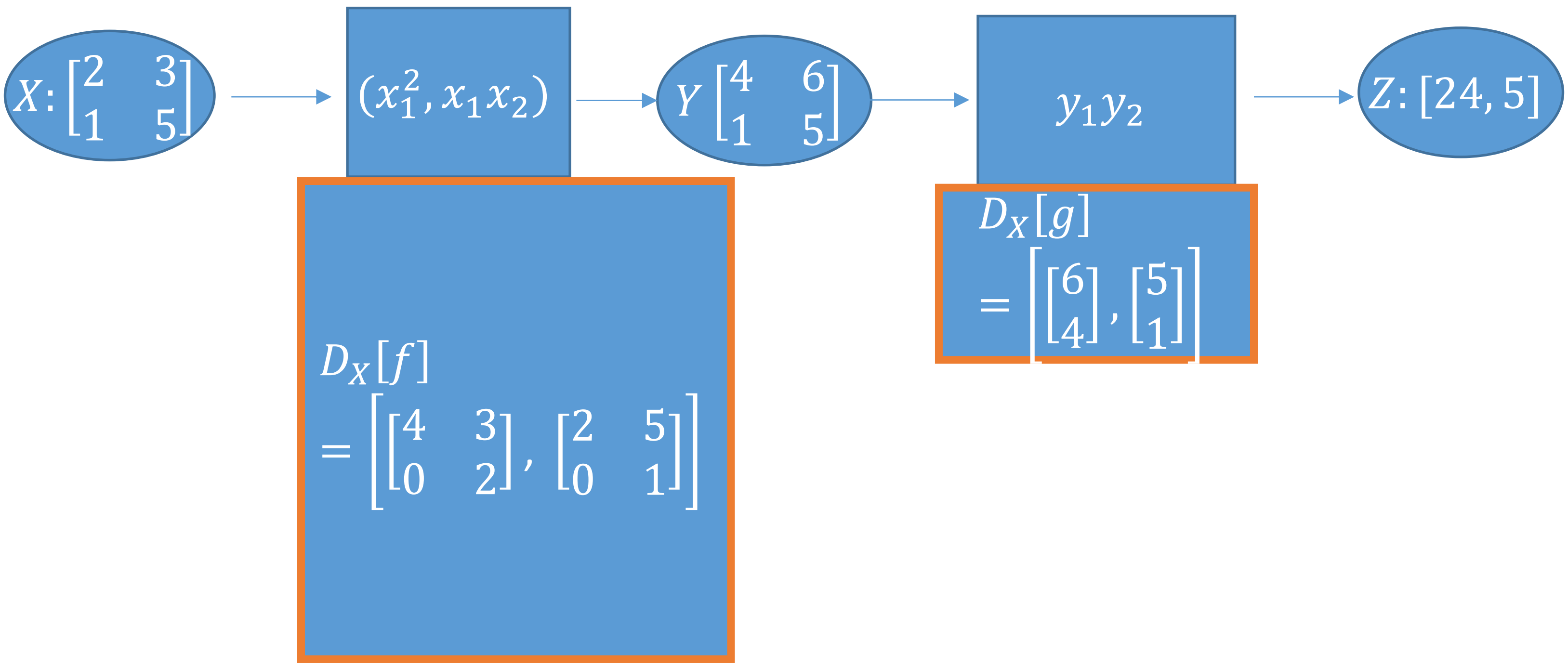
Derivatives of Batched functions

- Given a function $f: \mathbb{R}^n \rightarrow \mathbb{R}^d$, there is a *batched* function that distributed f along a batch dimension.
- $f_{batched}: \mathbb{R}^{B \times n} \rightarrow \mathbb{R}^{B \times d}$
- $f_{batched}(X)[i] = f(x[i])$
- All the functions on your homework are batched functions.
- To compute derivatives of batched functions, compute derivatives of each individual row.

