Pytorch Quick Intro

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Outline

Why pytorch?

- easy to debug in native python
- currently popular in research
  http://horace.io/pytorch-vs-tensorflow/[1]
- nowadays pytorch and tensorflow are very similar
  https://towardsdatascience.com/pytorch-vs-tensorflow-in-2020-fe237862fae1
- automatic differentiation / autograd: computes derivatives of functions for you.
- for those who never heard of it: torchvision model zoo – many networks with pretrained weights ready to load

[1] Older frameworks?

Key content I

- pytorch tensors: numpy with GPU transfer option
  - linear algebra similar to numpy
  - data is stored in `.data` field
- pytorch broadcasting rules
- torch.einsum for general tensor multiplications with summing
- **pytorch $\rightarrow$ math:** be able to write down mathematically what a certain pytorch operation does
- **math $\rightarrow$ pytorch:** be able to decide how math formula can be realized by which pytorch operations

Key content II

- pytorch autograd:
  - records graph of function computations
  - capable of computing gradient of weighted sum of Jacobi matrix
- when one needs to use only data or handle gradients, tensor have `.data` and `.grad.data` fields

Readings

- Installation https://pytorch.org/get-started/locally/
- quick intro: https://pytorch.org/tutorials/beginner/deep_learning_60min_blitz.html
- cheat sheet: https://pytorch.org/tutorials/beginner/ptcheat.html

Pytorch modules

Package	Description
torch	The top-level PyTorch package and tensor library.
torch.nn	A subpackage that contains modules and extensible classes for building neural networks.
torch.autograd	A subpackage that supports all the differentiable Tensor operations in PyTorch.
torch.nn.functional	A functional interface that contains typical operations used for building neural networks like loss functions, activation functions, and convolution operations.
torch.optim	A subpackage that contains standard optimization operations like SGD and Adam.
torch.utils	A subpackage that contains utility classes like data sets and data loaders that make data preprocessing easier.
torchvision	A package that provides access to popular datasets, model architectures, and image transformations for computer vision.

Tensor mathematically:

- 1-tensor: a linear mapping $v_1 \mapsto L(v_1)$, representable as $L(v_1) = u \cdot v_1$ by a vector $u = (u_j)$
- 2-tensor: a bilinear mapping $v_1, v_2 \mapsto L(v_1, v_2)$, representable as $L(v_1, v_2) = v_1^t A v_2 = \sum_{ij} v_{1,i} v_{2,j} A_{ij}$ by a matrix $A = (A_{ij})$
- 3-tensor: a trilinear mapping $v_1, v_2, v_3 \mapsto L(v_1, v_2, v_3)$, representable as $L(v_1, v_2, v_3) = \sum_{ijk} v_{1,i} v_{2,j} v_{3,k} A_{ijk}$ by a 3-dim array $A = (A_{ij})$
- n-tensor ... n-linear mapping ... representable by a n-dim array $A = (A_{i_1 \cdots i_n})$
- n-tensors $\leftrightarrow$ n-dim arrays

Tensor?

Same as in physics lectures

- 1-tensor: object/array with 1-dimensional way to index it, vector
  $a[i] \leftrightarrow a_i$
- 2-tensor: object/array with 2-dimensional way to index it, matrix
  $a[i, k] \leftrightarrow a_{i,k}$
- 3-tensor: object/array with 3-dimensional way to index it
  $a[i, k, l] \leftrightarrow a_{i,k,l}$
- n-tensor: object/array with n-dimensional way to index it
- Tensor in pytorch:

  a representation of an numpy-array-like structure
  A_i, $A_{i,j,k}$, $A_{i,j,k}$ or $A_{i_1,\ldots,i_n}$ with benefits (for storing computed gradients).

