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Autograd: A cool software trick for avoiding maths

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Why?

Most parameter optimization involves taking gradients

$$f(x) = \frac{1}{x} * \mathrm{e}^{x}$$

$$f'(x) = \frac{e^{x}}{x}\left(1 - \frac{1}{x}\right)$$

```
def f(x):
    return (1/x) * exp(x)

def df(x):
    return (exp(x)/x)*(1-1/x)


y = f(x)
z = df(x)
```

Why?

Most parameter optimization involves taking gradients

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```
def f(x):
    return (1/x) * exp(x)
```

```
def df(x):
    return (exp(x)/x)*(1-1/x)
```

```
df = grad(f) # Autodiff!

y = f(x)
z = df(x)
```

Get away with writing that instead of implementing df(x)

What AutoDiff isn't

Finite differences

- Expensive (Multiple evaluations for each partial derivative)
- Unstable (Involves division of a small number by a small number)

Symbolic differentiation

- Returns actual derivatives, not an expression for them (Mathematica)
- Keeps track of repeated expression evaluation

What AutoDiff is

A source of exact analytical gradients

- Returns actual derivatives

Efficient

- Uses memoization (stores intermediate values for later reuse)

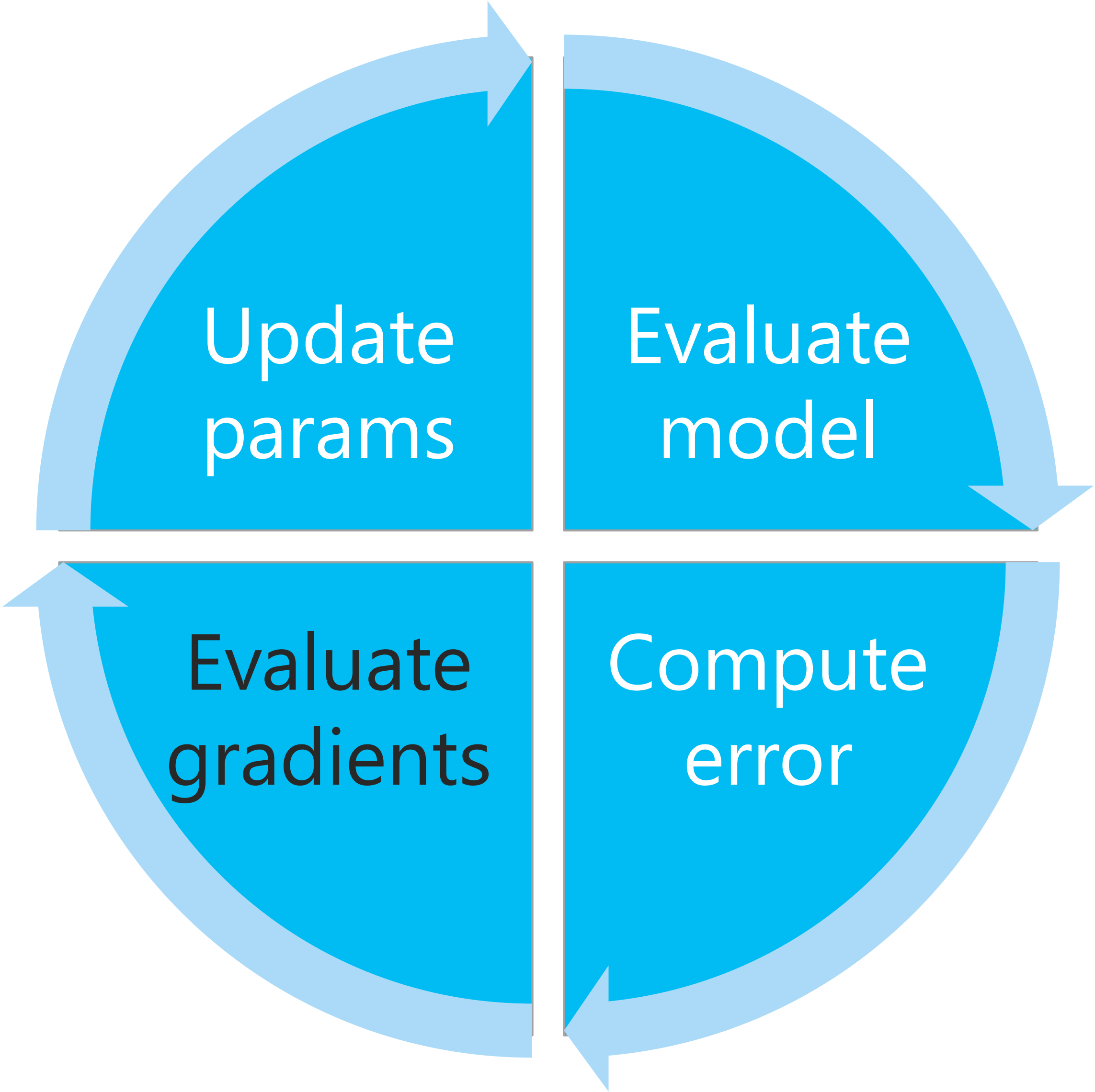
Terminology

Back propagation (Backprop)

- Optimizes model parameters using repeated application of the chain rule of derivatives
- Can be implemented efficiently using reverse-mode differentiation

AutoGrad is a particular AutoDiff package

Optimization using backprop



An example

Given a nested function

$$L = F\Big(G\big(H(x)\big)\Big)$$

Derivative using Chain rule

$$\frac{dL}{dx} = \frac{\partial F}{\partial G} * \frac{\partial G}{\partial H} * \frac{\partial H}{\partial x}$$

$$x \rightarrow \boxed{H} \rightarrow \boxed{G} \rightarrow \boxed{F} \rightarrow L$$

