Automatic differentiation

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Deep Learning course seminar

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January 12, 2018

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  - How do matrices and vectors fit into the story of derivatives?

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- Large gap between:
  - Backpropagation materials
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- *Every* tutorial focuses on deriving specific neural network architectures
- Many other equally confusing things
  - How do matrices and vectors fit into the story of derivatives?
  - Do we really need so many complex rules of derivation?

Claims

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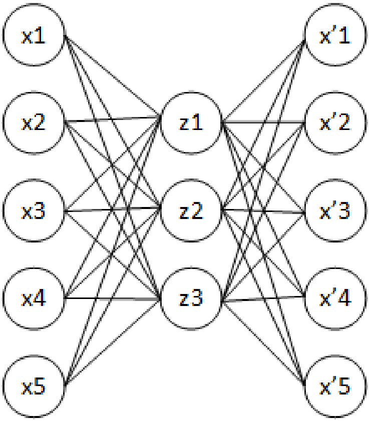
- Backpropagation is a function that maps one computational graph to another
- Not connected to linear algebra
- Arbitrary tensor contraction operations can be generalized with Einstein summation
- With Einsum, calculating derivatives is elegant

Computational graphs



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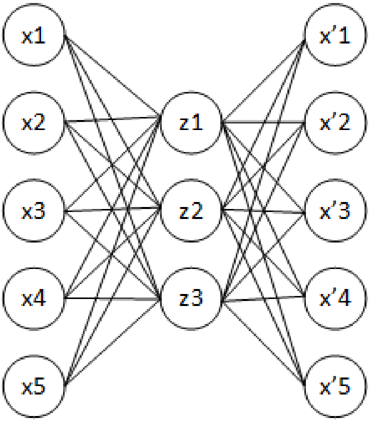

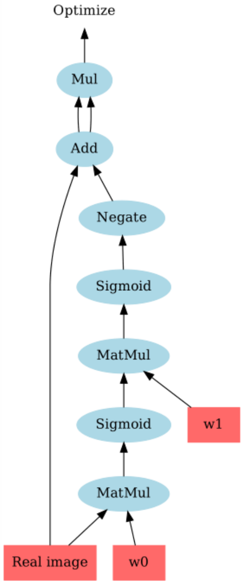

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- One operation - one class

Composition of many smaller operations

- Instead of defining every neural network by hand, we define many small parts of it and we set up ways to combine them
- Main idea - let's build a minimal implementation of autodiff during the course of this talk
- One operation - one class
- Each operation takes a Node and returns a value

Code snippet - Variable

```
class Variable:
    def __init__(self, value, name="Variable"):
        self.value = value

    def _eval(self):
        return self.value
```

Code snippet

```python
class Exp:
    def __init__(self, node, name="Exp"):
        self.node = node

    def _eval(self):
        return np.exp(self.node._eval())
```

Code snippet

```
class Add:
    def __init__(self, node1, node2, name="Add"):
        self.node1 = node1
        self.node2 = node2

    def _eval(self):
        return node1._eval() + node2._eval()
```

Code snippet

```
class Sigmoid:
    def __init__(self, node, name="Sigmoid"):
        self.node = node

    def _eval(self):
        return 1 / (1 + np.exp(-self.node._eval()))
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Let’s abstract some common stuff

```python
class Node:
    def __init__(self, nodes, name="Node"):
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    def __call__(self, *args, **kwargs):
        return self.eval()
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    def __call__(self, *args, **kwargs):
        return self.eval()

    def eval(self):
        if self.cached is None:
            self.cached = self._eval()

        return self.cached
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Let's abstract some common stuff - caching!

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        if self.cached is None:
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        return self.cached
```

Code snippet - refactored

```
class Exp(Node):
    def __init__(self, node, name="Exp"):
        super().__init__([node])

    def _eval(self):
        return np.exp(self.nodes[0]())
```

Code snippet - refactored

```
class Add(Node):
    def __init__(self, node1, node2, name="Add"):
        super().__init__([node1, node2])

    def _eval(self):
        return self.nodes[0]() + self.nodes[1]()
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class Sigmoid(Node):
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- We can define arbitrary computation graphs...
- But how do we *train* them?
- Where are all the derivatives?
- Where is the neural network here?
- Turns out, we're missing two things:
  - Matrix operations
  - Gradient calculation

Let’s quickly add matrix multiplication

```
class MatMul(Node):
    def __init__(self, node1, node2, name="MatMul"):
        super().__init__([node1, node2])

    def _eval(self):
        return self.nodes[0]() @ self.nodes[1]()
```

Backpropagation

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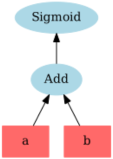

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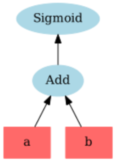
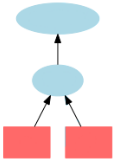


Backpropagation - we don't need to know the types



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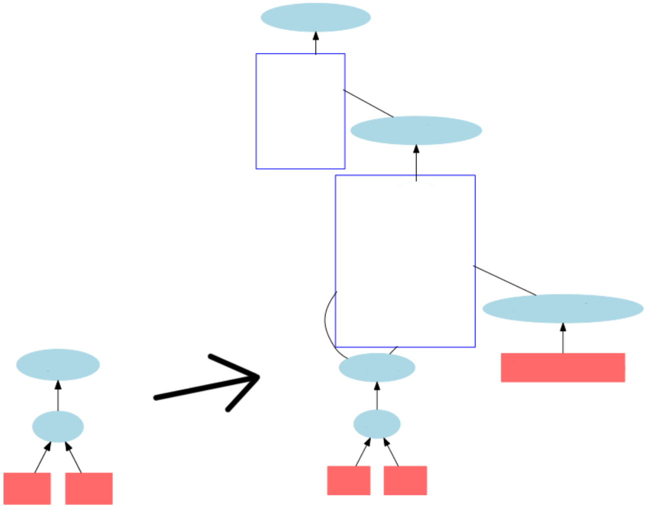

