

Automatic differentiation

Matthew J Johnson (mattjj@google.com)

Deep Learning Summer School
Montreal 2017



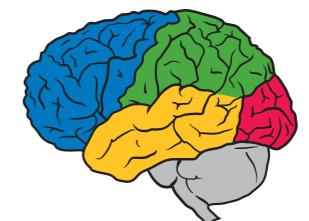
Dougal Maclaurin



David Duvenaud



Ryan P Adams



Our awesome new world

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- TensorFlow, Stan, Theano, Edward, PyTorch, MinPy
- Only need to specify forward model
- Autodiff + optimization / inference done for you

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- debugger?
- a second compiler/interpreter to satisfy
- a new mini-language to learn

Autograd

- github.com/hips/autograd

- differentiates native Python code
- handles most of Numpy + Scipy
- loops, branching, recursion, closures
- arrays, tuples, lists, dicts, classes, ...
- derivatives of derivatives
- a one-function API
- small and easy to extend



Dougal Maclaurin

Autograd examples

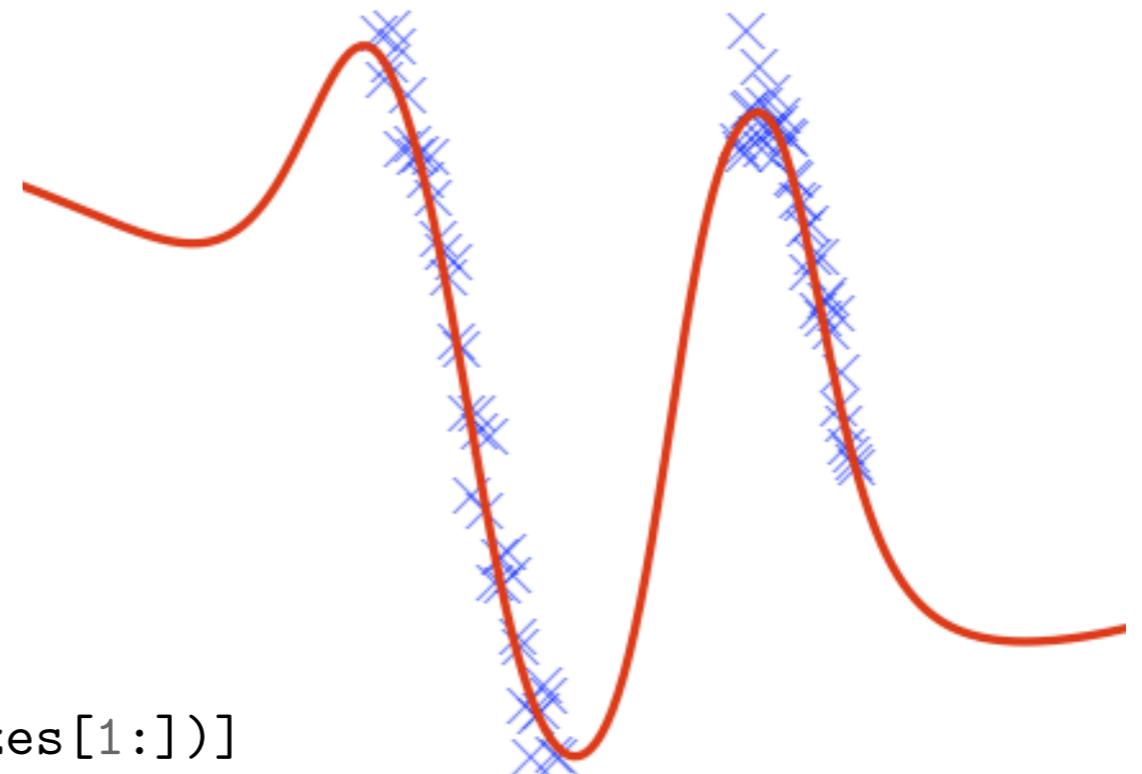
```
import autograd.numpy as np
import autograd.numpy.random as npr
from autograd import grad

def predict(weights, inputs):
    for W, b in weights:
        outputs = np.dot(inputs, W) + b
        inputs = np.tanh(outputs)
    return outputs

def init_params(scale, sizes):
    return [(npr.randn(m, n) * scale,
             npr.randn(n) * scale)
            for m, n in zip(sizes[:-1], sizes[1:])]

def logprob_fun(params, inputs, targets):
    preds = predict(weights, inputs)
    return np.sum((preds - targets)**2)

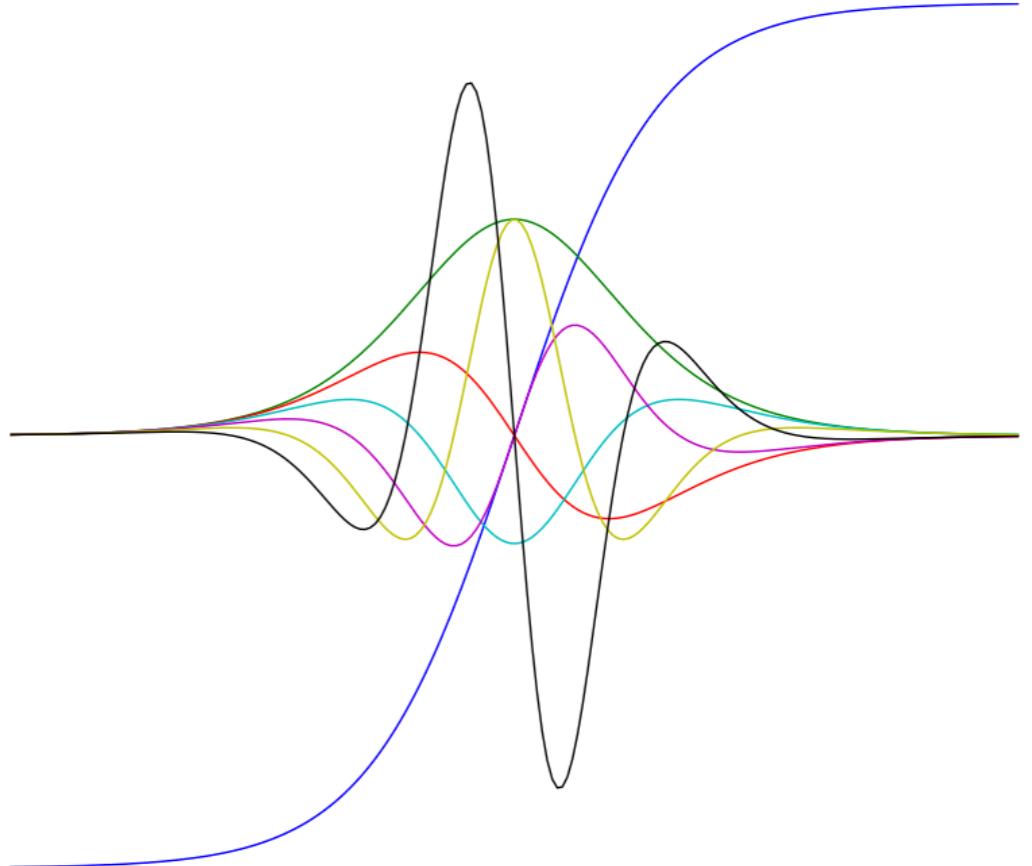
gradient_fun = grad(logprob_fun)
```



Autograd examples

```
import autograd.numpy as np
from autograd import grad
import matplotlib.pyplot as plt

x = np.linspace(-7, 7, 200)
plt.plot(x, np.tanh(x),
          x, grad(np.tanh)(x),
          x, grad(grad(np.tanh))(x),
          x, grad(grad(grad(np.tanh)))(x),
          x, grad(grad(grad(grad(np.tanh))))(x),
          x, grad(grad(grad(grad(grad(np.tanh)))))(x),
          x, grad(grad(grad(grad(grad(grad(np.tanh))))))(x))
```



Hessians and HVPs

```
from autograd import grad, jacobian

def hessian(fun, argnum=0):
    return jacobian(jacobian(fun, argnum), argnum)

def hvp(fun):
    def grad_dot_vector(arg, vector):
        return np.dot(grad(fun)(arg), vector)
    return grad(grad_dot_vector)
```

$$\nabla^2 f(x) \cdot v = \nabla_x (\nabla_x f(x) \cdot v)$$

Black-box inference in a tweet



Ryan Adams @ryan_p_adams · 7 Nov 2015

@DavidDuvenaud

```
def elbo(p, lp, D, N):  
    v=exp(p[D:])  
    s=randn(N,D)*sqrt(v)+p[:D]  
    return mvn.entropy(0, diag(v))+mean(lp(s))  
gf = grad(elbo)
```

1

7

22

...

Tutorial goals

1. Jacobians and the chain rule
 - Forward and reverse accumulation
2. Autograd's implementation
 - Fully closed tracing autodiff in Python
3. Advanced autodiff techniques
 - Checkpointing, forward from reverse, differentiating optima and fixed points

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$$F:\mathbb{R}^n\rightarrow \mathbb{R}$$

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$$\begin{array}{ccc} F : & \begin{array}{c} \textcolor{gray}{\boxed{}} \\ \mapsto \\ \textcolor{red}{y} \in \mathbb{R} \end{array} & \xrightarrow{} \\ & \textcolor{blue}{x} \in \mathbb{R}^n & \end{array}$$

$$F:\mathbb{R}^n\rightarrow \mathbb{R}$$

$$F:\begin{array}{|c|}\hline\textcolor{gray}{\square}\\\hline\end{array}\mapsto \textcolor{red}{y}\in\mathbb{R}$$

$$\textcolor{blue}{x}\in\mathbb{R}^n$$

$$F = D \circ C \circ B \circ A$$

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$$F = D \circ C \circ B \circ A$$

$$\textcolor{red}{y}=F(\textcolor{blue}{x})=D(C(B(A(\textcolor{blue}{x}))))$$

$$F : \mathbb{R}^n \rightarrow \mathbb{R}$$

$$F : \begin{array}{c} \text{A tall gray rectangle} \\ \mapsto \\ \text{A small gray square} \end{array} \quad y \in \mathbb{R}$$

$x \in \mathbb{R}^n$

$$F = D \circ C \circ B \circ A$$

$$y = F(\textcolor{blue}{x}) = D(C(B(A(\textcolor{blue}{x}))))$$

$$\textcolor{red}{y} = D(\boldsymbol{c}), \quad \boldsymbol{c} = C(\boldsymbol{b}), \quad \boldsymbol{b} = B(\boldsymbol{a}), \quad \boldsymbol{a} = A(\textcolor{blue}{x})$$

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$$F'(\textcolor{blue}{x})=\frac{\partial \textcolor{red}{y}}{\partial \textcolor{blue}{x}}=\left[\frac{\partial \textcolor{red}{y}}{\partial \textcolor{blue}{x}_1}\quad\cdots\quad\frac{\partial \textcolor{red}{y}}{\partial \textcolor{blue}{x}_n}\right]$$

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$$F'(\textcolor{blue}{x})=\begin{array}{l} \frac{\partial \textcolor{red}{y}}{\partial c} \end{array} \begin{array}{l} \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \end{array} \begin{array}{l} \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \end{array} \begin{array}{l} \frac{\partial \boldsymbol{a}}{\partial \textcolor{blue}{x}} \end{array}$$

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$$\frac{\partial \textcolor{red}{y}}{\partial \mathbf{c}} = D'(\mathbf{c})$$



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$$\frac{\partial \mathbf{c}}{\partial \mathbf{b}} = C'(\mathbf{b})$$

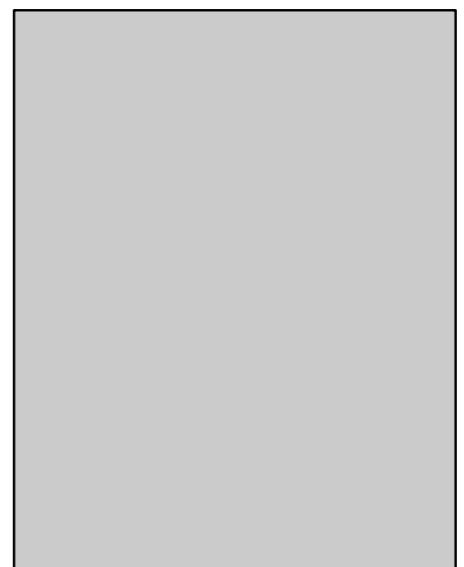
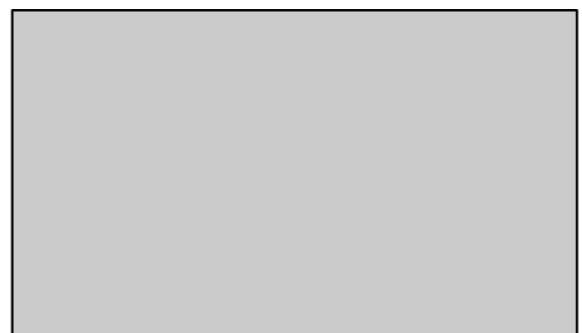


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$\frac{\partial \textcolor{red}{y}}{\partial \mathbf{c}} = D'(\mathbf{c})$ $\frac{\partial \mathbf{c}}{\partial \mathbf{b}} = C'(\mathbf{b})$ $\frac{\partial \mathbf{b}}{\partial \mathbf{a}} = B'(\mathbf{a})$ $\frac{\partial \mathbf{a}}{\partial \textcolor{blue}{x}} = A'(\textcolor{blue}{x})$



$$F'(\textcolor{blue}{x}) = \frac{\partial \textcolor{red}{y}}{\partial c} \left(\frac{\partial c}{\partial b} \begin{pmatrix} \frac{\partial b}{\partial a} & \frac{\partial a}{\partial \textcolor{blue}{x}} \end{pmatrix} \right)$$

$$F'(\mathbf{x}) = \frac{\partial \mathbf{y}}{\partial \mathbf{c}} \left(\underbrace{\frac{\partial \mathbf{c}}{\partial \mathbf{b}} \begin{pmatrix} \frac{\partial \mathbf{b}}{\partial \mathbf{a}} & \frac{\partial \mathbf{a}}{\partial \mathbf{x}} \end{pmatrix}}_{\text{ }} \right)$$
$$\frac{\partial \mathbf{b}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial b_1}{\partial \mathbf{x}_1} & \dots & \frac{\partial b_1}{\partial \mathbf{x}_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial b_m}{\partial \mathbf{x}_1} & \dots & \frac{\partial b_m}{\partial \mathbf{x}_n} \end{bmatrix}$$

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$$\frac{\partial \mathbf{y}}{\partial \mathbf{b}} = \begin{bmatrix} \frac{\partial \mathbf{y}}{\partial b_1} & \dots & \frac{\partial \mathbf{y}}{\partial b_m} \end{bmatrix}$$

$$F'(\mathbf{x}) = \frac{\partial \mathbf{y}}{\partial \mathbf{c}} \underbrace{\left(\frac{\partial \mathbf{c}}{\partial \mathbf{b}} \begin{pmatrix} \frac{\partial \mathbf{b}}{\partial \mathbf{a}} & \frac{\partial \mathbf{a}}{\partial \mathbf{x}} \end{pmatrix} \right)}_{\text{Forward accumulation}}$$