Forward mode

$$dL = \frac{\partial F}{\partial G} * \frac{\partial G}{\partial H} * \frac{\partial H}{\partial x} * dx$$

Output $\longleftarrow$ Input

An example

Given a nested function

$$L = F\Big(G\big(H(x)\big)\Big)$$

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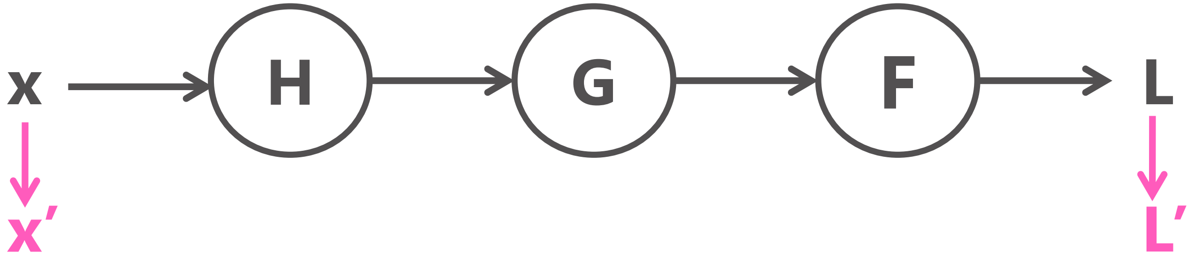


Forward mode

$$dL = \frac{\partial F}{\partial G} * \frac{\partial G}{\partial H} * \frac{\partial H}{\partial x} * dx$$

Output Input

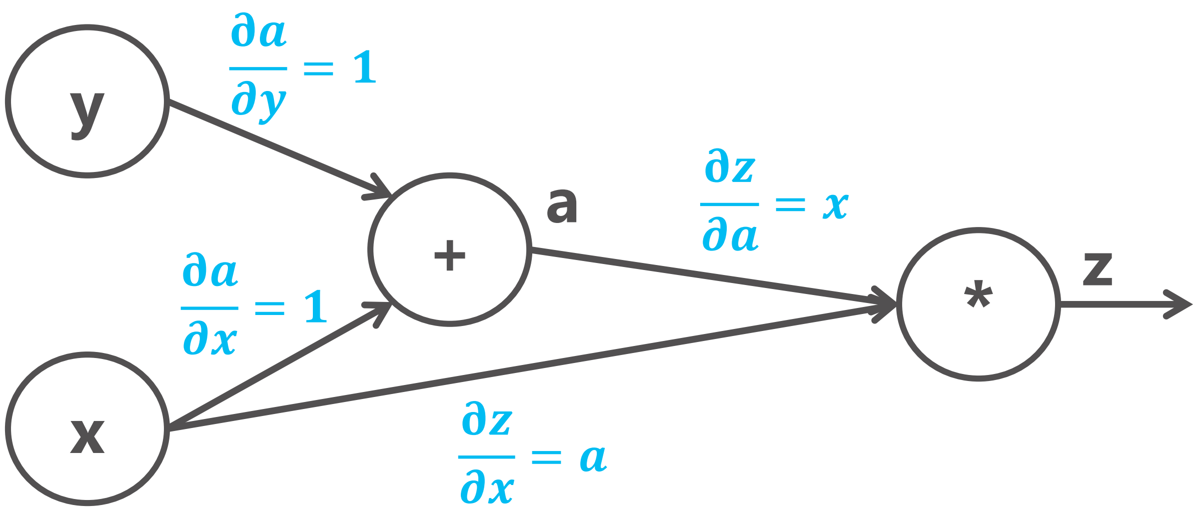
Reverse mode

$$\frac{d}{dx} = \frac{d}{dL} * \frac{\partial F}{\partial G} * \frac{\partial G}{\partial H} * \frac{\partial H}{\partial x}$$

Output Input

Multipath case

$$a(x, y) = x + y$$
$$z(a, x) = a * x$$



Computes derivative of outputs wrt an input

$$\nabla z = \left(\frac{\partial z(x,y,a)}{\partial x} \;,\; \frac{\partial z(x,y,a)}{\partial y} \right)$$