Derivatives of Batched Functions



Derivatives of Batched Functions



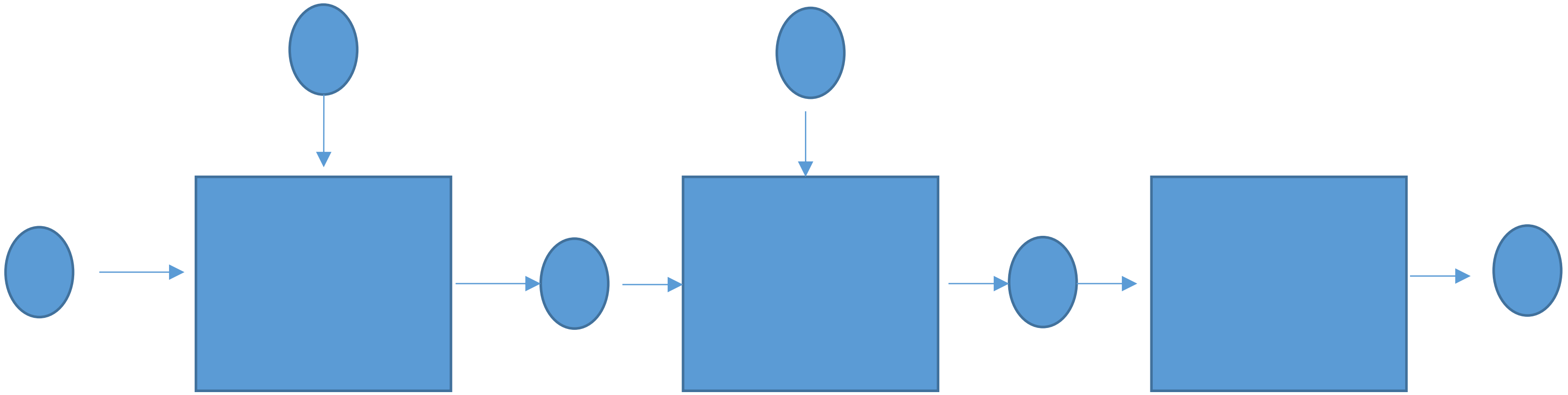
Derivatives of Matrix Functions

- To compute derivatives of a function that takes a matrix input, $f: \mathbb{R}^{n \times m} \rightarrow \mathbb{R}^d$, unroll the matrix into a vector.
- You will need to reshape the gradient back into the same shape as the matrix.
- To avoid unrolling, use matrix derivatives from HW 1.