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$$F'(\mathbf{x}) = \underbrace{\left(\left(\frac{\partial \mathbf{y}}{\partial \mathbf{c}} \quad \frac{\partial \mathbf{c}}{\partial \mathbf{b}} \right) \frac{\partial \mathbf{b}}{\partial \mathbf{a}} \right)}_{\text{Reverse accumulation}} \frac{\partial \mathbf{a}}{\partial \mathbf{x}}$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{b}} = \begin{bmatrix} \frac{\partial \mathbf{y}}{\partial b_1} & \dots & \frac{\partial \mathbf{y}}{\partial b_m} \end{bmatrix}$$

Forward
accumulation

Reverse
accumulation

$$F'(\textcolor{blue}{x})\ \textcolor{violet}{v} = \begin{array}{c}\frac{\partial \textcolor{red}{y}}{\partial c} \quad \frac{\partial c}{\partial b} \quad \frac{\partial b}{\partial a} \quad \frac{\partial a}{\partial \textcolor{blue}{x}}\end{array} \textcolor{violet}{v}$$

$$F'(\textcolor{blue}{x}) \ \textcolor{violet}{v} = \begin{matrix} \frac{\partial \textcolor{red}{y}}{\partial c} & \frac{\partial c}{\partial b} & \frac{\partial b}{\partial a} & \frac{\partial a}{\partial \textcolor{blue}{x}} \end{matrix} \ \textcolor{violet}{v}$$

$$F'(\textcolor{blue}{x}) \ \textcolor{violet}{v} = \frac{\partial \textcolor{red}{y}}{\partial c} \left(\frac{\partial c}{\partial b} \left(\frac{\partial b}{\partial a} \left(\frac{\partial a}{\partial \textcolor{blue}{x}} \ \textcolor{violet}{v} \right) \right) \right)$$

$$F'(\mathbf{x}) \ \mathbf{v} = \begin{matrix} \frac{\partial \mathbf{y}}{\partial \mathbf{c}} & \frac{\partial \mathbf{c}}{\partial \mathbf{b}} & \frac{\partial \mathbf{b}}{\partial \mathbf{a}} & \frac{\partial \mathbf{a}}{\partial \mathbf{x}} \end{matrix} \ \mathbf{v}$$

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Forward accumulation \leftrightarrow Jacobian-vector products

Build Jacobian one column at a time

$$F'(\mathbf{x}) \ \mathbf{v} = \begin{matrix} \frac{\partial \mathbf{y}}{\partial \mathbf{c}} & \frac{\partial \mathbf{c}}{\partial \mathbf{b}} & \frac{\partial \mathbf{b}}{\partial \mathbf{a}} & \frac{\partial \mathbf{a}}{\partial \mathbf{x}} \end{matrix} \ \mathbf{v}$$

$$F'(\mathbf{x}) \ \mathbf{v} = \frac{\partial \mathbf{y}}{\partial \mathbf{c}} \left(\frac{\partial \mathbf{c}}{\partial \mathbf{b}} \left(\frac{\partial \mathbf{b}}{\partial \mathbf{a}} \left(\frac{\partial \mathbf{a}}{\partial \mathbf{x}} \ \mathbf{v} \right) \right) \right)$$

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$$\textcolor{violet}{v}^\top F'(\textcolor{blue}{x}) = \quad \textcolor{violet}{v}^\top \frac{\partial \textcolor{red}{y}}{\partial c} \quad \frac{\partial c}{\partial b} \quad \frac{\partial b}{\partial a} \quad \frac{\partial a}{\partial \textcolor{blue}{x}}$$

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$$\boldsymbol{v}^\top F'(\boldsymbol{x}) = \begin{matrix} \boldsymbol{v}^\top \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{c}} & \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} & \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} & \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}} \end{matrix}$$

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Reverse accumulation \leftrightarrow vector-Jacobian products

Build Jacobian one row at a time

$$\boldsymbol{v}^\top F'(\boldsymbol{x}) = \begin{matrix} \boldsymbol{v}^\top \frac{\partial \mathbf{y}}{\partial \mathbf{c}} & \frac{\partial \mathbf{c}}{\partial \mathbf{b}} & \frac{\partial \mathbf{b}}{\partial \mathbf{a}} & \frac{\partial \mathbf{a}}{\partial \boldsymbol{x}} \end{matrix}$$

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Forward and reverse accumulation

- Forward accumulation
 - Jacobian-vector products
 - “push-forward”
 - build Jacobian matrix one column at a time
- Reverse accumulation
 - vector-Jacobian products
 - “pull-back”
 - build Jacobian matrix one row at a time

Non-chain composition

Non-chain composition

Fan-in

$$\textcolor{red}{y} = F(\textcolor{blue}{x}_1, \textcolor{blue}{x}_2)$$

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Fan-in

$$\textcolor{red}{y} = F(\textcolor{blue}{x}_1, \textcolor{blue}{x}_2)$$

$$\frac{\partial \textcolor{red}{y}}{\partial \textcolor{blue}{x}_1} = F'_1(\textcolor{blue}{x}_1, \textcolor{blue}{x}_2)$$

$$\frac{\partial \textcolor{red}{y}}{\partial \textcolor{blue}{x}_2} = F'_2(\textcolor{blue}{x}_1, \textcolor{blue}{x}_2)$$

Non-chain composition

Fan-in

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Fan-out

$$G(\textcolor{blue}{x}) = \begin{bmatrix} \textcolor{blue}{x} \\ \textcolor{blue}{x} \end{bmatrix} = \begin{bmatrix} I \\ I \end{bmatrix} \textcolor{blue}{x}$$

Non-chain composition

Fan-in

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$$G'(\textcolor{blue}{x}) = \begin{bmatrix} I \\ I \end{bmatrix}$$

$$\textcolor{violet}{v}^\top G'(\textcolor{blue}{x}) = [\textcolor{violet}{v}_1^\top \quad \textcolor{violet}{v}_2^\top] \begin{bmatrix} I \\ I \end{bmatrix} = \textcolor{violet}{v}_1^\top + \textcolor{violet}{v}_2^\top$$

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Autodiff implementations

1. Read and generate source code ahead-of-time
 - source and target language could be Python
 - or a “computation graph” language (TensorFlow)
2. Monitor function execution at runtime

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- source and target language could be Python
- or a “computation graph” language (TensorFlow)

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Autograd's ingredients

1. Tracing the composition of primitive functions
2. Defining a vector-Jacobian product (VJP) operator for each primitive
3. Composing VJPs backward

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1. Tracing the composition of primitive functions
2. Defining a vector-Jacobian product (VJP) operator for each primitive
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`numpy.sum`

primitive

autograd.numpy.sum

numpy.sum

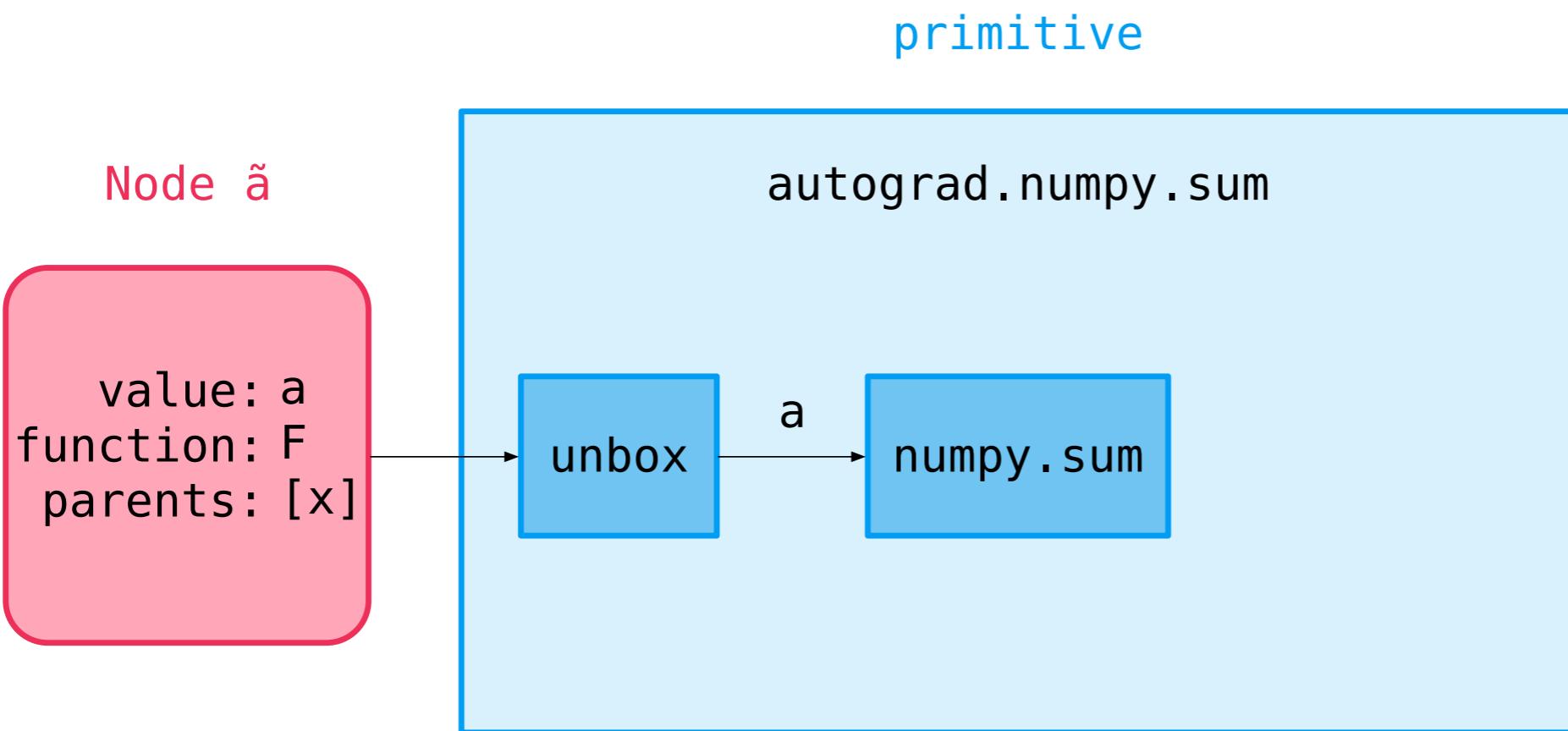
Node \tilde{a}

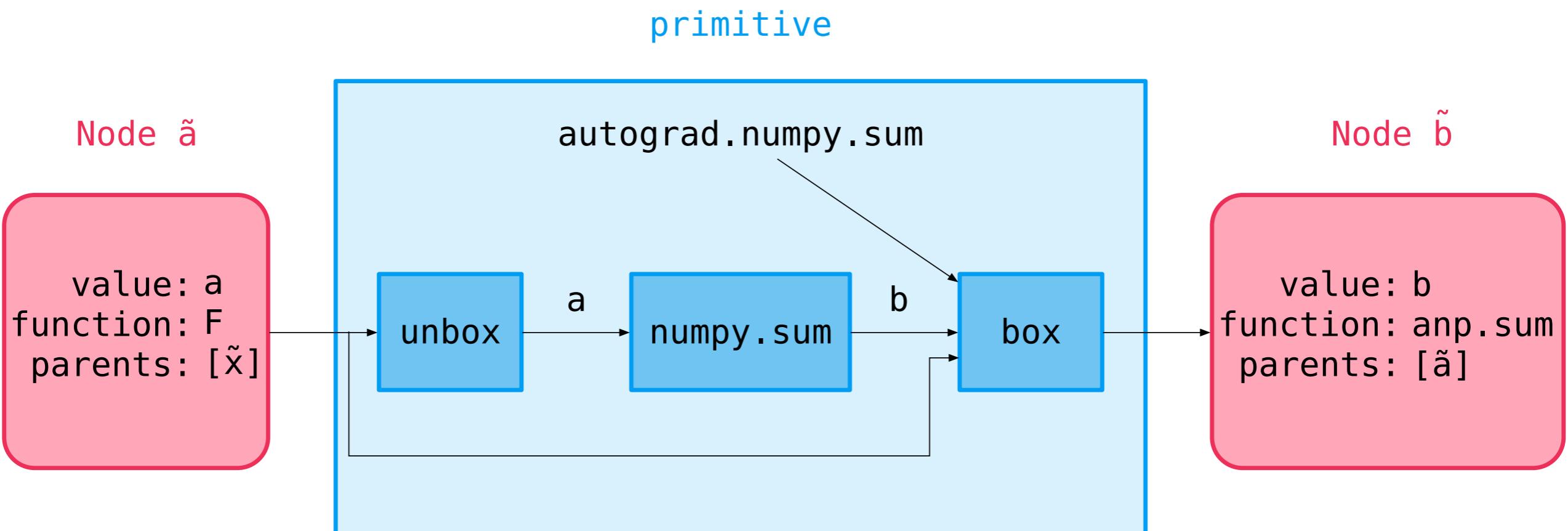
value: a
function: F
parents: [x]

primitive

autograd.numpy.sum

numpy.sum





```
class Node(object):
    __slots__ = ['value', 'recipe', 'progenitors', 'vspace']

    def __init__(self, value, recipe, progenitors):
        self.value = value
        self.recipe = recipe
        self.progenitors = progenitors
        self.vspace = vspace(value)
```

```
class primitive(object):
    def __call__(self, *args, **kwargs):
        argvals = list(args)

        parents = []
        for argnum, arg in enumerate(args):
            if isnode(arg):
                argvals[argnum] = arg.value
                if argnum in self.zero_vjps: continue
                parents.append((argnum, arg))

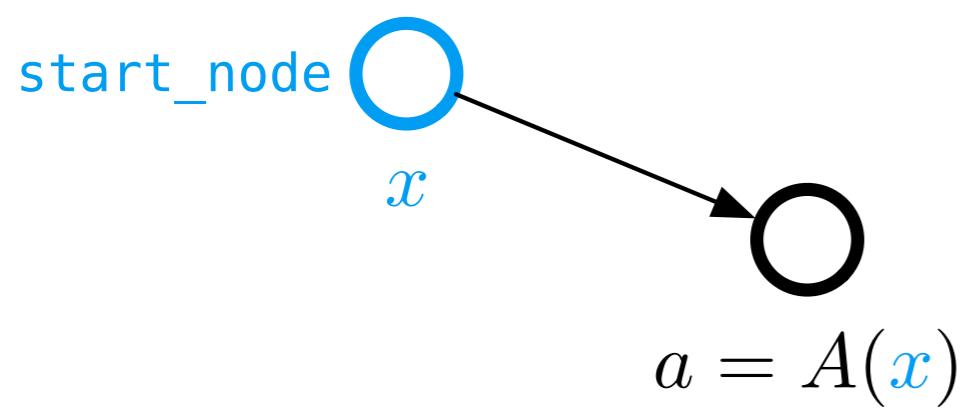
        result_value = self.fun(*argvals, **kwargs)
        return new_node(result_value, (self, args, kwargs, parents), )
```