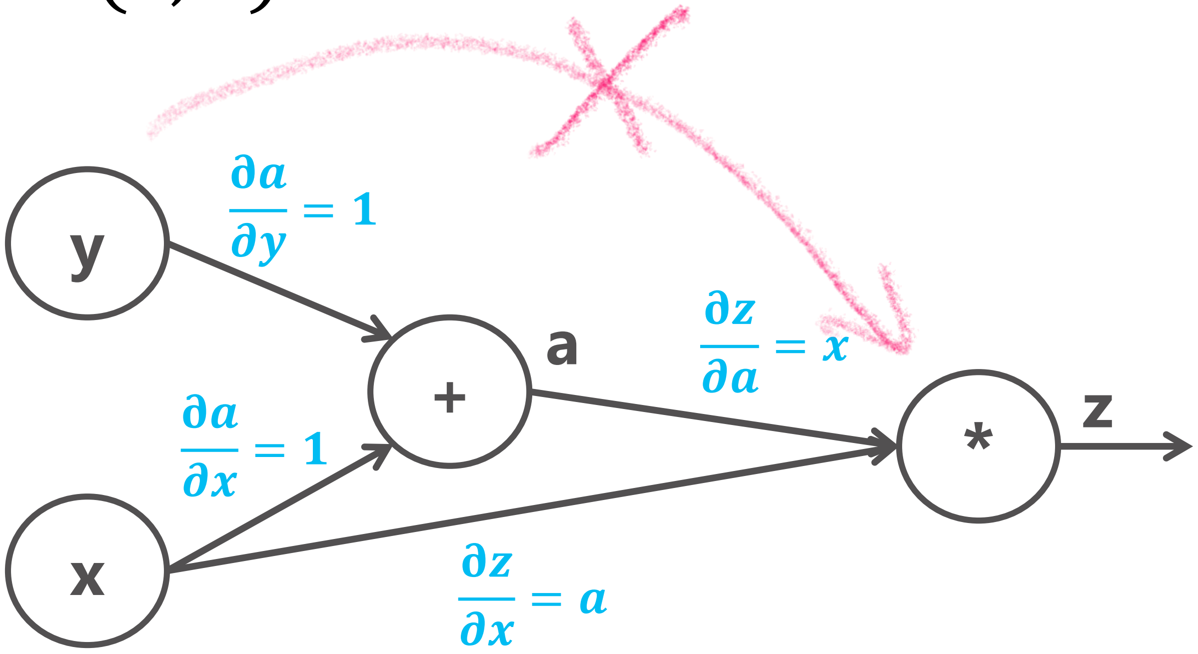
$$\frac{\partial z(x,y,a)}{\partial x} = \frac{\partial z}{\partial x} + \frac{\partial z}{\partial a} * \frac{\partial a}{\partial x}$$

$$\frac{\partial z(x,y,a)}{\partial y} = \frac{\partial z}{\partial y} + \frac{\partial z}{\partial a} * \frac{\partial a}{\partial y}$$

Total derivative rule

Multipath case

$$a(x, y) = x + y$$
$$z(a, x) = a * x$$



Computes derivative of outputs wrt an input

$$\nabla z = \left(\frac{\partial z(x,y,a)}{\partial x} , \frac{\partial z(x,y,a)}{\partial y} \right)$$

$$\frac{\partial z(x,y,a)}{\partial x} = \frac{\partial z}{\partial x} + \frac{\partial z}{\partial a} * \frac{\partial a}{\partial x}$$

$$\frac{\partial z(x,y,a)}{\partial y} = \cancel{\frac{\partial z}{\partial y}} + \frac{\partial z}{\partial a} * \frac{\partial a}{\partial y}$$

Total derivative rule

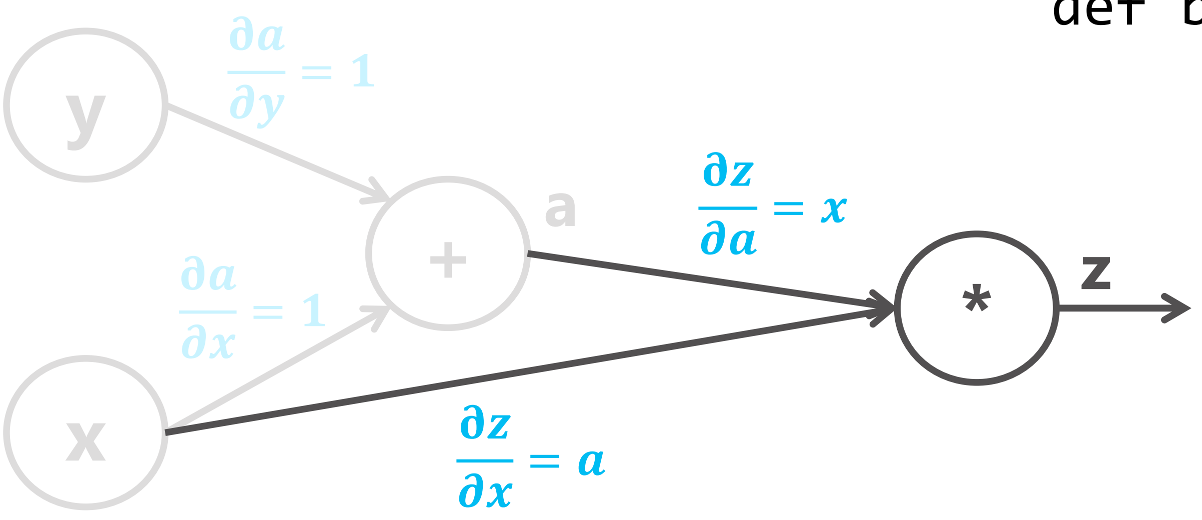
Prod

$$z = a * x$$