DIY: useful tricks and more examples

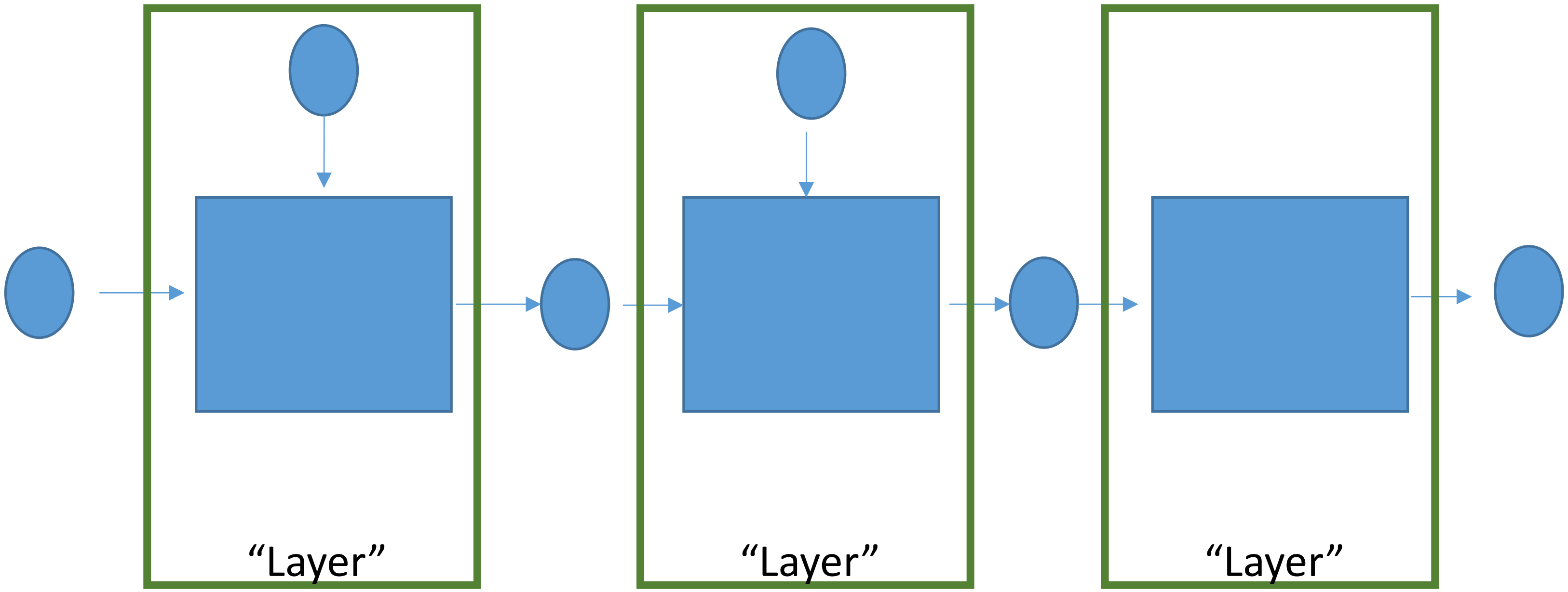
Simplified Graphs (on HW)

- Consider only graphs like:



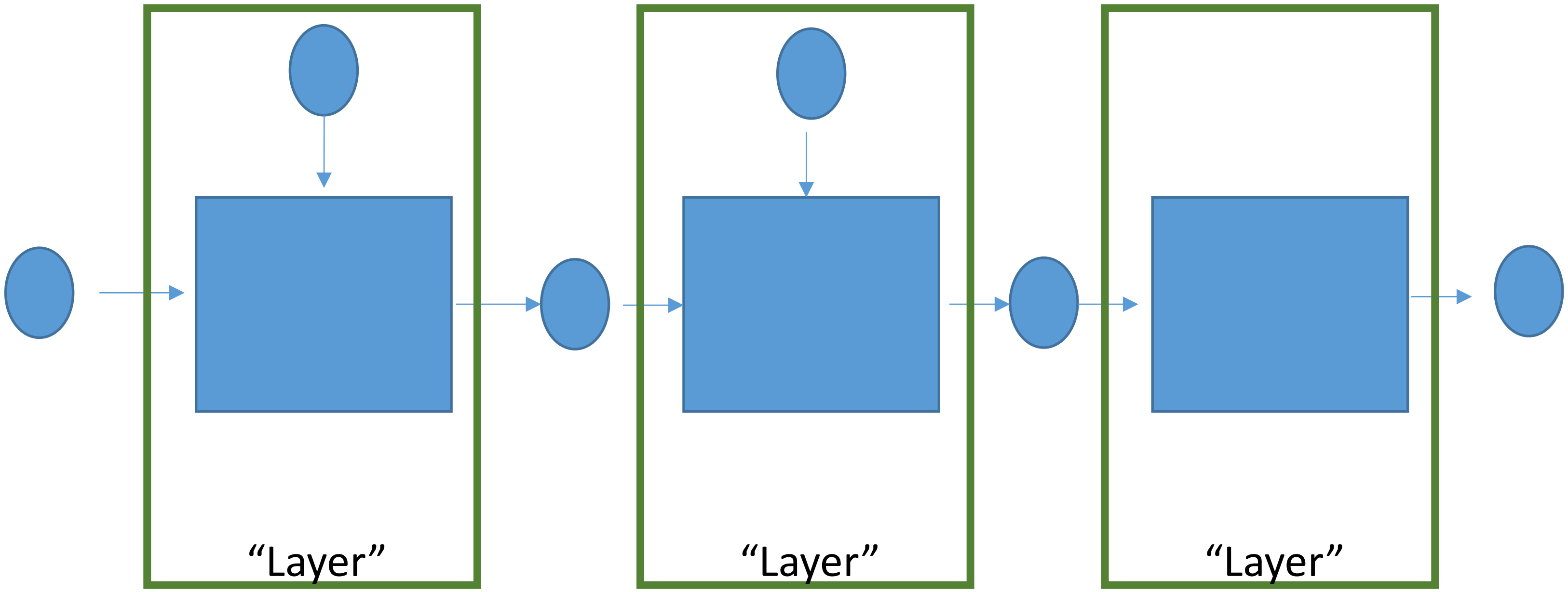
Simplified Graphs (on HW)