- with fixed values:

```
x= torch.zeros((5,1))
y= torch.ones((5))
z= torch.empty((3,2,3))
a = torch.empty((64,32,3,3)).fill_(32.) # initializes to some val
b= a.new_full((3,2),42.) # with same type and device as tensor a
c = torch.full((2, 3), 3.141592)
d = torch.randn((2, 3))
```

- from a saved tensor:
  https://pytorch.org/docs/stable/generated/torch.save.html
  https://pytorch.org/docs/stable/generated/torch.load.html

- from numpy:

```
a=np.random.normal(5,size=(2,3)).astype('float32')
x=torch.tensor(a) # this copies data
x2=torch.as_tensor(a) # this does NOT COPY data,
#and does nothing if its already a tensor with right type, etc.
x3=torch.from_numpy( a) # this does NOT COPY data
#when this can be inappropriate? not resizable tensor as limitati
```

- to numpy:

```
nparr = a.data.numpy() # a.numpy() works only if it has no grad f
```

```
x= torch.empty((2,3)) #empty tensor
```

A tensor has three important properties:

- its `.size()` or `.shape`
- the dtype: its type of numerical elements (most nns use `torch.float32`)
- device it is placed on (e.g. cpu, cuda:0, cuda:1)
- getting its size: output is a `torch.Size()` object.

```
print(x.size())
print(x.shape) # This is a {\tt torch.Size} class instance.
```

Use tuple or list to convert it:

```
xsize=tuple(x.size())
```

get its dtype:

```
print(x.dtype)
```

get its device placement

```
print(x.device) #is a {\tt torch.device} class instance
```

if you need strings, use `.__repr__()`.

Test for equality with

```
x.device==torch.device('cuda:0')
x.dtype==torch.float #rhs is a torch.dtype object
x.dtype.__repr__()=='torch.float32'
```

Important: you can print these anywhere in your execution code. no ugly fixed graph surprises.

https://pytorch.org/docs/stable/tensors.html

```
>>> a.to('blabladevice')
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
RuntimeError: Expected one of cpu, cuda, mkldnn, opengl, opencl, ideep, hip, msn
pu, xla device type at start of device string: blabladevice
>>>
```

HIP for AMD

XLA-compiler driven TPUs

https://pytorch.org/xla/release/1.7/index.html. Can try those in google Colab:

https://colab.research.google.com/notebooks/intro.ipynb

Type casting

```
print(a.dtype)
b= a.to(torch.float64) # see also the legacy method .type()
c= a.type(torch.DoubleTensor)
```

Device placement

```
print(a.device)
b= a.to('cuda:0')
```

```
x=torch.ones((10))
y=x.view((2,5))
z=x.view((-1,5)) #-1 joker
```

- Be careful: Which elements ends up where in this case?

```
x=torch.ones((4,2,3))
y=x.view((-1,12))
```

```
a= torch.full((2,3),3.)
b= torch.full((5,1,3),3.)
c= a+b
```

What will `c.shape` be ?

https://pytorch.org/docs/stable/notes/broadcasting.html

same holds for many binary operators like $+ - */$

$$
\begin{aligned}
a &= torch.ones((4)) \\
b &= torch.ones((1,4)) \\
& \quad torch.add(a,b) && \rightarrow (1,4) \\
a &= torch.ones((4)) \\
b &= torch.ones((4,1)) \\
& \quad torch.add(a,b) && \rightarrow (4,4)!!! \\
a &= torch.ones((3)) \\
b &= torch.ones((4,1)) \\
& \quad torch.add(a,b) && \rightarrow (4,3) \\
a &= torch.ones((3)) \\
b &= torch.ones((1,4)) \\
& \quad torch.add(a,b) && \rightarrow ERR
\end{aligned}
$$

- smaller tensor gets filled **from the left** with singleton dimensions until he has same dimensionality as larger tensor, as if `.unsqueeze(0)` would be applied again and again

1– the smaller tensor gets filled **from the left** with singleton dimensions until he has same dimensionality as larger tensor, as if `.unsqueeze(0)` would be applied again and again

2– then check whether they are compatible – they are incompatible if in one dimension both tensors have sizes > 1 which are not equal. if they are incompatible, you will get an error.