```
class ProdNode(object):

    def forward(self, a, x):
        self.x = x    # store a,x for use
        self.a = a    # in backward later
        z = a * x
        return z

    def backward(self, dz):
        da = self.x * dz
        dx1 = self.a * dz
        return da, dx1
```



Memoization needed to access x and avoid recomputing a

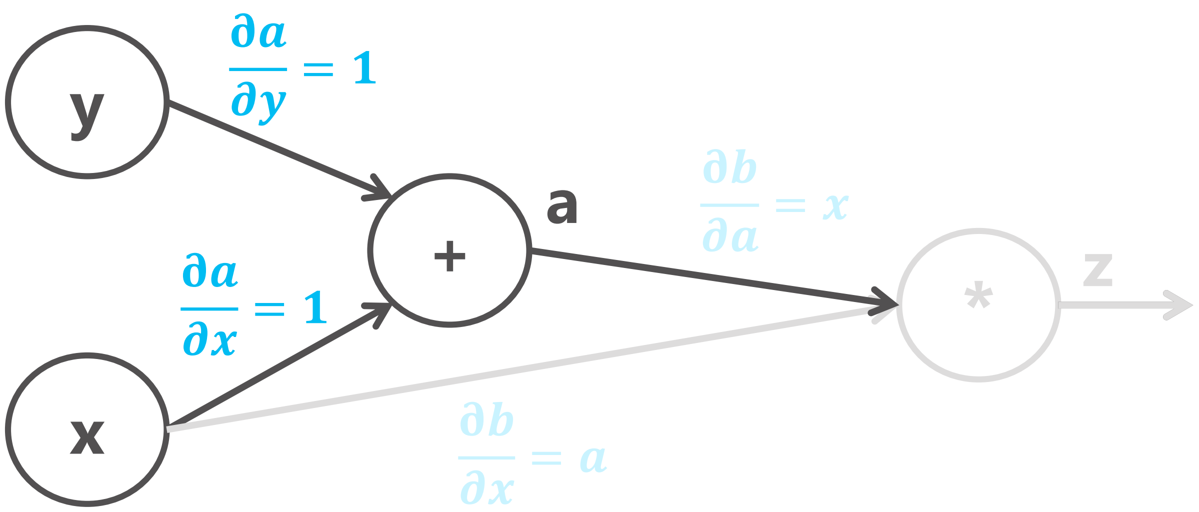
Add

```
class AddNode(object):

    def forward(self, x, y):
        a = x + y
        return a

    def backward(self, da):
        dx2 = 1 * da
        dy = 1 * da
        return dx2, dy
```

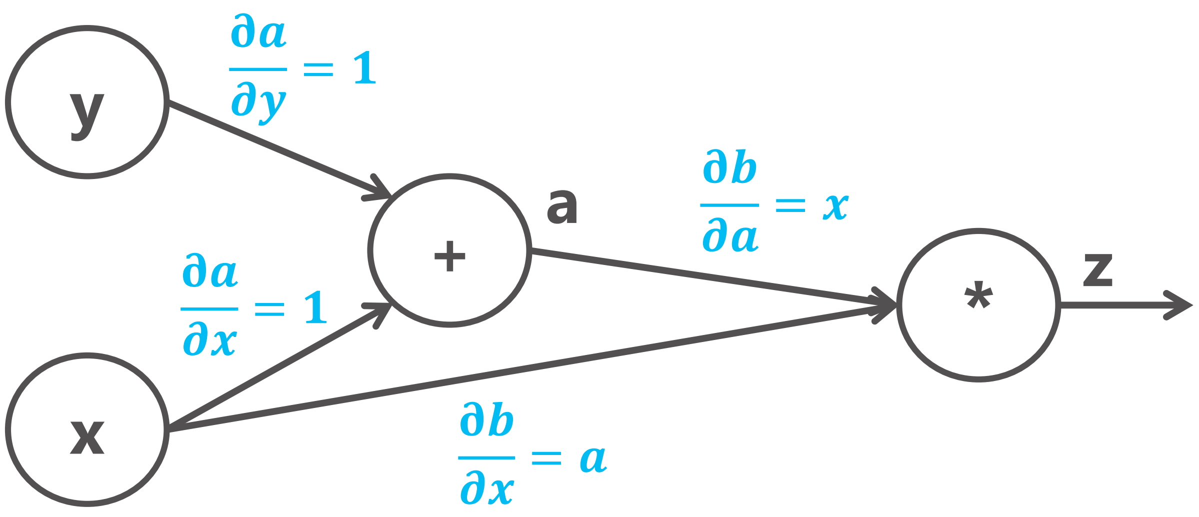
$$a = x + y$$



No memoization needed in this case

Combine

$$a = x + y$$