- Consider only graphs like:



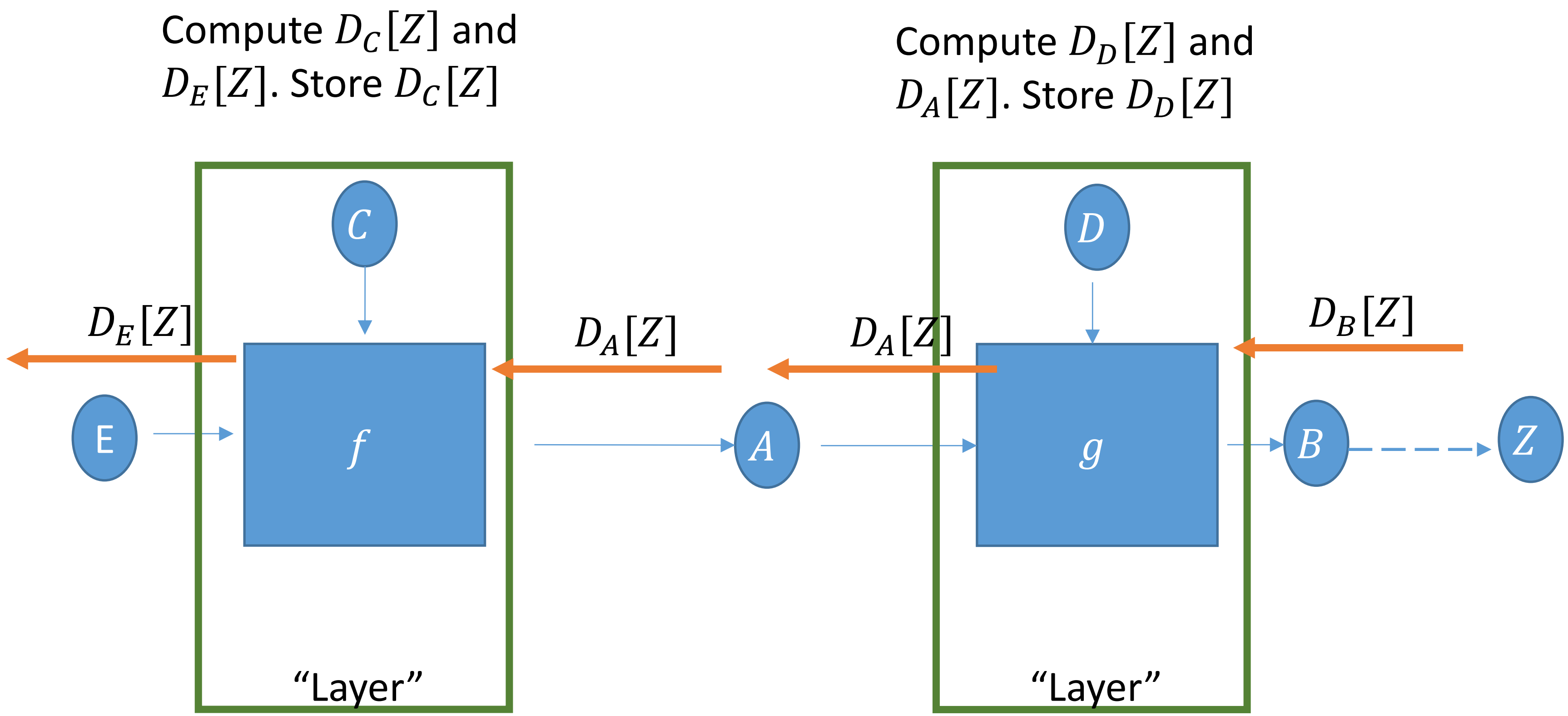
Simplified Graphs (on HW)