3– whenever a dimension with size 1 meets a dimension with a size $k > 1$, then the smaller vector is replicated/copied $k - 1$ times in this dimension until he reaches in this dimension size k and your actual operation is applied

Example:

start	after insert	after copying
(4,1)	(4,1)	(4,4)
(4)	(1,4)	(4,4)

More examples:

start	after insert	after copying
(1,3)	(1,3)	(1,3)
(3)	(1,3)	(1,3)

start	after insert	after copying
(2,3)	(1,2,3)	(5,2,3)
(5,1,3)	(5,1,3)	(5,2,3)

start	after insert	after copying
(1,7)	(1,1,1,7)	(5,2,3,7)
(5,2,3,7)	(5,2,3,7)	(5,2,3,7)

start	after insert	after copying
(4,1)	(1,4,1)	ERR
(2,3,7)	(2,3,7)	ERR

if broadcasting is too ... , then apply `.unsqueeze(dim)` on your tensor, until both tensors have the same number of dimension axes. The only thing what is done then, is copying along $dim = 1$ axes.

`torch.mm(a,b)` dot product, not broadcasting. a, b must be 1-tensors

$$a.size() = (d), \;\; b.size() = (d)$$
$$torch.dot(a, b) = \sum_{d'} a_{d'} b_{d'} = \sum_{d'} a[d']b[d']$$
$$\rightarrow torch.dot(a, b).size() = ()$$

`torch.mm(A,B)` matrix multiplication, not broadcasting. A, B must be 2-tensors

$$A.size() = (i, k), \;\; B.size() = (k, l)$$
$$torch.mm(A, B)[i, l] = \sum_{k'} A_{i,k'} B_{k',l} = \sum_{k} A[i, k']B[k', l]$$
$$\rightarrow torch.mm(A, B).size() = (i, l)$$

`torch.bmm(A,B)` **batched** matrix multiplication, not broadcasting. A, B must be 3-tensors. multiplication along last dim of A and second dim of B.

$$A.size() = (b, i, k), \;\; B.size() = (b, k, l)$$

$$torch.bmm(A, B)[b, i, l] = \sum_{k'} A_{b,i,k'} B_{b,k',l} = \sum_{k} A[b, i, k'] B[b, k', l]$$

$$\rightarrow torch.bmm(A, B).size() = (b, i, l)$$

> `torch.bmm(A,B)` performs for every index k a matrix multiplication between $A[k, :, :]$ and $B[k, :, :]$
> – its a for loop over k of `torch.mm(A[k,:,:], B[k,:,:])`

Think: $torch.bmm(A, B)$ given a known shape of A puts what restrictions on B??

example: want to compute matrix vector product by `mm(.)`
$(vA)_l = \sum_k^K v_k A_{k,l}$, $v.shape = (K)$.

v is 1-tensor, cannot use `torch.mm(`v, A`)`. add a dim in v:

$torch.mm(v.unsqueeze(0), A)$	$(1, K) \cdot (K, L) \to (1, L)$
$torch.mm(v.unsqueeze(0), A).squeeze(0)$	$(1, K) \cdot (K, L) \to (1, L) \to (L)$

`torch.squeeze(A,dim=2)` - remove singleton dim
$(a, b, 1, c) \to (a, b, c)$
`torch.unsqueeze(A,dim=1)` - insert singleton dim
$(a, b, c) \to (a, 1, b, c)$
`torch.unsqueeze(A,dim=0)` - insert singleton dim
$(a, b, c) \to (1, a, b, c)$

...

`torch.transpose(A,dim1,dim2)` swaps two dimensions

`torch.Tensor.permute(*dims)` permutes a set of dimensions rather than just swapping two

I have to implement:

$$T_{i,n,r,s} = \sum_{k,m,o} A_{i,k,m,n,o} B_{m,o,r} C_{k,m,r,s}$$

Outline

a general way to do all kinds of batched and non-batched tensor multiplications: torch.einsum