```
for i in range(num_steps):
    # Evaluate at current params
    a = add.forward(x,y)
    z = prod.forward(a,x)
    dz = z - z_hat
    # Compute param update
    da, dx2 = prod.backward(dz)
    dx1, dy = add.backward(da)
    dx = dx1 + dx2
    # Update params
    x = x - lr*dx
    y = y - lr*dy
```

Autograd package

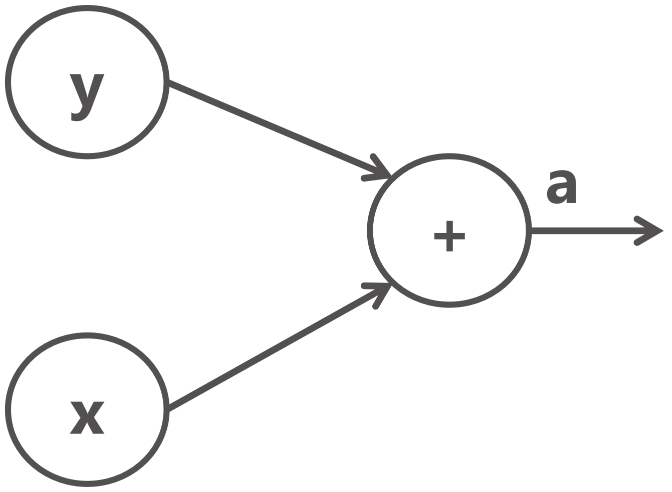
- Lightweight automatic differentiation package that automates the computation of gradients of a function
- Function must be expressed using common python, numpy and scipy primitives (those with .deriv defined)

Alternatives

- AutoDidact, only 200 lines of Python
- PyTorch, JAX: GPU support

Autograd: Simple

$$a = x + y$$



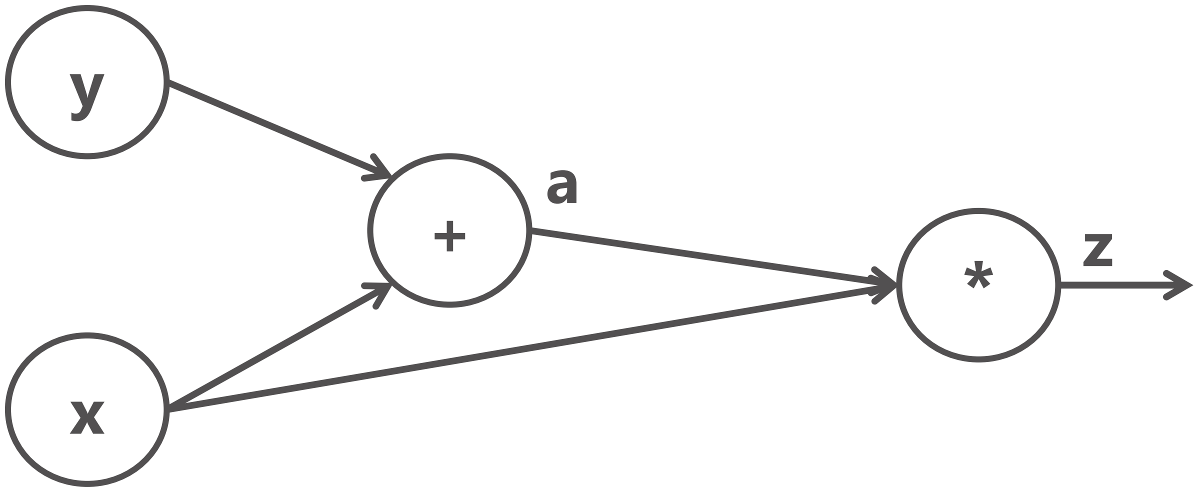

```
from autograd import grad
def add(x, y):
    return x + y

grad_layer = grad(add,(0,1))

for i in range(num_steps):
    # Evaluate at current params
    a = add(x,y)
    da = np.float64(a - a_hat)
    # Compute param update
    grads = grad_add(x,y)
    dx, dy = (g*da for g in grads)
    # Update params
    x = x - lr*dx
    y = y - lr*dy
```

Autograd: Nested

$$a = x + y$$
$$z = x * y$$




```
from autograd import grad
add = lambda x, y: x + y
node = lambda x, y: x * add(x, y)

grad_layer = grad(node,(0,1))

for i in range(num_steps):
    # Evaluate at current params
    z = node(x, y)
    dz = np.float64(z - z_hat)
    # Compute param update
    grads = grad_node(x, y)
    dx, dy = (g*dz for g in grads)
    # Update params
    x = x - lr*dx
    y = y - lr*dy
```

PyTorch