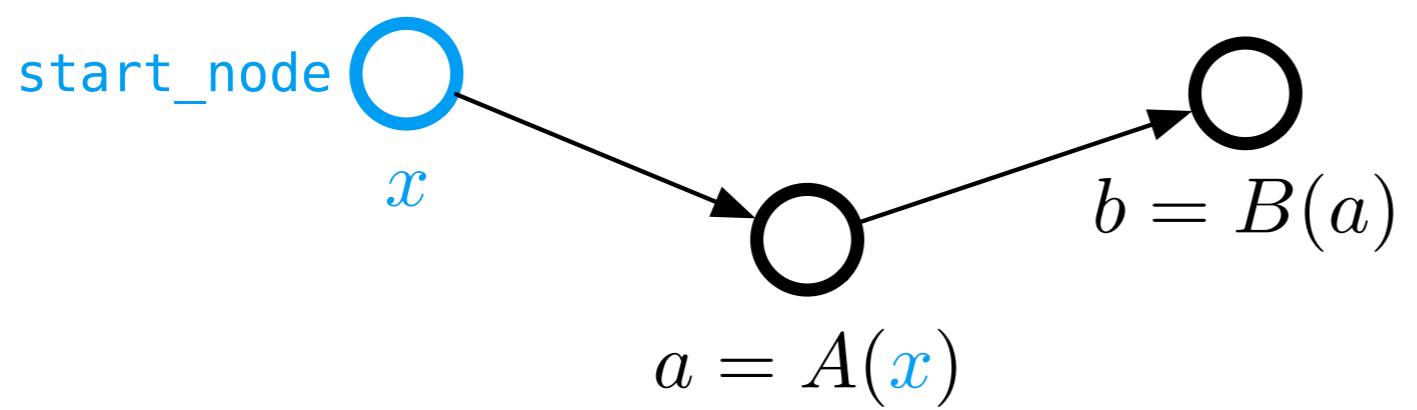
```
class primitive(object):
    def __call__(self, *args, **kwargs):
        argvals = list(args)
        progenitors = set()
        parents = []
        for argnum, arg in enumerate(args):
            if isnode(arg):
                argvals[argnum] = arg.value
                if argnum in self.zero_vjps: continue
                parents.append((argnum, arg))
                progenitors.update(arg.progenitors & active_progenitors)

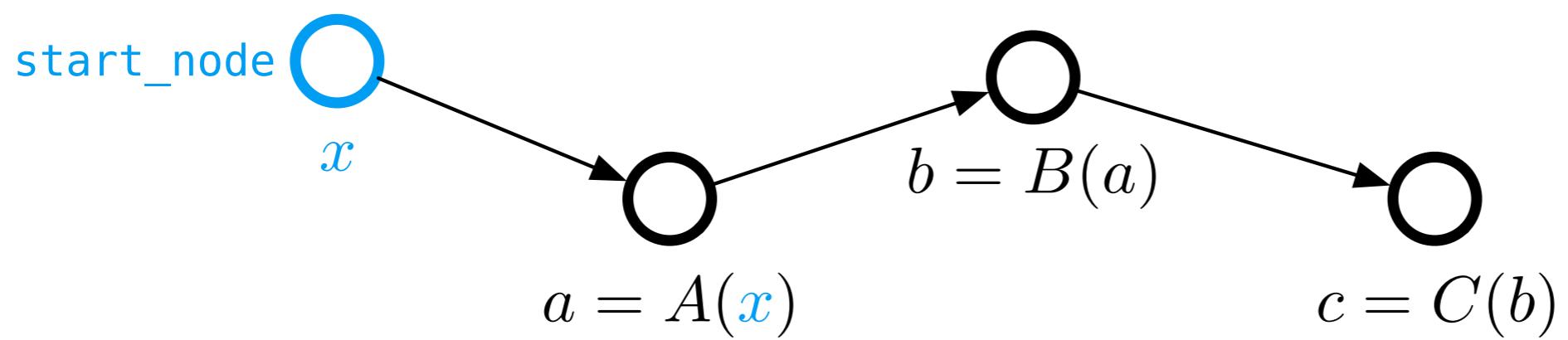
        result_value = self.fun(*argvals, **kwargs)
        return new_node(result_value, (self, args, kwargs, parents), progenitors)
```

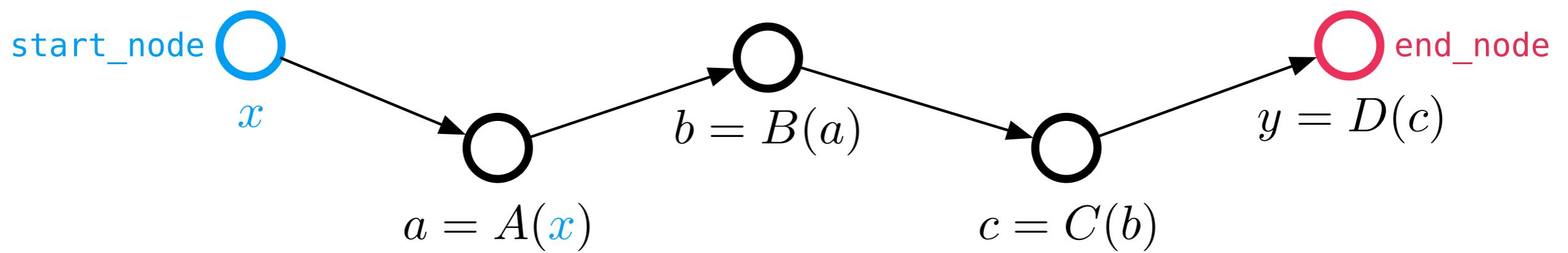
```
def forward_pass(fun, args, kwargs, argnum=0):
    args = list(args)
    start_node = new_progenitor(args[argnum])
    args[argnum] = start_node
    active_progenitors.add(start_node)
    end_node = fun(*args, **kwargs)
    active_progenitors.remove(start_node)
    return start_node, end_node
```

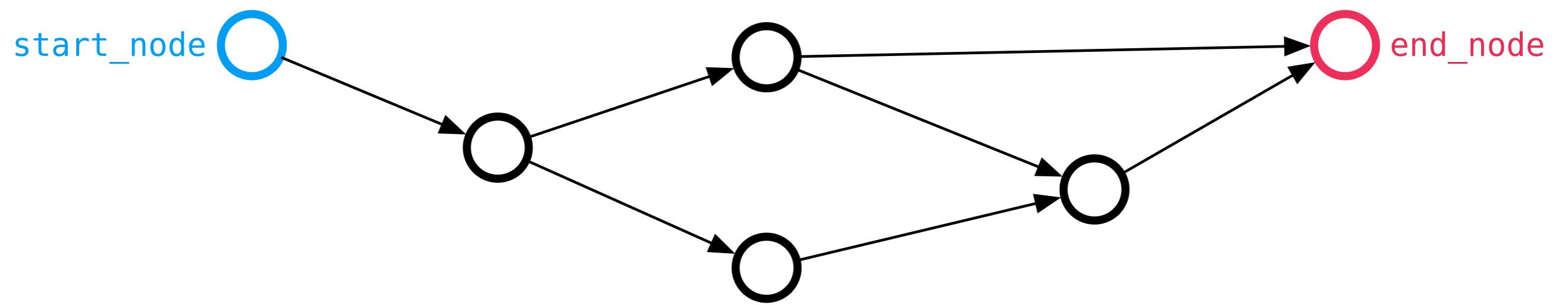
start_node 
 x

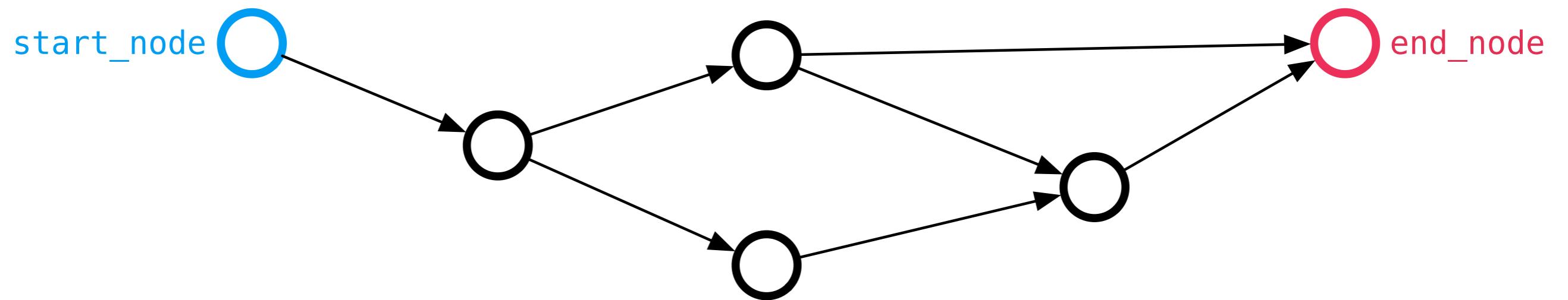












No control flow!

Autograd's ingredients

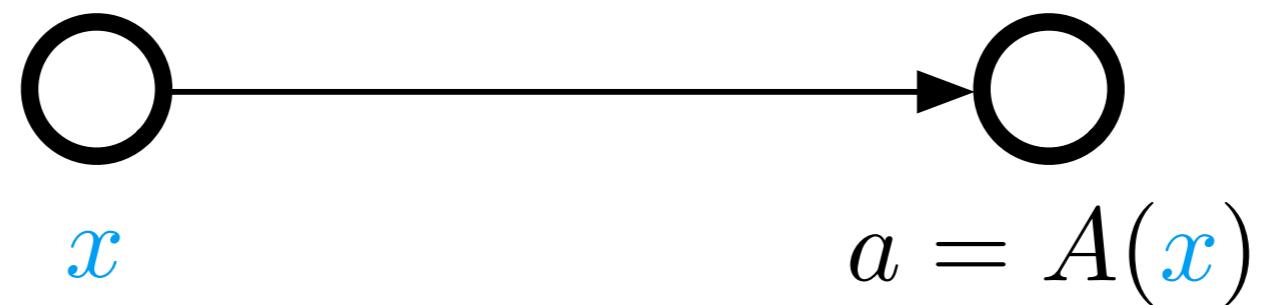
1. Tracing the composition of primitive functions
2. Defining a vector-Jacobian product (VJP) operator for each primitive
3. Composing VJPs backward



$\textcolor{blue}{x}$

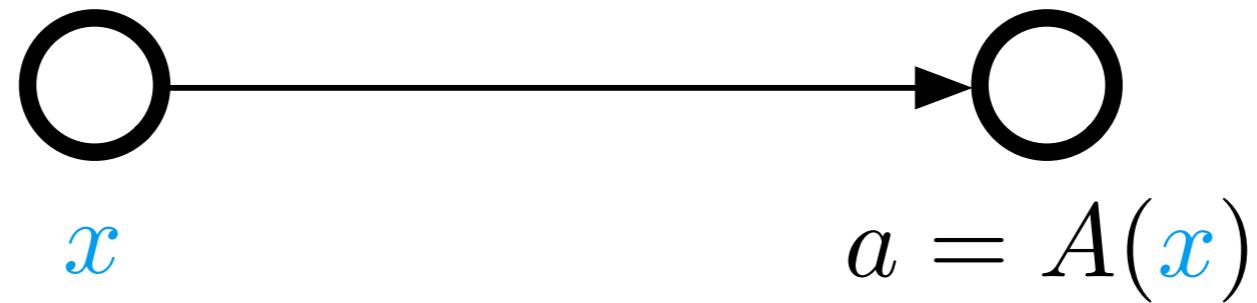
$a = A(\textcolor{blue}{x})$

$$\frac{\partial \textcolor{red}{y}}{\partial a}$$

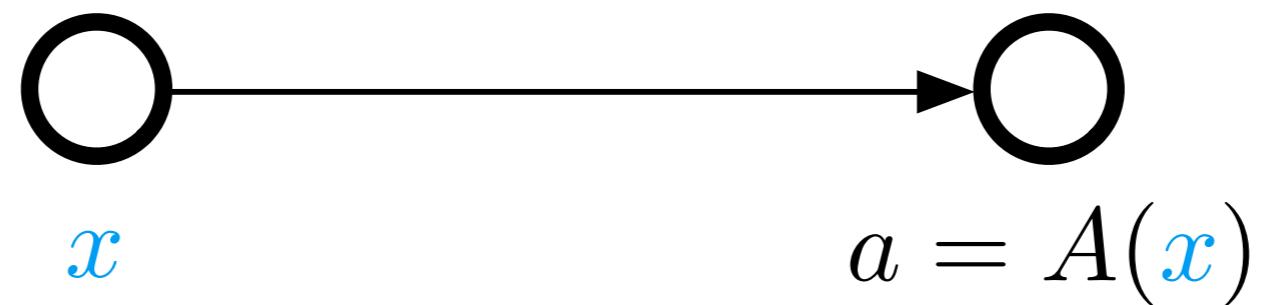


$$\frac{\partial \textcolor{red}{y}}{\partial \textcolor{blue}{x}} = ?$$

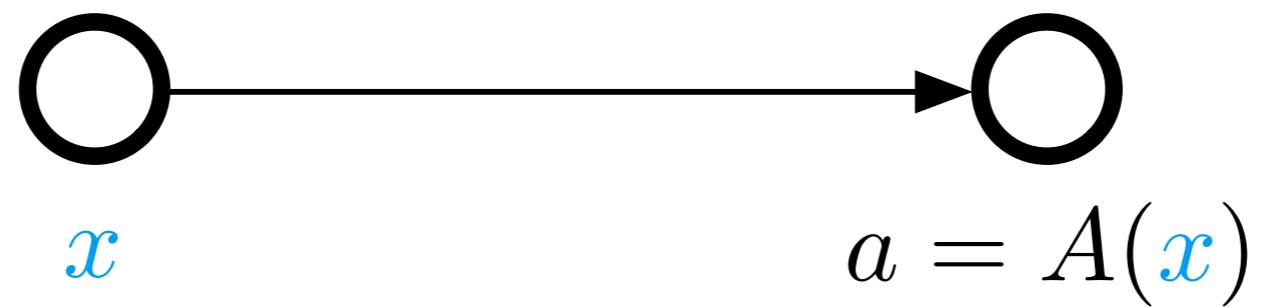
$$\frac{\partial \textcolor{red}{y}}{\partial a}$$



$$\frac{\partial \textcolor{red}{y}}{\partial \textcolor{blue}{x}} = \frac{\partial \textcolor{red}{y}}{\partial a} \cdot \frac{\partial a}{\partial \textcolor{blue}{x}}$$
$$\frac{\partial \textcolor{red}{y}}{\partial a}$$



$$\frac{\partial \textcolor{red}{y}}{\partial \textcolor{blue}{x}} = \frac{\partial \textcolor{red}{y}}{\partial a} \cdot A'(\textcolor{blue}{x}) \quad \frac{\partial \textcolor{red}{y}}{\partial a}$$