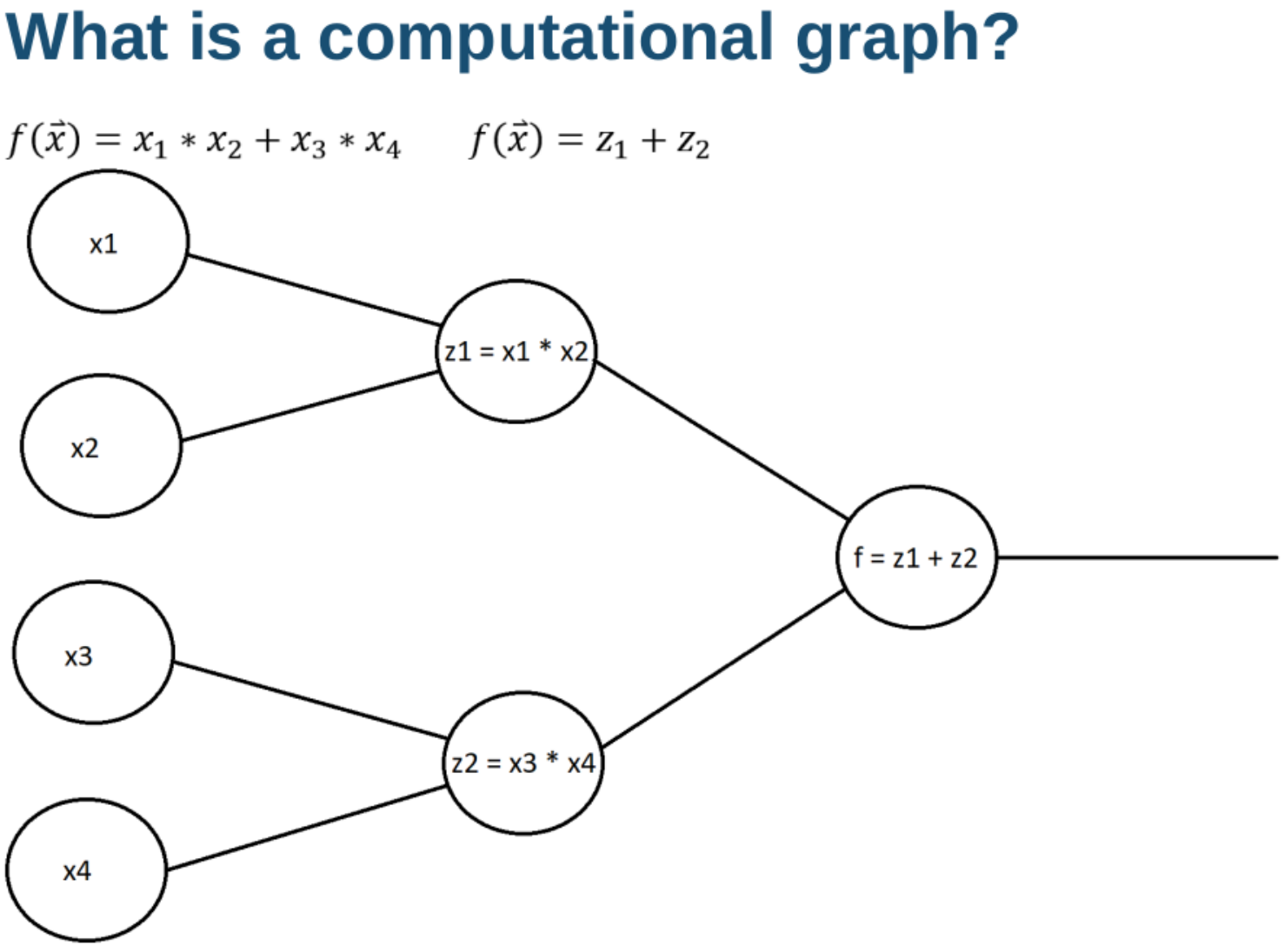
https://rockt.github.io/2018/04/30/einsum

rule:

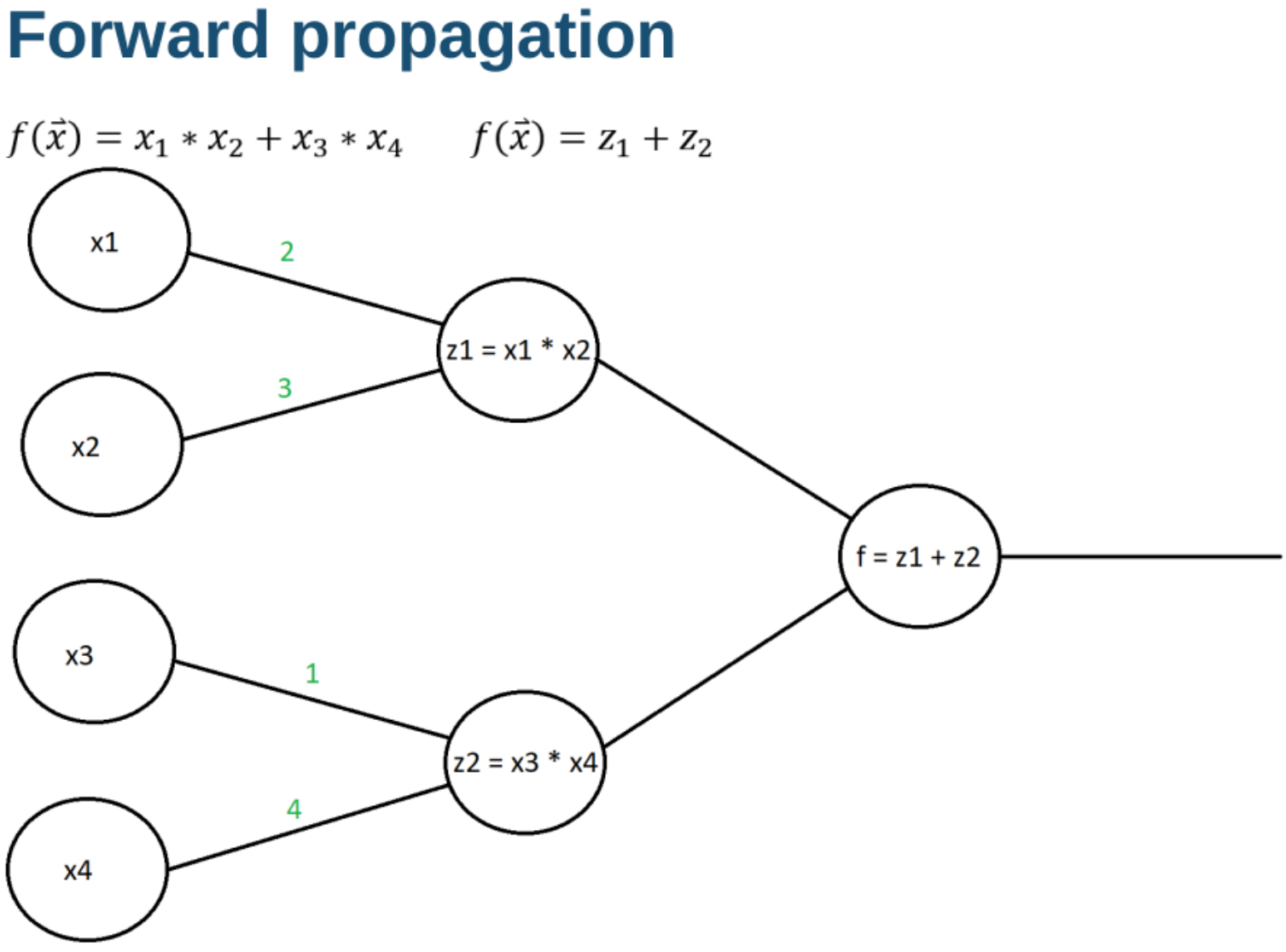
- left of $->$: all tensors separated by , which are to be multiplied and summed.
- **indices that have same name in multiple tensors, will get multiplied together**
- right of $->$ the result tensor with remaining indices.
- **All indices missing right of $->$ are summed out so that they vanish in the result.**

Outline

A directed-graph representation of computations done.