```
# AutoGrad
for i in range(50):
    z = net(x,y)
    dz = np.float64(z - z_hat)
    # assumes dz = 1.0
    # i.e. returns dx/da and dy/da
    # so post-multiply by dz
    grads = grad_net(x,y)
    dx, dy = (g*dz for g in grads)

    x = x - lr*dx
    y = y - lr*dy
```

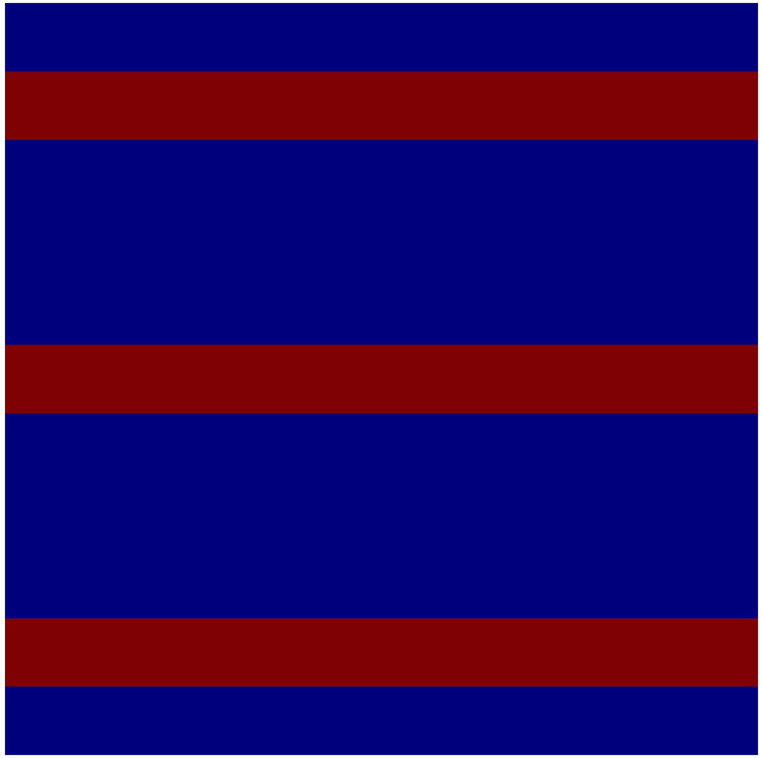
```
# PyTorch
model = Net().to(device)
optimiser = optim.SGD(model.parameters(), lr=lr, momentum=momentum)
model.train()
for i, (data, target) in enumerate(train_loader):
    data, target = data.to(device), target.to(device)
    # sets w.grad = 0 for all params w
    # this step does not affect the computational graph,
    # only changes the values of params w
    optimiser.zero_grad()
    # computational graph is created here, during the fwd pass
    # the computation graph is available through loss.grad_fn
    output = model(data)
    loss = F.nll_loss(output, target)
    # computes dloss/dw for every param w with requires_grad=true
    # the computational graph in loss.grad_fn
    # is used to compute gradients
    loss.backward()
    # updates the value of w using w.grad
    # For SGD, w += -lr * w.grad
    # this step does not affect the computational graph
    optimiser.step()
```

AutoGrad applications

Fluid simulation

Simulates realistic fluid flows by solving Navier-Stokes equations for optimal visual quality

Source: github.com/HIPS/autograd/