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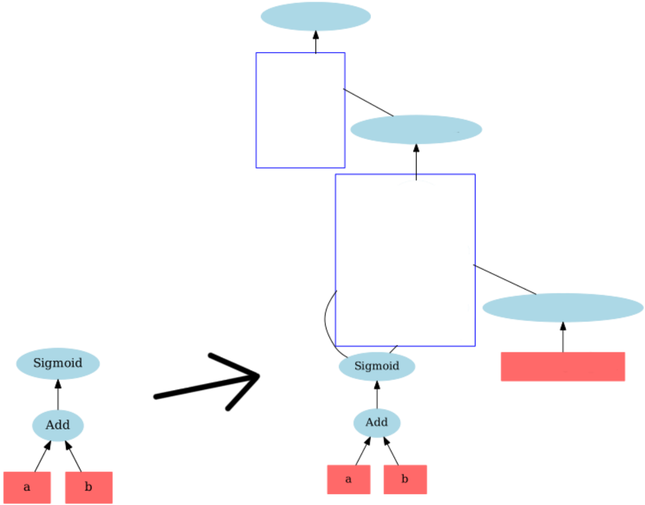

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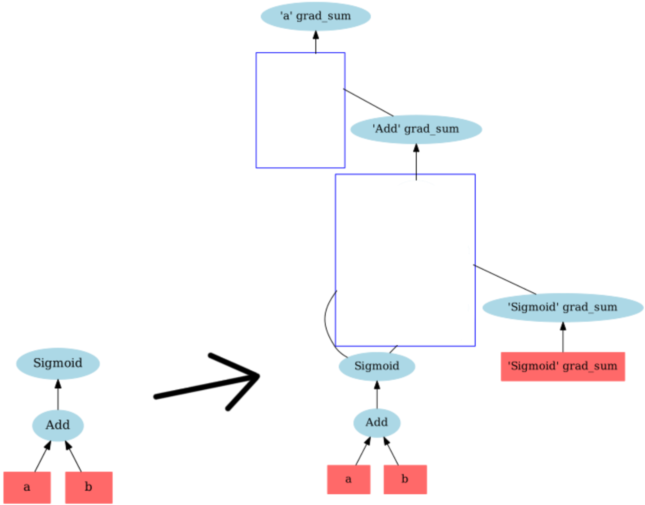

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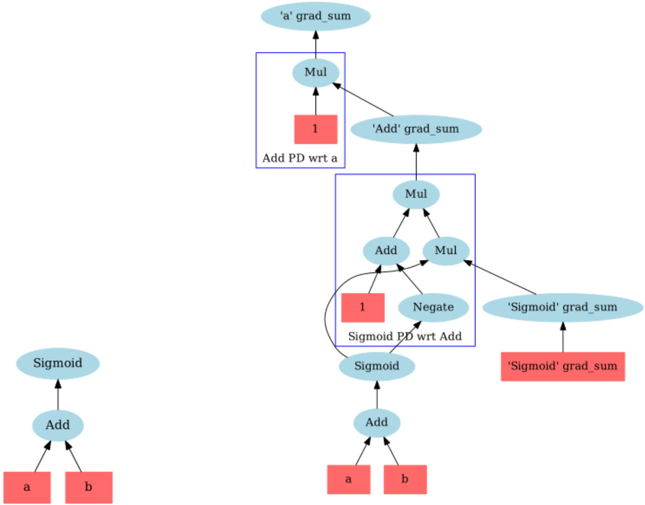

We need derivatives!

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class Node:
    def __init__(self, nodes, name="Node"):
        self.nodes = nodes

    # other stuff ...

    def _eval(self):
        raise NotImplementedError()
```

We need derivatives!

```python
class Node:
    def __init__(self, nodes, name="Node"):
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    # other stuff ...

    def _eval(self):
        raise NotImplementedError()

    def _partial_derivative(self, wrt, previous_grad):
        raise NotImplementedError()
```

Code snippet - add

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class Add(Node):
    def __init__(self, node1, node2, name="Add"):
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    def _partial_derivative(self, wrt, previous_grad):
        return previous_grad * self.nodes.count(wrt)
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Code snippet - Sigmoid

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    def _eval(self):
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    def _partial_derivative(self, wrt, previous_grad):
        if wrt == self.node:
            return previous_grad * self * (1 - self)
        return 0
```

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- When constructing the partial derivative, by not “stepping down" from our graphs into real numbers, we get higher-order gradients for free!

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    dct[top_node] += [previous_grad]
    def add_partials(dct, node):
        dct[node] = Add(*dct[node], name=add_sum_name(node))
        for child in set(node.children):
            dct[child] += [node.partial_derivative(wrt=child,
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    dct = functools.reduce(add_partials,
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    return [dct[wrt] if dct[wrt] != [] else Variable(0) for wrt in wrt_list]
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- *Backprop as a Functor*

Thank you!