# Automatic Differentiation in PyTorch

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# What is automatic differentiation?

- AD is a higher-order function which either:
  - Accepts a function and returns a second function which gives, when evaluated, the sensitivity at *any location*, $AD : (f) \mapsto f'$
  - Accepts a function and an input to be evaluated, and evaluates the function and its derivative, *at that specific location* $AD : (f, x) \mapsto (f(x), f'(x))$
- These two views correspond to static and dynamic AD
  - For mathematical expressions, the static approach is preferred
  - For computer programs, the dynamic approach is preferred

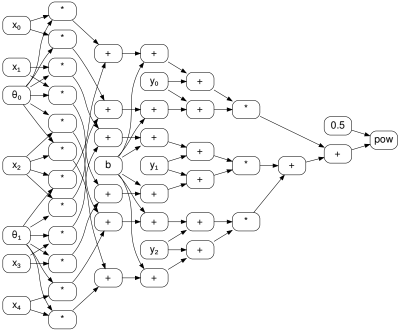
# Static and Dynamic Representations

Programs are dynamical systems, graphs are static objects.

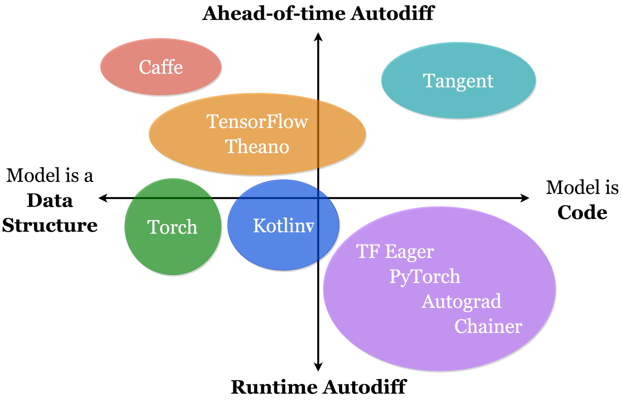
**Program**

```
sum = 0
l = [0, 0, 0, 0]
for i in range(0, 4):
  l[i] += t[i] * x[i]
for i in range(0, 4):
  l[i] -= y[i] - b
for i in range(0, 4):
  l[i] *= l[i]
for i in range(0, 4):
  sum += l[i]
l = sqrt(sum)
```

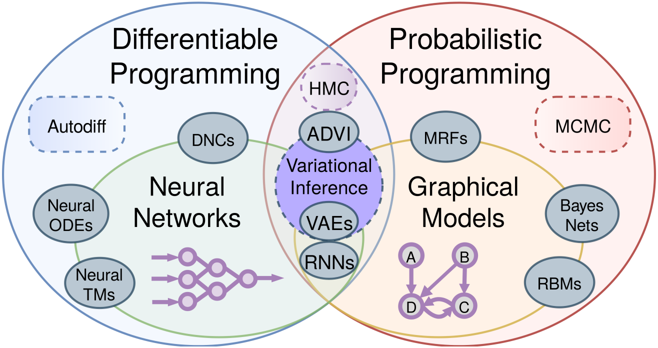
**Computation Graph**



# Dimensions of AD frameworks



# What is a differentiable program?



# What is a derivative?

To understand AD, you just need to remember two simple rules:

$$
\begin{aligned}
D(f + g) &= D(f) + D(g) \\
D(f \cdot g) &= D(f) \cdot g + f \cdot D(g)
\end{aligned}
$$

The derivative is a *linear map* between function spaces.

$$
\begin{aligned}
D(f + g) &= D(f) + D(g) \\
\alpha D(f) &= D(\alpha f)
\end{aligned}
$$

# Picrograd / PyTorch in a single slide

```
class Var:
  def __init__(self, val, grad_fn=lambda: []):
    self.v, self.grad_fn = val, grad_fn

  def __add__(self, other):
    return Var(self.v + other.v,
      lambda: [(self, 1.0), (other, 1.0)])

  def __mul__(self, other):
    return Var(self.v * other.v,
      lambda: [(self, other.v), (other, self.v)])

  def grad(self, bp = 1.0, dict = {}):
    dict[self] = dict.get(self, 0) + bp
    for input, val in self.grad_fn():
        input.grad(val * bp, dict)
    return dict
```