- Consider only graphs like:



- Only need gradients for variables inside layers

Backward Function (on HW)



Only consider the case $Z \in \mathbb{R}$, so that the shape of $D_X[Z]$ is always the same as X for all variables.

np.einsum

- Super-useful function used to express complicated matrix manipulations
- There are good tutorials online: see https://ajcr.net/Basic-guide-to-einsum/

np.einsum example

- `np.einsum('abc, bad -> ab', X, Y)`
- X and Y are both 3-dimensional matrices (tensors).
- X is associated with the string 'abc'
- Y is associated with the string 'bad'
- If X has shape [A, B, C], then Y has shape [B, A, D] for some other D.
- The output is a 2-dimensional tensor of shape [A, B]

np.einsum example

- `np.einsum('abc, bad -> ab', X, Y)`

- Let Z be the output. Then

- $Z[i,j] = \sum_{k,w} X[i,j,k] \times Y[j,i,w]$

- We summed over indices *not* present in Z

Another example

- `np.einsum('abcd, daa, be -> adf', X, Y, Z)`
- Inputs X, Y and Z have shapes [A, B, C, D], [D, A, A] and [B, E]
- Output W has shape [A, D, F]

- $W[a, d, f] = \sum_{b,c,e} X[a, b, c, d] \times Y[d, a, a] \times Z[b, e]$

Some familiar examples

- `Z= np.einsum('ij, jk -> ik', X, Y)`
- $Z[i,k] = \sum_j X[i,j] Y[j,k]$
  - Matrix multiplication

- `Z= np.einsum('ij-> ji', X)`
- $Z[j,i] = X[i,j]$
  - Matrix transpose

- `Z = np.einsum('ii->', X)`
- $Z = \sum_i X[i,i] = trace(X)$

Batched matrix multiplication

- $X \in \mathbb{R}^{B \times n}$
- $M \in \mathbb{R}^{B \times n \times m}$
- X is a batch of n dimensional vectors.
- M is a batch of $n \times m$ matrices.
- We want to compute $Y \in \mathbb{R}^{B \times m}$, where the ith row of Y is $X[i]M[i] \in \mathbb{R}^{m}$.
- How to write this?

Batched matrix multiply

- $X \in \mathbb{R}^{B \times n}$
- $M \in \mathbb{R}^{B \times n \times m}$
- We want to compute $Y \in \mathbb{R}^{B \times m}$, where the ith row of Y is $X[i]M[i] \in \mathbb{R}^m$.
- $Y[i,j] = \sum_k X[i,k]M[i,k,j]$
- `Y = np.einsum('ik, ikj -> ij', X, M)`

- Einsum in general is very good for batched operations.

Matrices and Tensors

- A matrix in $\mathbb{R}^{n \times m}$ is an n by m two dimensional array of real numbers.
  - A "list of lists". The outer list is size n, the inner lists are all size m.
- A tensor in $\mathbb{R}^{d_1 \times \cdots \times d_n}$ is a d_1 by d_2 by… by d_n n-dimensional array of real numbers.
  - A "list of lists of … of lists". Outer list has d_1 elements, inner-most lists all have d_n elements.
- We say a tensor in $\mathbb{R}^{a \times b \times c}$ has "shape" $[a, b, c]$.
- We access a tensor via multi-indices: $A[0,2,3]$.