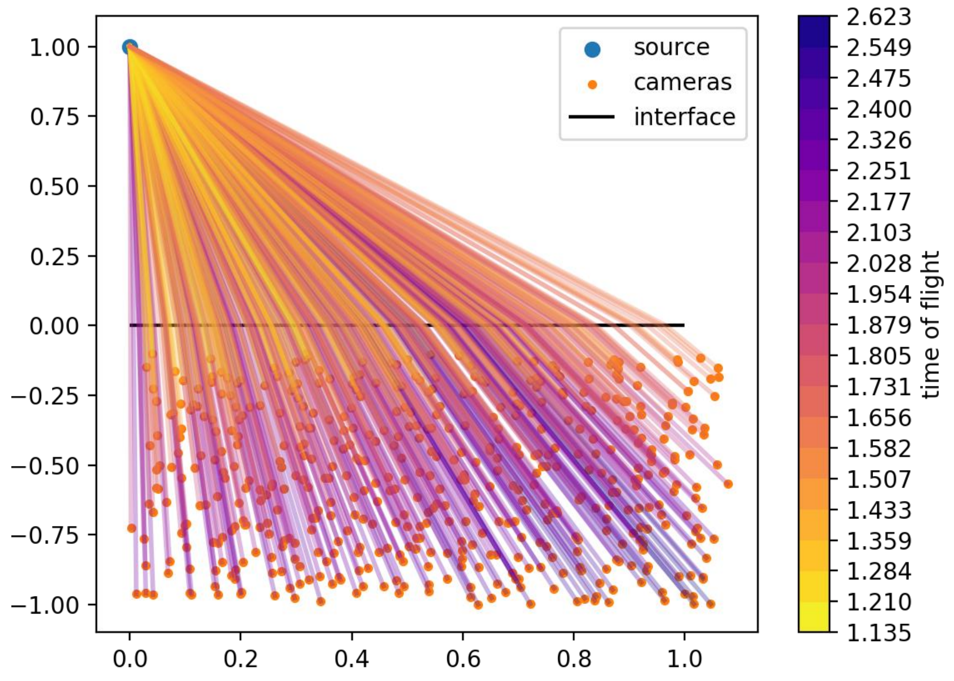
Electromagnetic simulation

Calculates the effect of a single input parameter on simulation output using forward mode

Forward-Mode Differentiation of Maxwell's Equations arXiv:1908.10507 PyPI: ceviche

AutoGrad applications

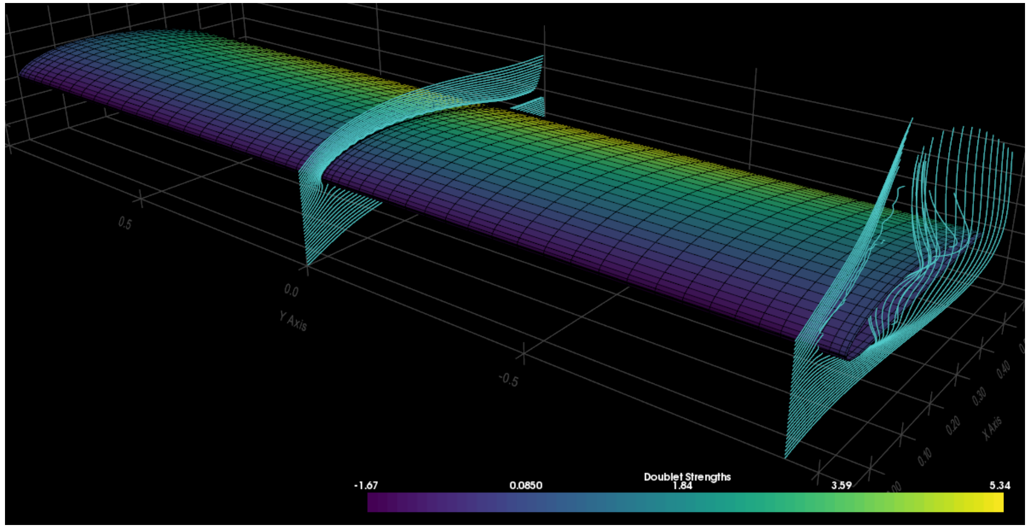
Ray tracing



Finds ray with minimum time of flight

Source: http://flothesof.github.io/ray-tracing-numpy-autograd.html

Aircraft design



Calculates aerodynamic performance & sensitivity wrt large number of design variables

Source: github.com/peterdsharpe/AeroSandbox

Recent advances

- *PyTorch (Python)*
  Direct/Indirect access to AutoGrad, GPU implementation

- JAX (Python)
  AutoGrad with XLA-jit for GPU and TPU

- Message passing (C#)
  Generalization of approximate automatic differentiation
  Useful when functions don't have closed form analytical derivatives

References

1. Autograd https://github.com/HIPS/autograd
2. AutoDidact https://github.com/mattjj/autodidact
   AutoGrad light (200 lines of Python)
3. PyTorch https://pytorch.org/
   AutoGrad + GPU support
4. JAX https://github.com/google/jax
   AutoGrad + GPU/TPU JIT compilation
5. T Minka, From automatic differentiation to message passing
   https://tminka.github.io/papers/acmll2019/ ACMLL 2019
   Approximate automatic differentiation

Code: https://notebooks.azure.com/pashmina-cameron/projects/autodiff