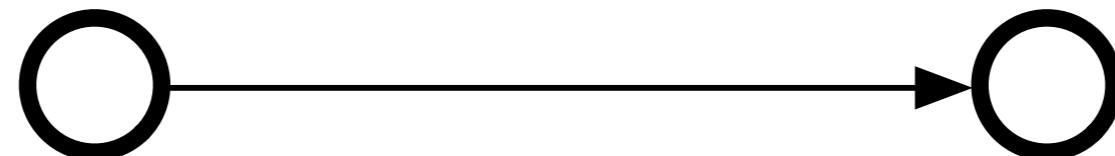


vector-Jacobian product



$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial \mathbf{y}}{\partial a} \cdot A'(\mathbf{x})$$

$$\frac{\partial \mathbf{y}}{\partial a}$$



$$\mathbf{x}$$

$$a = A(\mathbf{x})$$

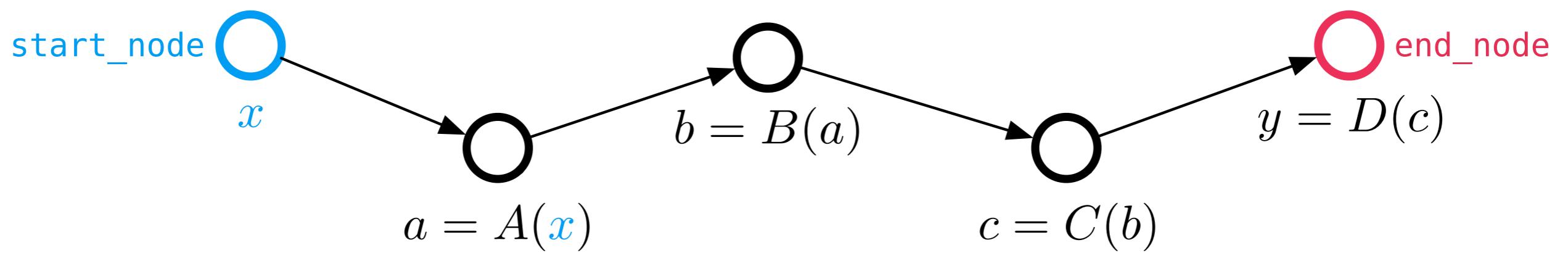
```
anp.sinh.defvjp(lambda g, ans, vs, gvs, x: g * anp.cosh(x))
anp.cosh.defvjp(lambda g, ans, vs, gvs, x: g * anp.sinh(x))
anp.tanh.defvjp(lambda g, ans, vs, gvs, x: g / anp.cosh(x)**2)

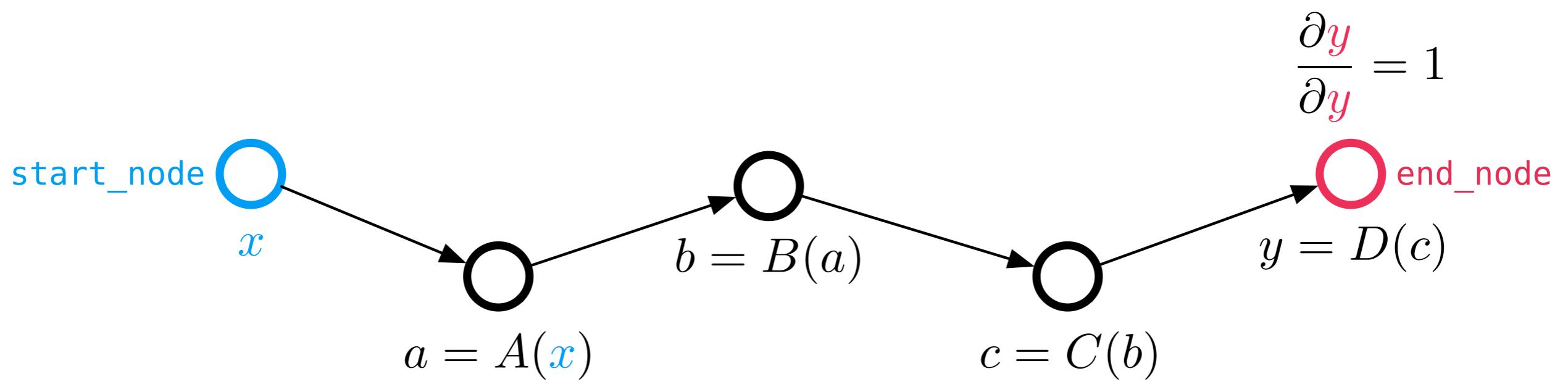
anp.cross.defvjp(lambda g, ans, vs, gvs, a, b, axisa=-1, axisb=-1, axisc=-1, axis=None:
                  anp.cross(b, g, axisb, axisc, axisa, axis), argnum=0)

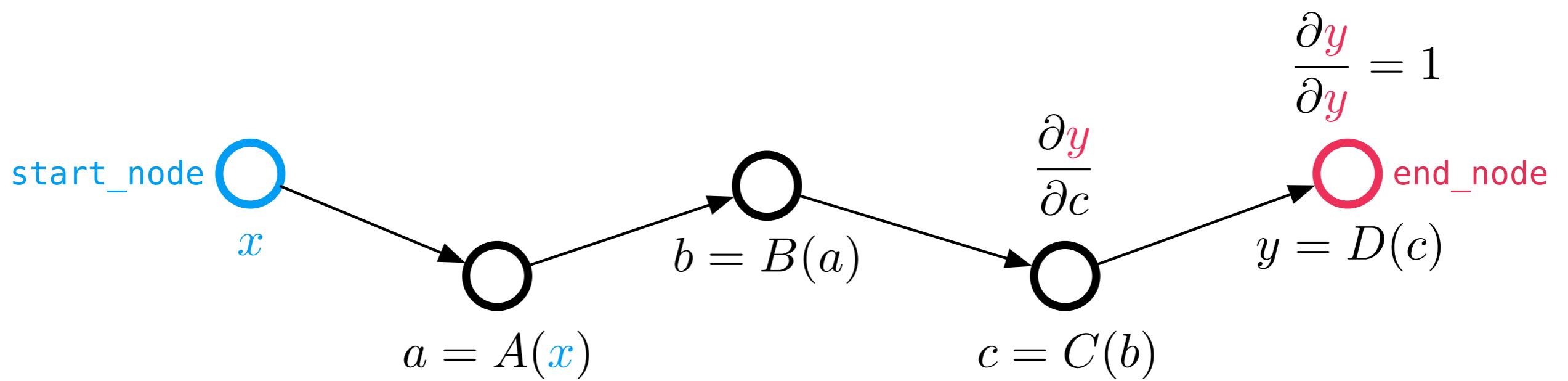
def grad_sort(g, ans, vs, gvs, x, axis=-1, kind='quicksort', order=None):
    sort_perm = anp.argsort(x, axis, kind, order)
    return unpermute(g, sort_perm)
anp.sort.defvjp(grad_sort)
```

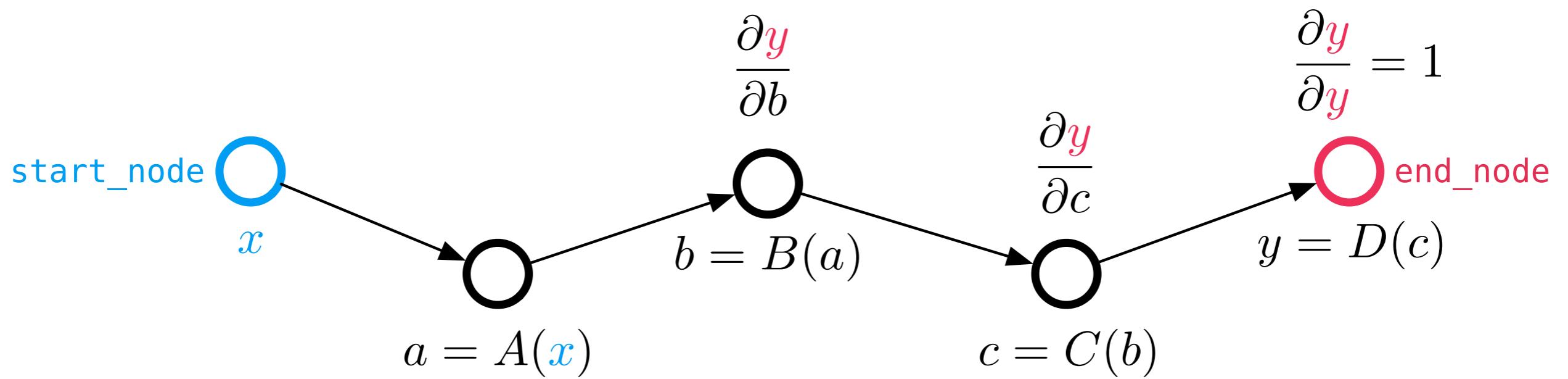
Autograd's ingredients

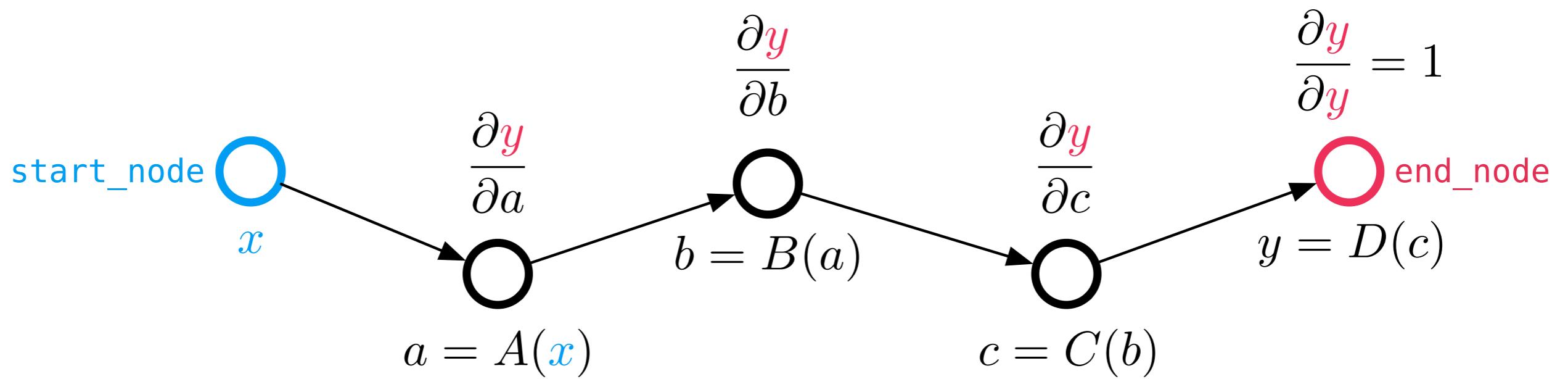
1. Tracing the composition of primitive functions
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3. Composing VJPs backward