Forward pass: the actual computation

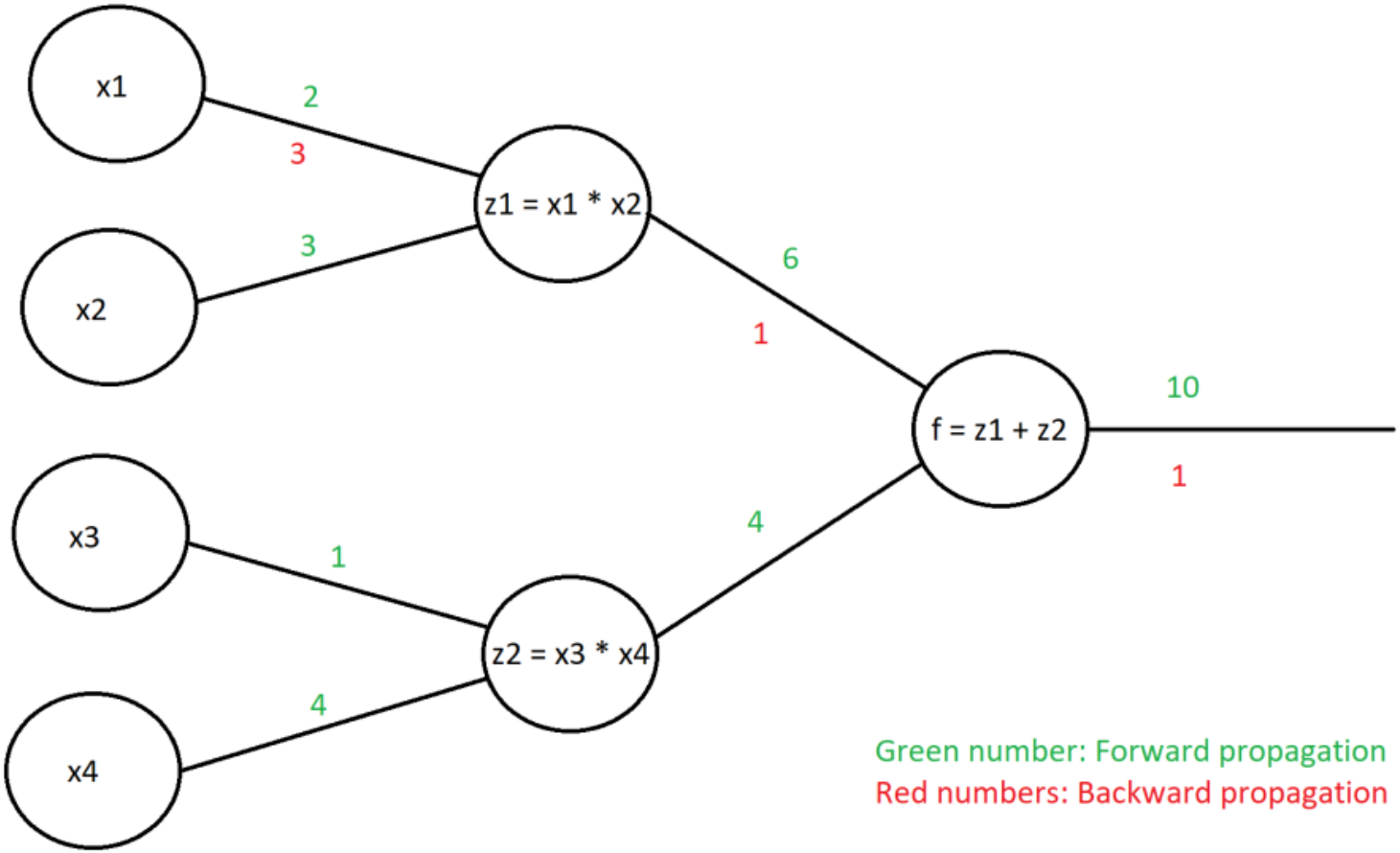


Backward pass: computing derivates

Backward propagation

What if we want to get the derivative of *f* with respect to the *x1*?