# Higher-order and higher-rank AD

The *gradient*, $\nabla : (\mathbb{R}^m \to \mathbb{R}) \to \mathbb{R}^m$ maps a function $Q$ to:

$$\nabla Q(q_1, \ldots, q_m) = \left[\frac{\partial Q}{\partial q_1}, \ldots, \frac{\partial Q}{\partial q_m}\right]$$

The *Jacobian*, $\mathcal{J} : (\mathbb{R}^m \to \mathbb{R}^n) \to \mathbb{R}^{n \times m}$ is a matrix of partials:

$$\mathcal{J} \circ \mathbf{f} = \begin{bmatrix} \frac{\partial \mathbf{f}}{\partial x_1} & \cdots & \frac{\partial \mathbf{f}}{\partial x_m} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \cdots & \frac{\partial f_n}{\partial x_m} \end{bmatrix} = \begin{bmatrix} \nabla f_1 \\ \vdots \\ \nabla f_m \end{bmatrix}$$

# Higher-order chains

Suppose we have a function $P(X) = p_k \circ p_{k-1} \circ \cdots \circ p_1 \circ X$. The derivative of a linear composition can be expressed as a product:

$$\frac{dP}{dp_1} = \frac{dp_k}{dp_{k-1}} \frac{dp_{k-1}}{dp_{k-2}} \dots \frac{dp_2}{dp_1} = \prod_{i=1}^{k-1} \frac{dp_{i+1}}{dp_i}$$

This also holds in higher dimensions, for example $\mathbf{P}_k : \mathbb{R}^m \to \mathbb{R}^n$:

$$\mathcal{J}\mathbf{P_k} = \prod_{i=1}^{k} \mathcal{J}p_i = \underbrace{\Big(\Big((\mathcal{J}p_k \mathcal{J}p_{k-1}) \dots \mathcal{J}p_2\Big)\mathcal{J}p_1\Big)}_{\textit{Reverse mode, VJP, Pullback}}$$
$$= \underbrace{\Big(\mathcal{J}p_k\Big(\mathcal{J}p_{k-1} \dots (\mathcal{J}p_2 \mathcal{J}p_1)\Big)\Big)}_{\textit{Forward mode, JVP, Pushforward}}$$

# Gradients in PyTorch

Suppose we have a scalar-valued vector function, $f : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$. `grad` is a function that takes $f$ and a tuple of input variables, and returns their gradients as a tuple.

```
x = torch.randn(2, requires_grad=True)
t = torch.tensor([2., 3.], requires_grad=True)
y = torch.randn(2)
f = sum((x*t - y)**2)**0.5

torch.autograd.grad(f, inputs=(x, t))
```

```
(tensor([-0.60,  2.85]), tensor([0.23, 1.47]))
```

# What is a vectorizing map? (vmap)

Suppose we have a scalar-valued function, $f : \mathbb{R} \to \mathbb{R}$. `vmap` is a function which takes $f$ and returns a function $g : \mathbb{R}^* \to \mathbb{R}^*$ that accepts a tensor $t : \mathbb{R}^*$, and maps $f$ over the tensor, elementwise.

---

```
function = lambda x: x**2 + x
tensor = torch.ones(3, 3, 3) * 2
vmap(function)(tensor)
```

---

```
torch.dot                   # [   D   ],[   D   ] ->    S
vd = vmap(torch.dot)        # [ N,D ],[ N,D ] -> [ N ]
vvd = vmap(vd)              # [N,D,C],[N,D,C] -> [N,D]
x, y = torch.ones(3, 2, 5), torch.ones(3, 2, 5)
vvd(x, y)
```

# Jacobians in PyTorch

```
def jacobian(fun, x) -> torch.Tensor:
  x = x.detach().requires_grad_()
  y = fun(x)
  vjp = lambda v: torch.autograd.grad(y, x, v)[0]
  vs = torch.eye(y.numel())\
          .view(y.numel(), *y.shape)
  result = vmap(vjp)(vs)
  return result.detach()

f = lambda x: x ** 3
jacobian(f, torch.ones(3))
```