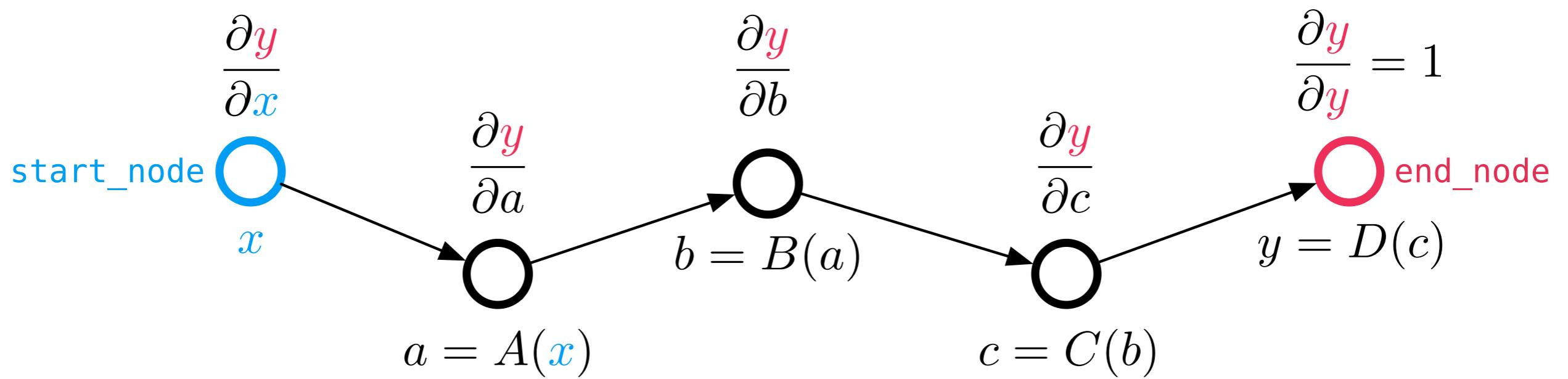






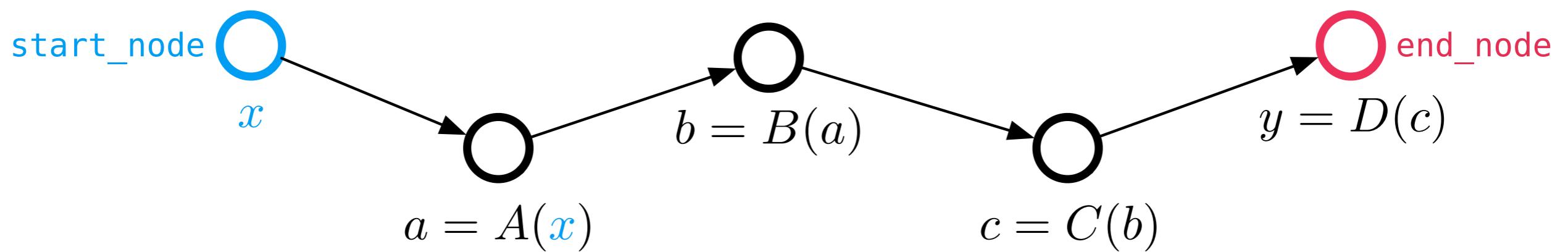


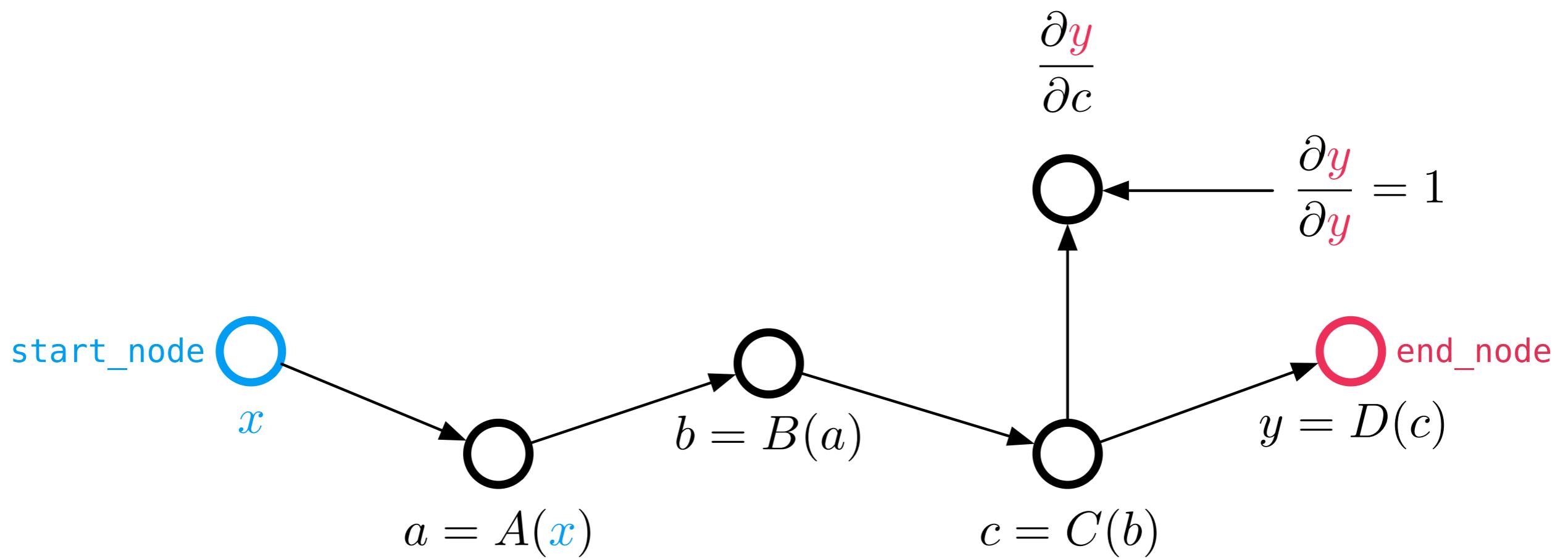


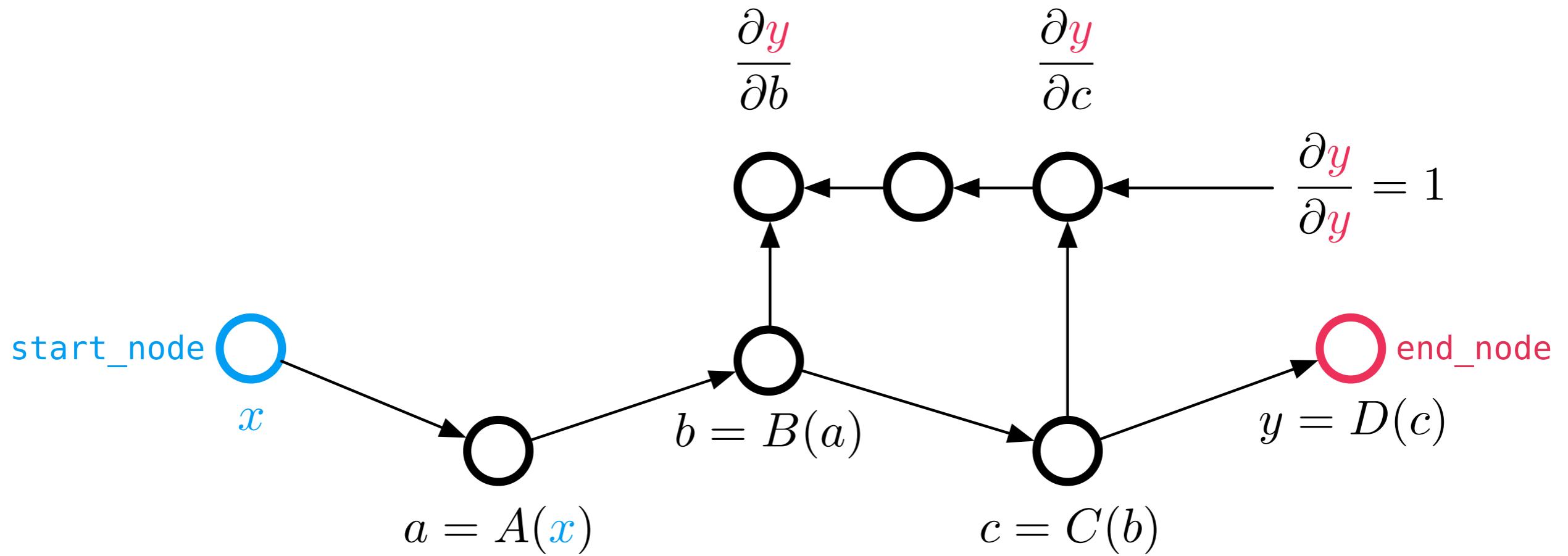


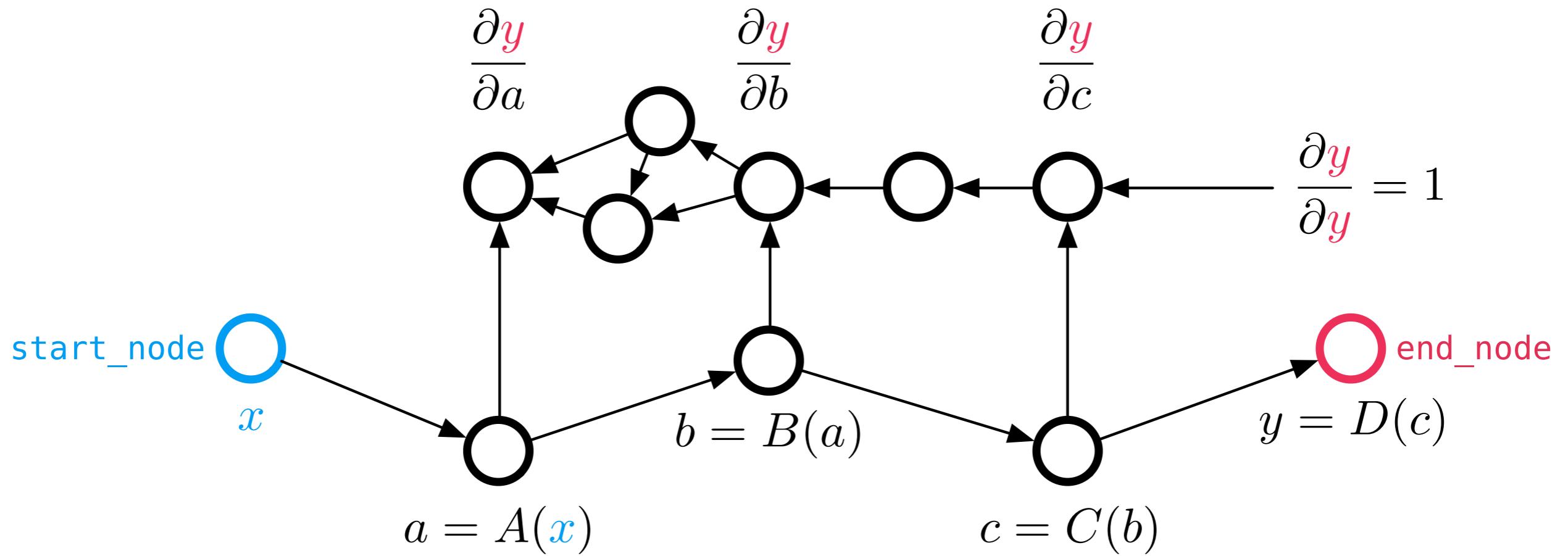
higher-order autodiff just works:
the backward pass can itself be traced

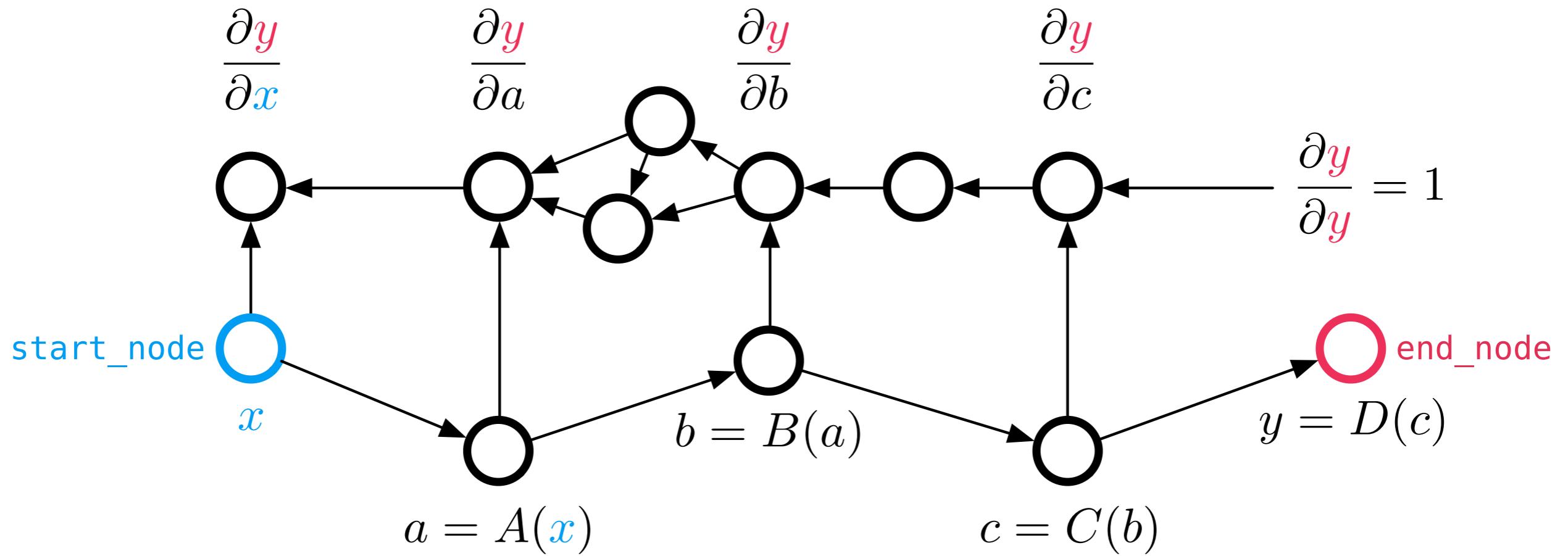
$$\frac{\partial \textcolor{red}{y}}{\partial y} = 1$$

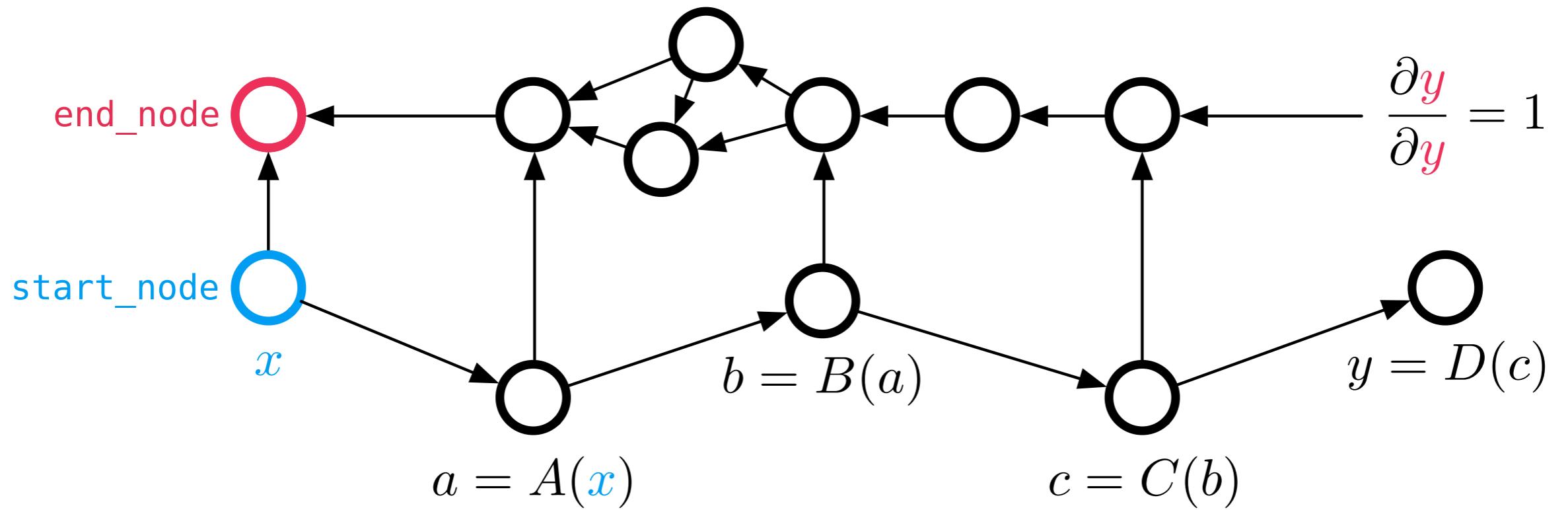













```
def grad(fun, argnum=0):
    def gradfun(*args, **kwargs):
        args = list(args)
        args[argnum] = safe_type(args[argnum])
        vjp, ans = make_vjp(fun, argnum)(*args, **kwargs)
        return vjp(vspace(getval(ans)).ones())
    return gradfun
```

```
def make_vjp(fun, argnum=0):
    def vjp_maker(*args, **kwargs):
        start_node, end_node = forward_pass(fun, args, kwargs, argnum)
        if not isnode(end_node) or start_node not in end_node.progenitors:
            warnings.warn("Output seems independent of input.")
            def vjp(g): return start_node.vspace.zeros()
        else:
            def vjp(g): return backward_pass(g, end_node, start_node)
        return vjp, end_node
    return vjp_maker
```

Autograd's ingredients

1. Tracing the composition of primitive functions
`Node`, `primitive`, `forward_pass`
2. Defining a vector-Jacobian product (VJP) operator for each primitive
`defvjp`
3. Composing VJPs backward
`backward_pass`, `make_vjp`, `grad`

Tradeoffs in forward vs reverse

Tradeoffs in forward vs reverse

- Reverse-mode requires tracing a program's execution
 - Memory cost scales like depth of program
 - Checkpointing can trade off time and memory

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 - But requires n calls to form Jacobian of $F : \mathbb{R}^n \rightarrow \mathbb{R}$
 - Autograd forward-mode by @j-towns: github.com/BB-UCL/autograd-forward

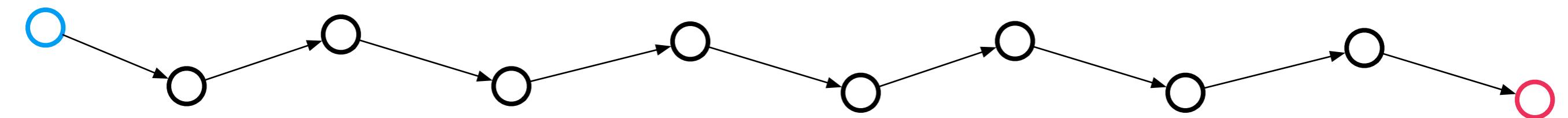
Tradeoffs in forward vs reverse

- Reverse-mode requires tracing a program's execution
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- Forward-mode evaluates a JVP with constant memory overhead
 - But requires n calls to form Jacobian of $F : \mathbb{R}^n \rightarrow \mathbb{R}$
 - Autograd forward-mode by @j-towns: github.com/BB-UCL/autograd-forward
- Can use both together (in autograd!) for mixed-mode

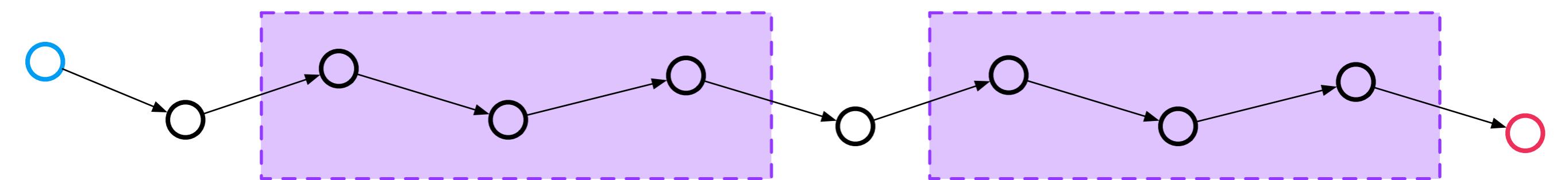
Tutorial goals

1. Jacobians and the chain rule
 - Forward and reverse accumulation
2. Autograd's implementation
 - Fully closed tracing autodiff in Python
3. Advanced autodiff techniques
 - Checkpointing, forward from reverse, differentiating optima and fixed points