$f(\vec{x}) = x_1 * x_2 + x_3 * x_4$ $f(\vec{x}) = z_1 + z_2$ $\frac{\partial f(\vec{x})}{\partial x_1} = \frac{\partial f}{\partial z_1}\frac{\partial z_1}{\partial x_1} = x_2$



What ? Automatic differentiation with respect to variables used in computations.
You can define a sequence of computations, then call `.backward()` or `torch.autograd.grad(...)`. see `autograf2.py`, `print_computationalgraph.py`

When ?

- If tensors are leaf tensors and have the `requires_grad=True` flag set, then they are marked for tracking operations along the computation sequence for later gradient computation.
- leaf tensor: not created as the result of an operation but defined by you as an input.

https://pytorch.org/tutorials/beginner/blitz/autograd_tutorial.html#sphx-glr-beginner-blitz-autograd-tutorial-py

...

if `e` is a tensor with `1` element, then `e.backward()` computes the gradient of `e` with respect to all its inputs that were involved in computing `e`.

see `print_computationalgraph.py`: the whole backward graph

if e is a tensor of $n \geq 2$ elements, then the gradient of e is a matrix, the Jacobi-matrix. Example for 3 elements:

$$e = (e_1, e_2, e_3)$$

$$de/dx = \begin{pmatrix} \frac{de_1}{dx_1} & \frac{de_2}{dx_1} & \frac{de_3}{dx_1} \\ \frac{de_1}{dx_2} & \frac{de_2}{dx_2} & \frac{de_3}{dx_2} \\ \vdots & \vdots & \vdots \\ \frac{de_1}{dx_8} & \frac{de_2}{dx_8} & \frac{de_3}{dx_8} \\ \vdots & \vdots & \vdots \\ \frac{de_1}{dx_D} & \frac{de_2}{dx_D} & \frac{de_3}{dx_D} \end{pmatrix}$$

if e is a tensor of $n \geq 2$ elements, then the gradient of e is a matrix, the Jacobi-matrix.
In this case: (for an example where e has 3 elements)
`e.backward(torch.tensor([-5,2,6]) )` computes the D-dim weighted gradient vector

$$\frac{de_1}{dx} * (-5) + \frac{de_2}{dx} * 2 + \frac{de_3}{dx} * 6$$

$$= \begin{pmatrix} \frac{de_1}{dx_1} * (-5) + \frac{de_2}{dx_1} * 2 + \frac{de_3}{dx_1} * 6 \\ \frac{de_1}{dx_2} * (-5) + \frac{de_2}{dx_2} * 2 + \frac{de_3}{dx_2} * 6 \\ \vdots \\ \frac{de_1}{dx_8} * (-5) + \frac{de_2}{dx_8} * 2 + \frac{de_3}{dx_8} * 6 \\ \vdots \\ \frac{de_1}{dx_D} * (-5) + \frac{de_2}{dx_D} * 2 + \frac{de_3}{dx_D} * 6 \end{pmatrix}$$

This is an inner product between the jacobi matrix and a vector that has as many elements as e in the forward pass.

Autograd

- Autograd tracks the graph of computations
- Tracked computations will be used to compute a gradient automatically
- use `with torch.no_grad():` environment to **not** record computations for gradient calculations for some larger block of code that is reused – use case: everything outside of handling training data, e.g. computing validation or test scores.[a]
- outlook / out of class: for GAN-training `sometensor.detach()` prevents the gradient flowing from `sometensor` to all those parts used to compute sometensor.

[a] Why you dont want to track gradient computations in this case?

Note: If you have a tensor with attached gradient, then the `.data` stores the tensor values, and `.grad.data` the gradient values

```
vals=x.data.numpy() #exports function values to numpy
g_vals=x.grad.data.numpy() #exports gradient values to numpy
```

- useful stuff: standard operations like mean or max, `torch.random`, `torch.nn.functional`
- Things behaving unexplainably weird? check your version: `print(torch.__version__)`

The end

Questions?!