---

```
tensor([[3., 0., 0.],
        [0., 3., 0.],
        [0., 0., 3.]])
```

# Higher-order and higher-rank AD

The *Hessian* $\mathbf{H} : (\mathbb{R}^m \to \mathbb{R}) \to \mathbb{R}^{m\times m}$ maps scalar functions to $\partial^2$:

$$\mathbf{H}(Q) = \begin{bmatrix} \frac{\partial^2 Q}{\partial x_1^2} & \frac{\partial^2 Q}{\partial x_1\,\partial x_2} & \cdots & \frac{\partial^2 Q}{\partial x_1\,\partial x_m} \\ \frac{\partial^2 Q}{\partial x_2\,\partial x_1} & \frac{\partial^2 Q}{\partial x_2^2} & \cdots & \frac{\partial^2 Q}{\partial x_2\,\partial x_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 Q}{\partial x_m\,\partial x_1} & \frac{\partial^2 Q}{\partial x_m\,\partial x_2} & \cdots & \frac{\partial^2 Q}{\partial x_m^2} \end{bmatrix}$$

The Hessian and Jacobian are related by $\mathbf{H}(Q)^\top = \mathcal{J} \circ \nabla Q$.

# Hessians in PyTorch

```
def hessian(fun, x) -> torch.Tensor:
    def grad0(x: torch.Tensor):
        y = fun(x)
        assert y.dim() == 0
        return torch.autograd.grad(y, x,
           create_graph=True)[0]
    return jacobian(grad0, x)

g = lambda x: (x ** 3).sum()
hessian(g, torch.ones(3))
```

---

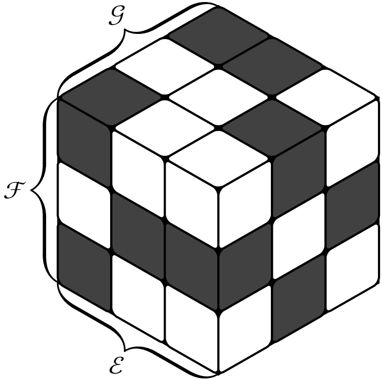
```
tensor([[6., 0., 0.],
        [0., 6., 0.],
        [0., 0., 6.]])
```

# What is a tensor?

**Rank-2**

$$\begin{bmatrix} 1 & 0 & \cdots & 1 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & \cdots & 1 \end{bmatrix}$$

**Rank-3**



# Checking matrix multiplication

Suppose we have two tensors, $A : \mathbb{R}^{x \times y \times \cdots}$ and $B : \mathbb{R}^{y \times z \times \cdots}$
Then `C = A @ B` has type $C : \mathbb{R}^{x \times z \times \cdots}$. For example:

```
state = torch.ones(9, 5, names=('batch', 'D'))
trans = torch.randn(5, 5, names=('in', 'out'))
next_state = state @ trans
print(next_state.names)
```

```
('batch', 'out')
```

# Runtime type checking: name mismatch

What happens if we try to sum dimensions with different names?

---

```
x = torch.ones(3, names=('X',))
y = torch.ones(3, names=('Z',))
z = x + y
```

---

```
----RuntimeError
Traceback (most recent call last)[...]
      2 x = torch.ones(3, names=('X',))
      3 y = torch.ones(3, names=('Y',))
----> 4 xpz = x + z
RuntimeError: Error attempting to broadcast
dims ['X'] and dims ['Y']: dim 'X' and dim 'Y'
are at the same position from the right
```

# Tips for Parallelism: Vectorization

- Stateful computation extremely difficult to parallelize
- Sequentiality is the essence of parallelism
- If necessary to use CPU, use `torch.multiprocessing`
- Use vectorization where possible, e.g. `vmap`, `pmap`

# Parallelism Tips: Loading data incrementally

- Loading the entire dataset into memory generally undesirable
- Start by timing. How long does it take to load a batch?
- Need to keep the GPU busy to maximize throughput
- When in doubt, check utilization `nvidia-smi`, `nvtop`

```
X, Y = torch.load('training.pt')
```
✗

---

```
ts = Dataset(partition['train'], labels)
tg = torch.utils.data.DataLoader(ts, ...)
```
✓

# References

- `torch.vmap` documentation
- Named Tensor Notation
- Introduction to Named Tensors in PyTorch
- PyTorch Data Loading Tutorial
- Model parallel best practices