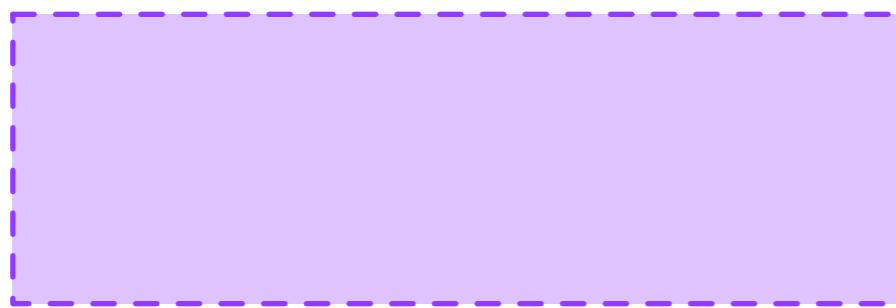
Checkpointing



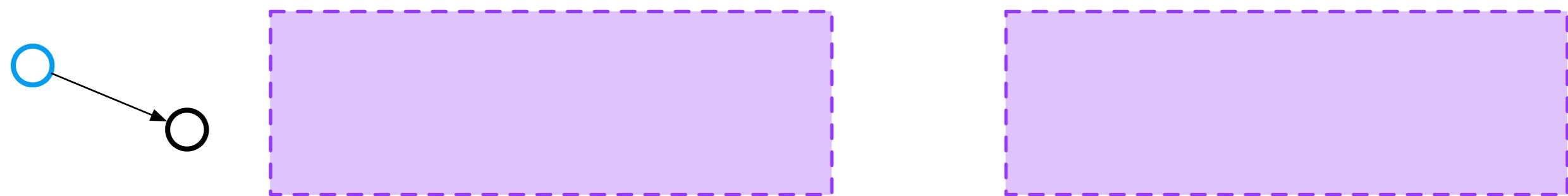
Checkpointing



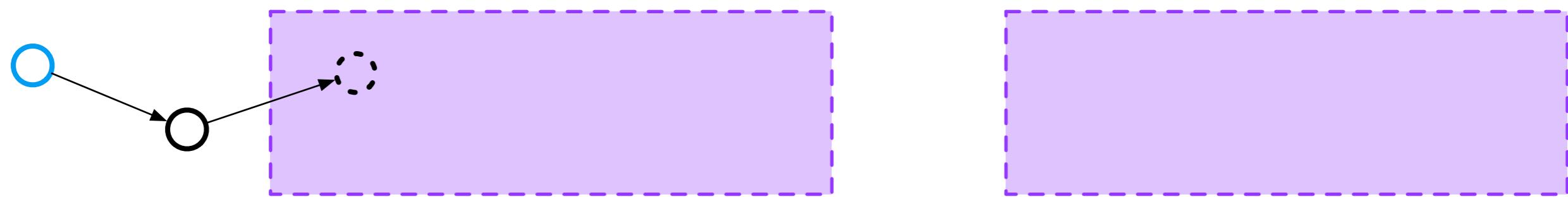
Checkpointing



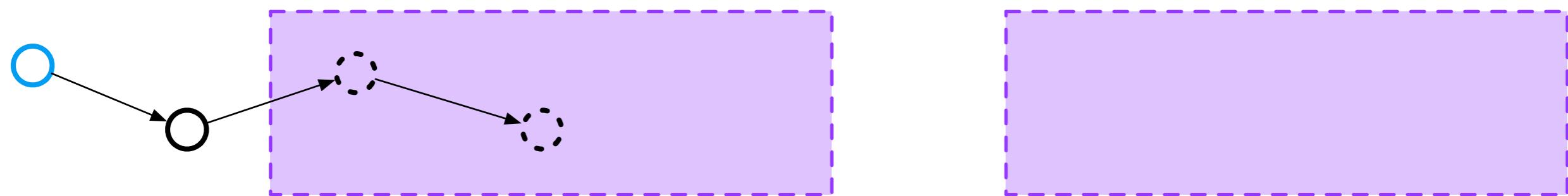
Checkpointing



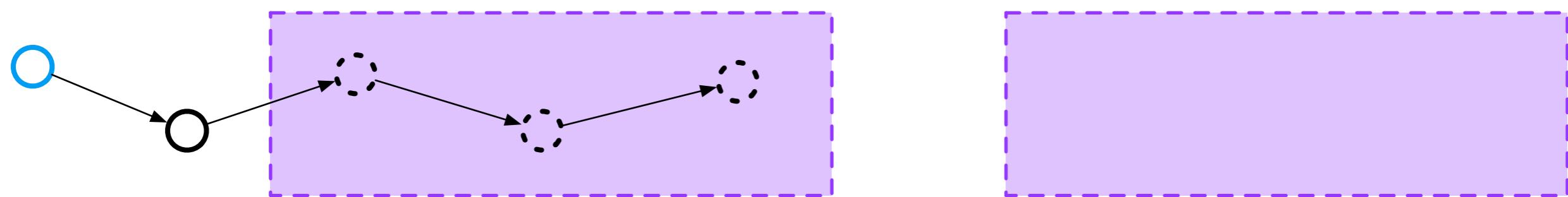
Checkpointing



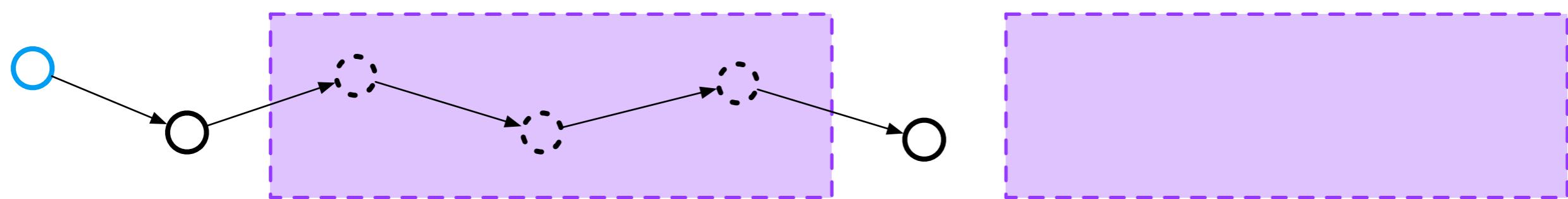
Checkpointing



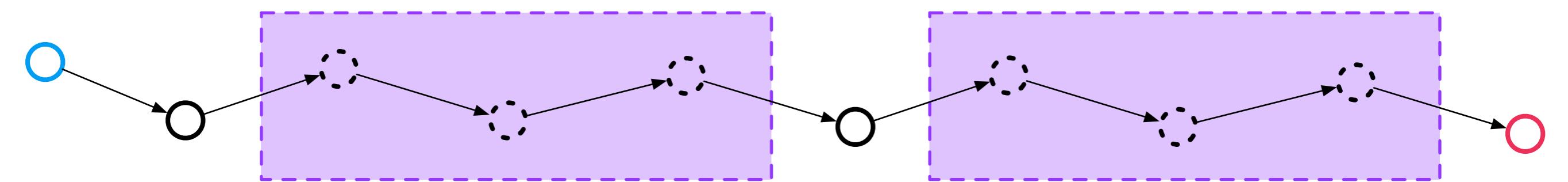
Checkpointing



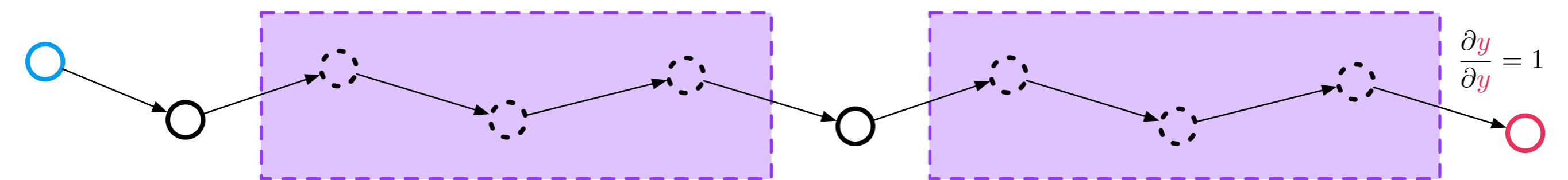
Checkpointing



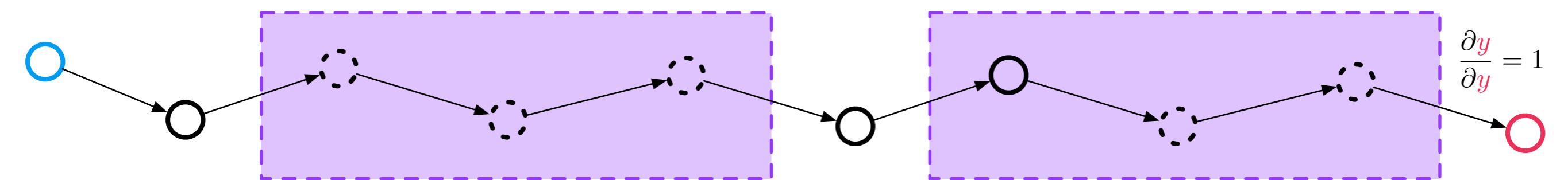
Checkpointing



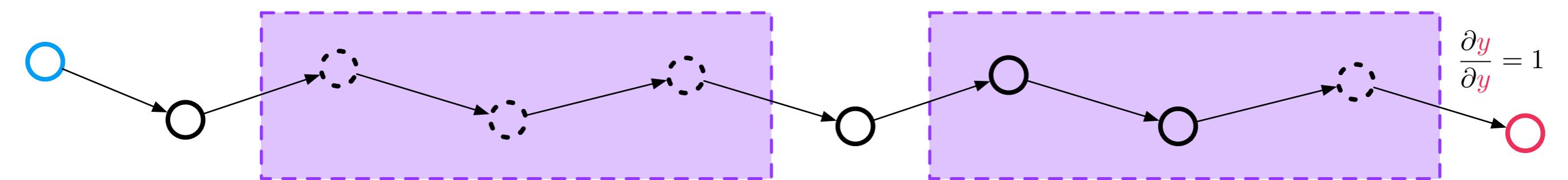
Checkpointing



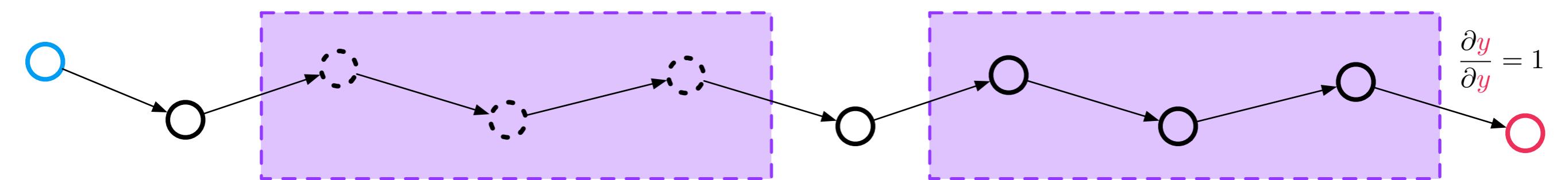
Checkpointing



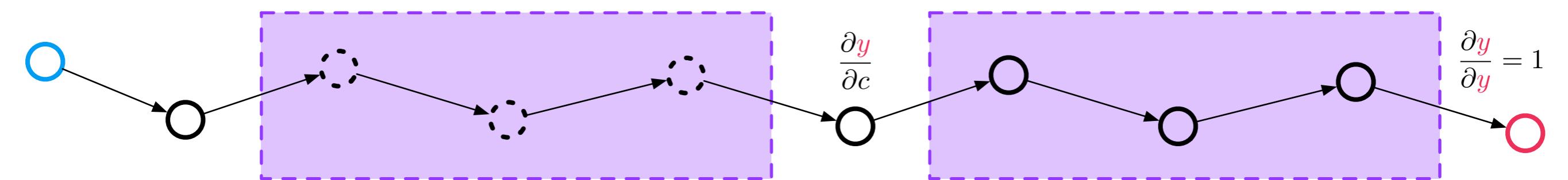
Checkpointing



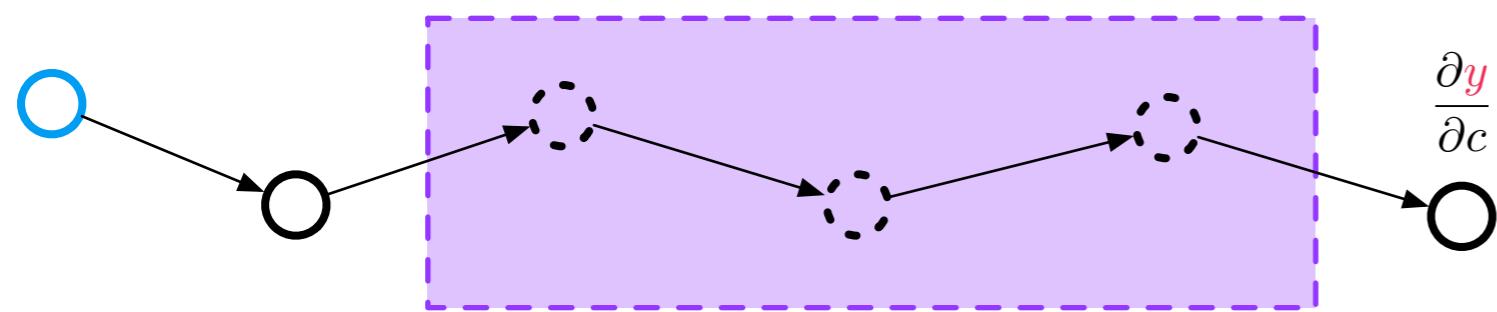
Checkpointing



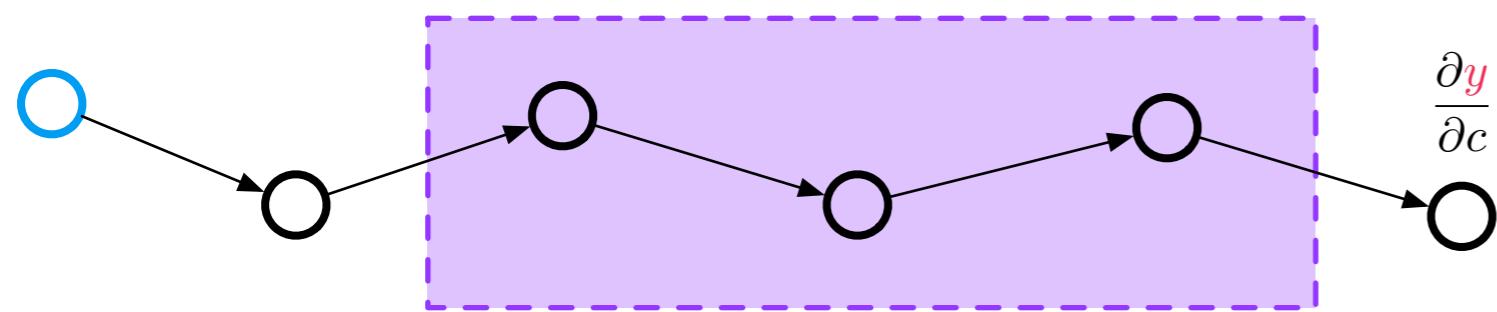
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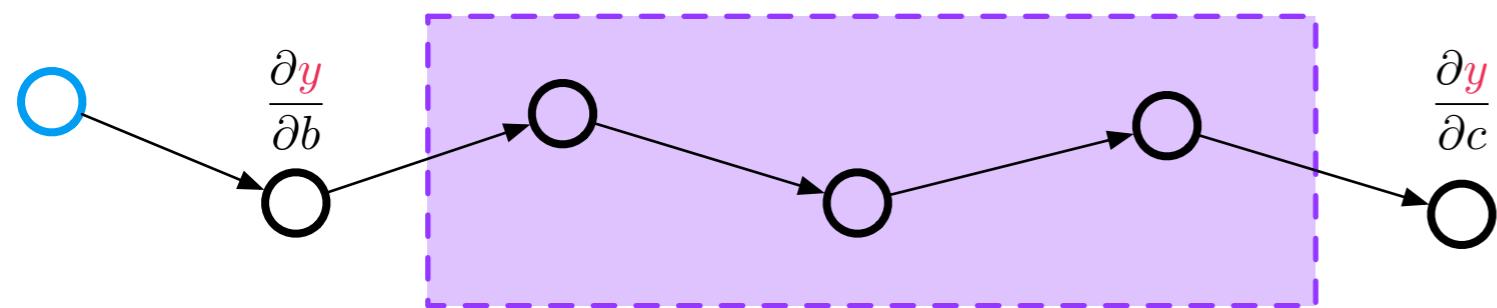
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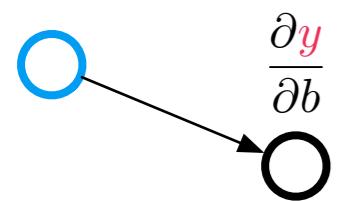
Checkpointing