Tensor Contraction

- Tensor contraction is the g generalization of matrix multiplication.
- Two tensors A and B can be contracted along one dimension if the last entry of A's shape is the same as the first entry of B's shape:
  - A has shape $[2, 45, 7]$ and B has shape $[7, 3, 67]$
- The output will have shape given by removing the common entry from A and B's shape and concatenating the lists:
  - $contract(A, B)$ has shape $[2, 45, 3, 67]$

Tensor Contraction Formula

- If A has shape $[a_1, \ldots, a_n, c]$ and b has shape $[c, b_1, \ldots, b_m]$, then

$$contract(A, B)[a_1, \ldots, a_n, b_1, \ldots, b_m] = \sum_{i=1}^{c} A[a_1, \ldots, a_n, i] \cdot B[i, b_1, \ldots, b_m]$$

- If $n = m = 1$, this is just matrix multiplication:

$$contract(A, B)[a, b] = \sum_{i=1}^{c} A[a, i] \cdot B[i, b]$$

Contraction along Many Dimensions

- Contraction along one dimension requires the last dimension of A to match the first dimension of B.
- Contraction along d dimensions requires the last d dimensions of A to match the first d dimensions of B.
- If $shape(A) = [2,5,4,6]$ and $shape(B) = [4,6,8,2]$, then A and B can be contracted along 2 dimensions.
  - The shape of $contract(A, B, 2)$ is [2,5,8,2].
- This is the `tensordot` function in `numpy`.

Contraction along Many Dimensions

- If A has shape $[a_1, \ldots, a_n, c_1, \ldots, c_k]$ and B has shape $[c_1, \ldots, c_{1=k}, b_1, \ldots, b_m]$, then $contract(A, B, k)$ has shape $[a_1, \ldots, a_n, b_1, \ldots, b_m]$.
- The conctraction is computed by:
$contract(A, B, k)[a_1, \ldots, a_n, b_1, \ldots, b_m]$
$= \sum_{i_1=1}^{c_1} \ldots \sum_{i_k=1}^{c_k} A[a_1, \ldots, a_n, i_1, \ldots i_k] \cdot B[i_1, \ldots, i_k, b_1, \ldots, b_m]$

What is the point of contraction?

- Using tensor contraction, we can write a linear map that takes matrices as both inputs and outputs.
- Let A have shape $[2, 3, 4, 5]$. Then A specifies a linear map that takes 2×3 matrices as input, and outputs 4×5 matrices:
- $A(M) = contract(M\ , A, 2)$
- Tensor contraction allows us to specify linear maps between arbitrary tensor shapes as also tensors of larger shape.

Derivatives of Tensor-valued functions

- Let $f: \mathbb{R}^{d_1 \times d_2 \times d_3} \to \mathbb{R}^{a \times b}$. The derivative is
$$D[f](x) \in \mathbb{R}^{d_1 \times d_2 \times d_3 \times a \times b}$$
- The derivative is a tensor that can contract all of the dimensions of the input and produce the dimensions of the output:
$$D[f](x): \mathbb{R}^{d_1 \times d_2 \times d_3} \to \mathbb{R}^{a \times b}$$
- The derivative formula:
$$D[f](x)[i,j,k,z,w] = \frac{df_{z,w}}{dx_{i,j,k}}(x)$$

Derivatives of Scalar-valued functions

- Let $f: \mathbb{R}^{d_1 \times d_2 \times d_3} \to \mathbb{R}$. The derivative is
$$D[f](x) \in \mathbb{R}^{d_1 \times d_2 \times d_3 \times 1}$$
- In this special case, we will usually drop the $\times 1$ of $D[f](x)$ to be in $\mathbb{R}^{d_1 \times d_2 \times d_3}$.
- The tensor contraction is:
$$contract\big(X, D[f](x)\big) = sum(X \odot D[f](x))$$
- Here $\odot$ is the coordinate-wise product (just normal multiplication in numpy), and sum just adds all the entries.