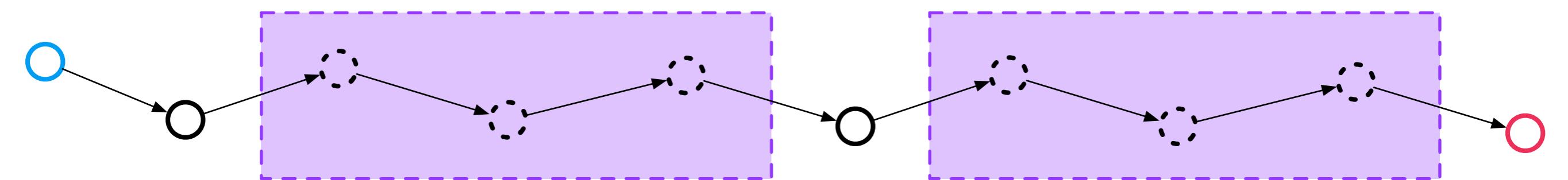
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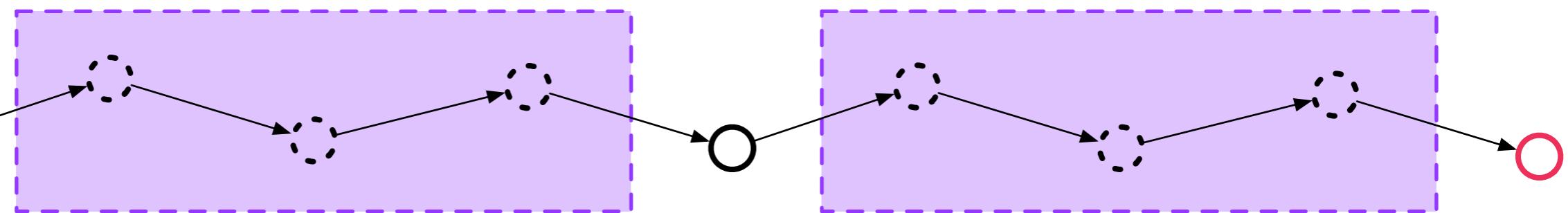
Checkpointing



Checkpointing



Checkpointing



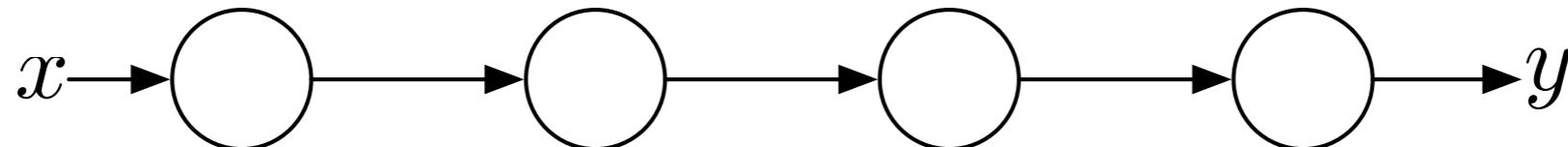
```
def checkpoint(fun):
    """Returns a checkpointed version of 'fun', where intermediate values
    computed during the forward pass of 'fun' are discarded and then recomputed
    for the backward pass. Useful to trade off time and memory."""
    def wrapped_grad(argnum, g, ans, vs, gvs, args, kwargs):
        return make_vjp(fun, argnum)(*args, **kwargs)[0](g)
    wrapped = primitive(fun)
    wrapped.vjp = wrapped_grad
    return wrapped
```

Getting forward from reverse

```
def make_jvp(fun, argnum=0):
    def jvp_maker(*args, **kwargs):
        vjp, y = make_vjp(fun, argnum)(*args, **kwargs)
        vjp_vjp, _ = make_vjp(vjp)(vspace(getval(y)).zeros()) # dummy vals
        return vjp_vjp # vjp_vjp is just jvp by linearity
    return jvp_maker
```

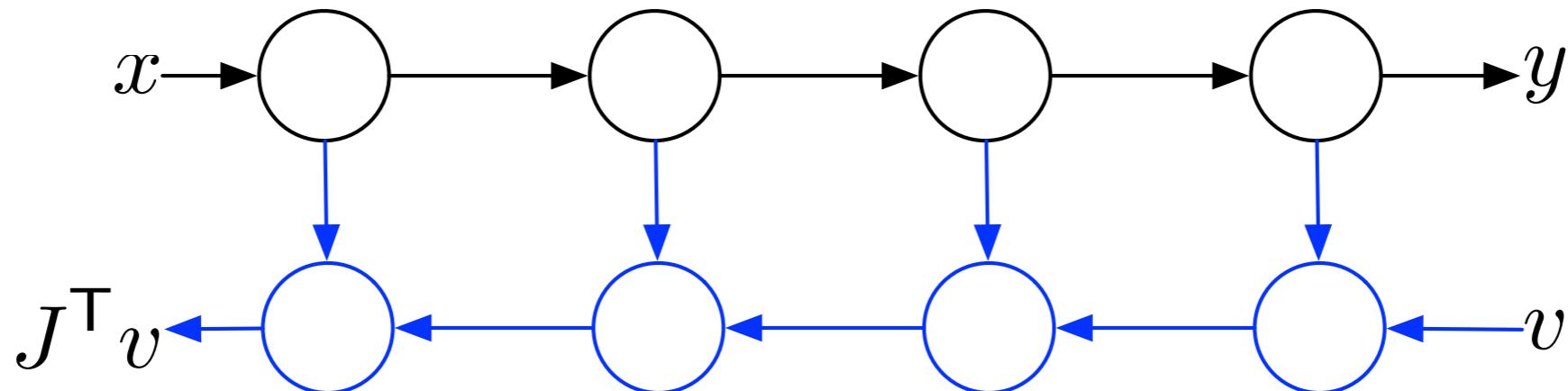
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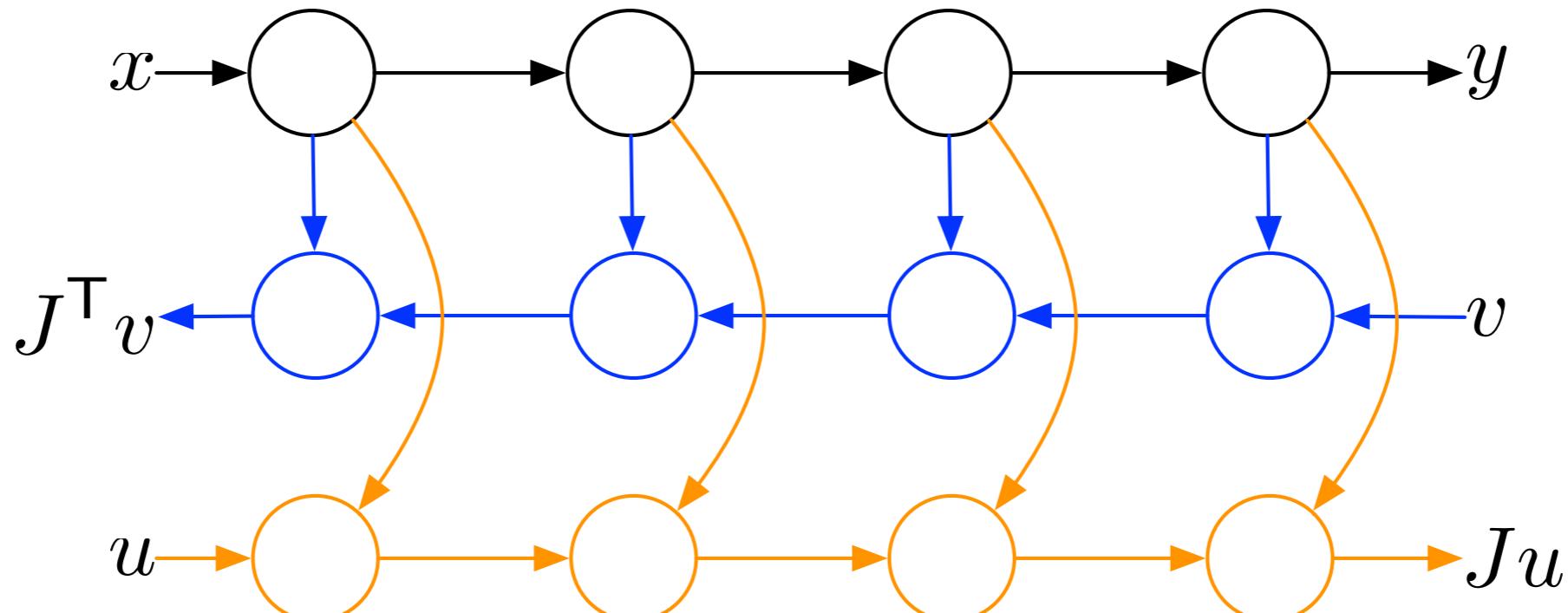
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Getting forward from reverse

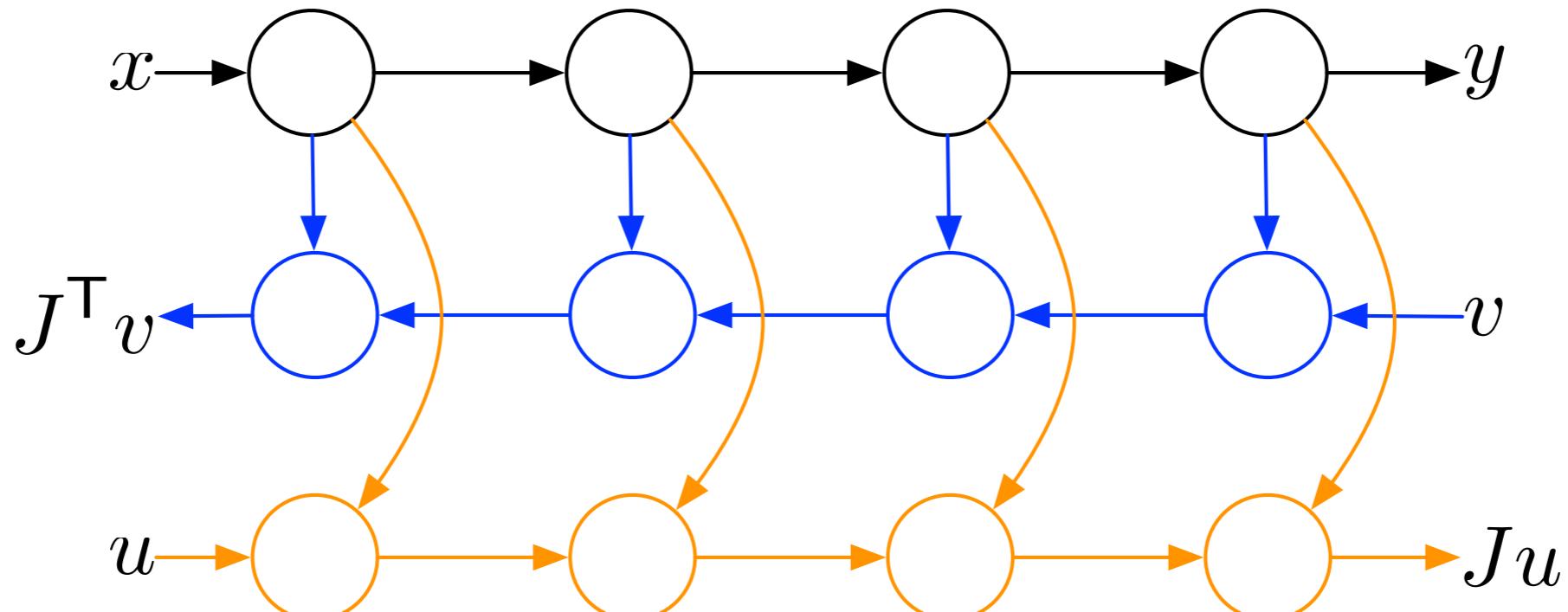
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    return jvp_maker
```



Getting forward from reverse

```
import tensorflow as tf

def fwd_gradients(ys, xs, d_xs):
    v = tf.placeholder(ys.dtype, shape=ys.get_shape()) # dummy variable
    g = tf.gradients(ys, xs, grad_ys=v)
    return tf.gradients(g, v, grad_ys=d_xs)
```



Solutions, optima, and fixed points

Solutions, optima, and fixed points

$$x^*(\textcolor{blue}{a}) = \arg \min_x f(\textcolor{blue}{a}, x)$$

$$\nabla x^*(\textcolor{blue}{a}) = ?$$

Solutions, optima, and fixed points

$$x^*(\textcolor{blue}{a}) = \arg \min_x f(\textcolor{blue}{a}, x)$$

$$\nabla x^*(\textcolor{blue}{a}) = ?$$

solve $g(\textcolor{blue}{a}, x) = 0$ for x

$$g(a, x^*(\textcolor{blue}{a})) = 0$$

$$\nabla x^*(\textcolor{blue}{a}) = ?$$

The implicit function theorem

$$g(a, x^*(\textcolor{blue}{a})) = 0$$

The implicit function theorem

$$g(a, x^*(\textcolor{blue}{a})) = 0$$

$$\nabla_a g(\textcolor{blue}{a}, x^*) + \nabla x^*(\textcolor{blue}{a}) \nabla_x g(\textcolor{blue}{a}, x^*) = 0$$

The implicit function theorem

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The implicit function theorem

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differentiate solutions / optima \leftrightarrow solve linearized systems

The implicit function theorem

$$g(a, x^*(\textcolor{blue}{a})) = 0$$

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$$\nabla x^*(\textcolor{blue}{a}) = -\nabla_a g(\textcolor{blue}{a}, x^*) \nabla_x g(\textcolor{blue}{a}, x^*)^{-1}$$

differentiate solutions / optima \leftrightarrow solve linearized systems

automatically generate a linear solver from the forward solver?

Differentiating fixed points

Differentiating fixed points

$x^*(\textcolor{blue}{a})$ solves $x = f(\textcolor{blue}{a}, x)$ for x

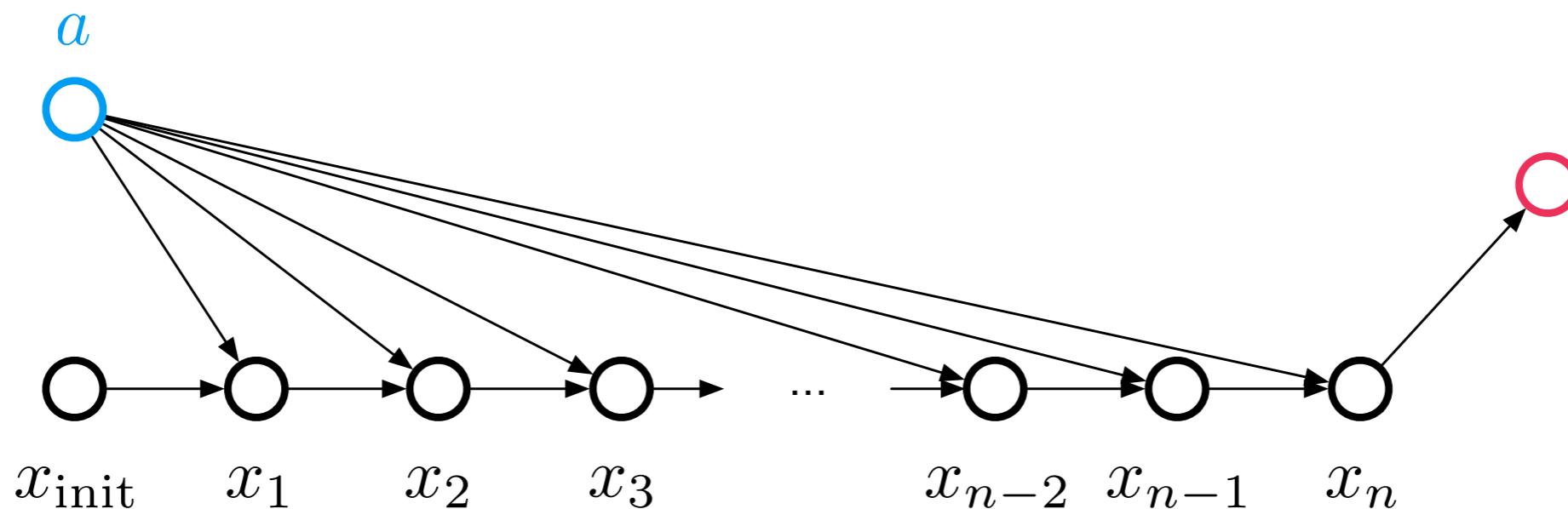
Differentiating fixed points

$x^*(a)$ solves $x = f(a, x)$ for x

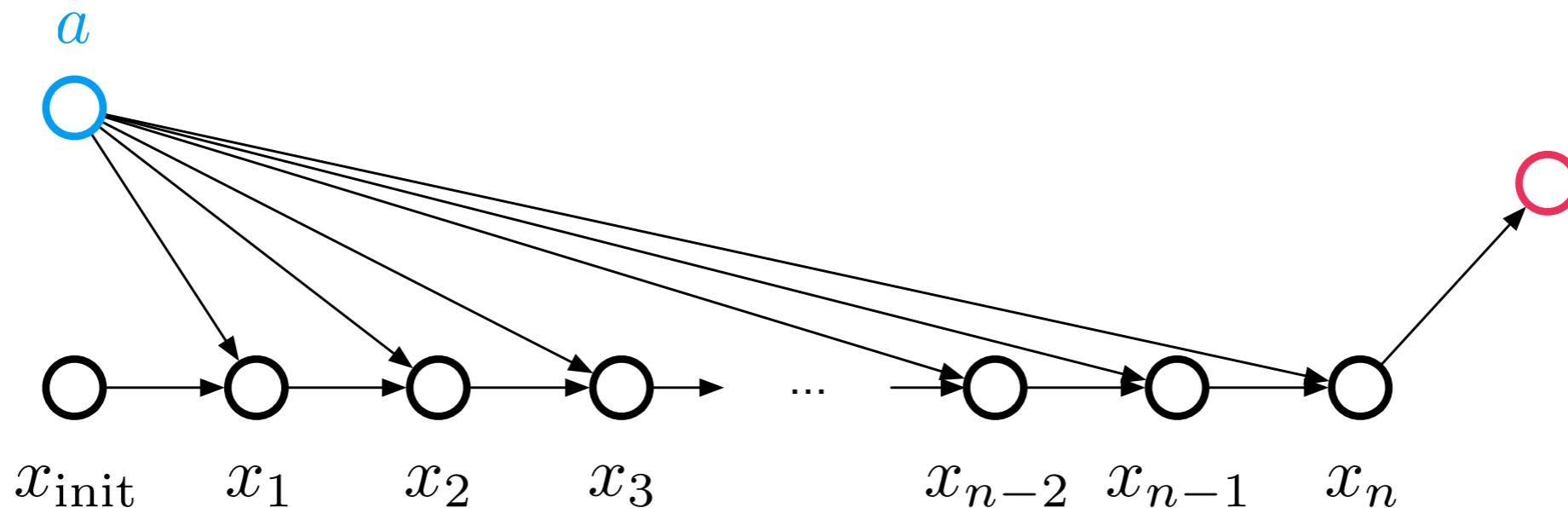
```
from autograd import primitive
from functools import partial

@primitive
def fixed_point(f, a, init, converged, max_iter):
    update = partial(f, a)
    current, prev = update(init), init
    for _ in xrange(max_iter):
        if converged(current, prev): break
        current, prev = update(current), current
    else:
        print 'fixed point iteration limit reached'
    return current
```

Differentiating fixed points



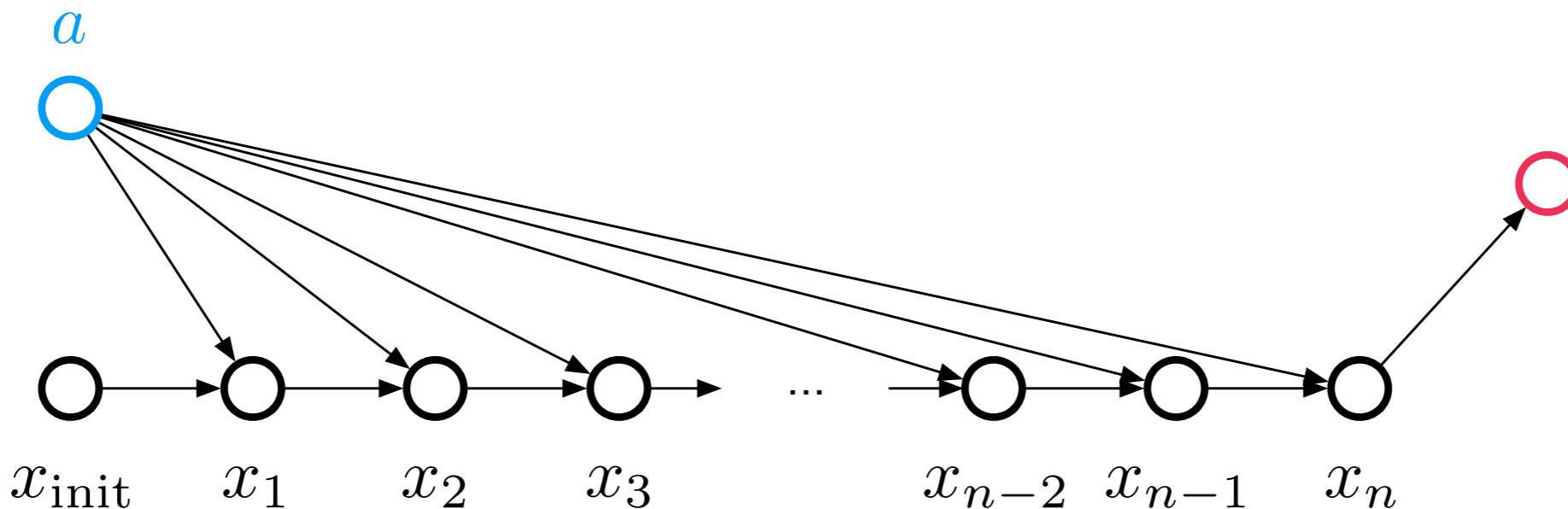
Differentiating fixed points



$$n \rightarrow \infty$$

$$x^* = x_n = x_{n-1} = x_{n-2} = \dots$$

Differentiating fixed points



```
from autograd import primitive, make_vjp, make_tuple
from autograd.util import flatten

def grad_fixed_point(g_fp, fp, vs, gvs, f, a, init, converged, max_iter):
    vjp, _ = make_vjp(lambda args: f(*args))(make_tuple(a, fp))
    g_a_flat, unflatten = flatten(vs.zeros())
    for _ in xrange(max_iter):
        if normsq(flatten(g)[0]) < 1e-6: break
        term, g = vjp(g)
        g_a_flat = g_a_flat + flatten(term)[0]
    else:
        print 'backward fixed point iteration limit reached'
    return unflatten(g_a_flat)
```

Differentiating fixed points

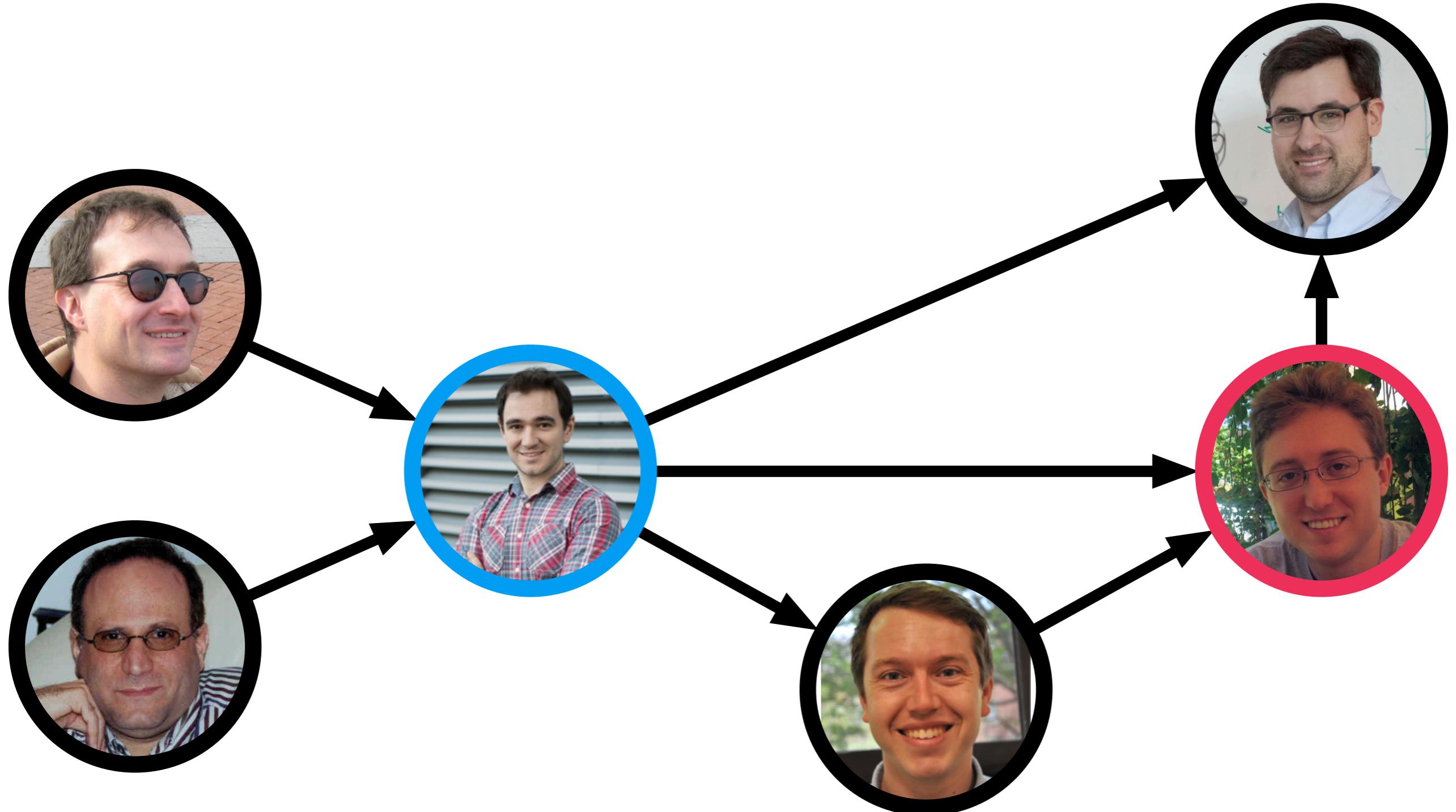
- Inherits structure from forward iteration
 - Forward is Newton \Rightarrow reverse requires only one step
 - Forward is block coordinate descent \Rightarrow reverse is block Gauss-Seidel
- May be preferable to decouple forward and reverse
 - Then choose any linear solver for implicit linearized system
 - Can reuse dual variables from forward solver

Second-order optimization

```
def make_hvp(fun, argnum=0):
    """Builds a function for evaluating the Hessian-vector product at a point,
    which may be useful when evaluating many Hessian-vector products at the same
    point while caching the results of the forward pass."""
    def hvp_maker(*args, **kwargs):
        return make_vjp(grad(fun, argnum), argnum)(*args, **kwargs)[0]
    return hvp_maker

def make_ggnvp(f, g=lambda x: 1./2*np.sum(x**2, axis=-1), f_argnum=0):
    """Builds a function for evaluating generalized-Gauss-Newton-vector products
    at a point. Slightly more expensive than mixed-mode."""
    def ggnvp_maker(*args, **kwargs):
        f_vjp, f_x = make_vjp(f, f_argnum)(*args, **kwargs)
        g_hvp, grad_g_x = make_vjp(grad(g))(f_x)
        f_vjp_vjp, _ = make_vjp(f_vjp)(vspace(getval(grad_g_x)).zeros())
        def ggnvp(v): return f_vjp(g_hvp(f_vjp_vjp(v)))
        return ggnvp
    return ggnvp_maker
```

Thanks!



References

- Dougal Maclaurin. Modeling, Inference and Optimization with Composable Differentiable Procedures. Harvard Physics Ph.D. Thesis, 2016. URL: <https://dougalmaclaurin.com/phd-thesis.pdf>
- github.com/hips/autograd