Introduction to PyTorch

Antoine Prouvost

NEXT Ai
a NEXT Canada program

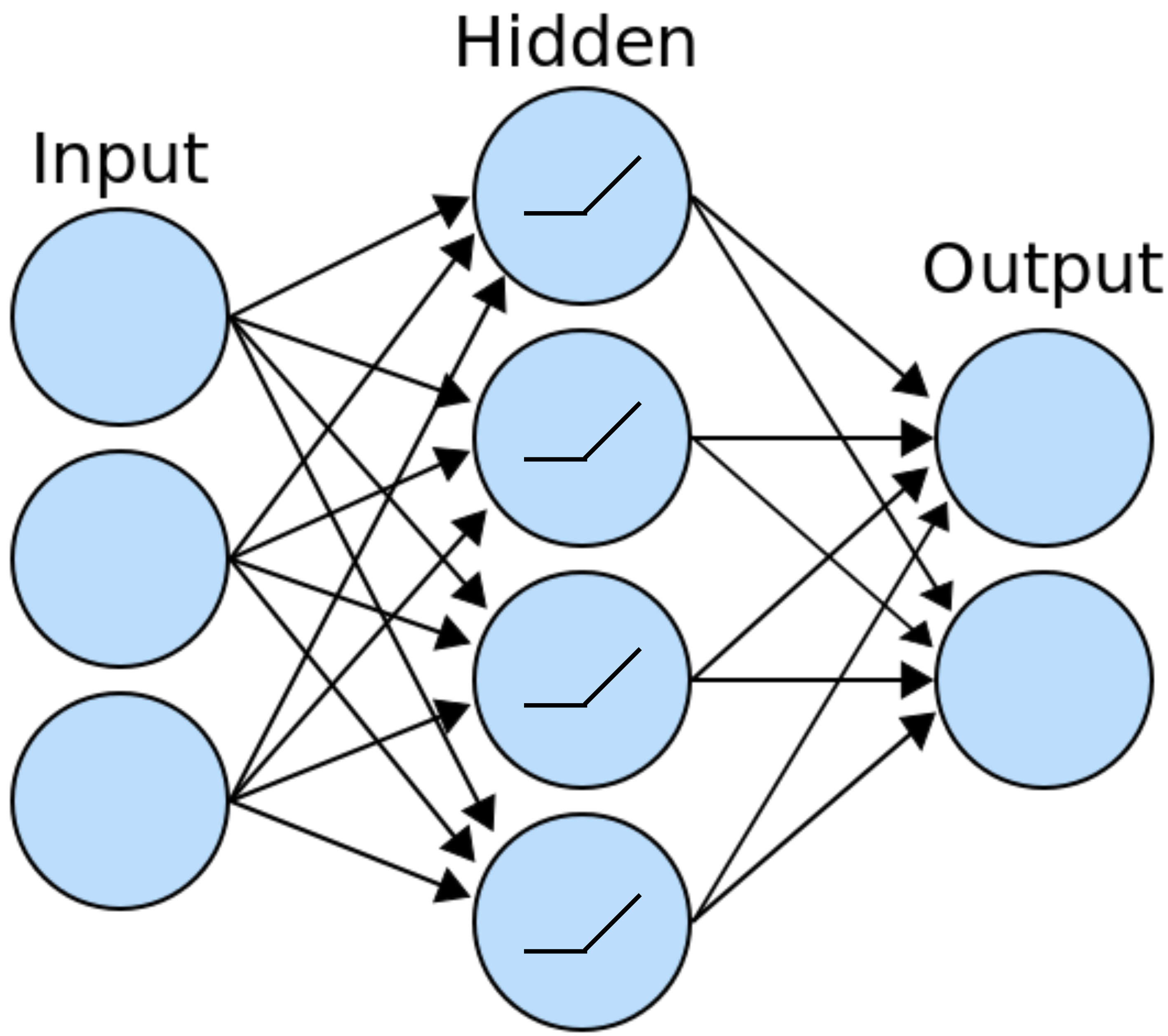
4th of March 2019

CANADA EXCELLENCE RESEARCH CHAIR
DATA SCIENCE FOR REAL-TIME DECISION-MAKING

Mila

POLYTECHNIQUE MONTRÉAL
WORLD-CLASS ENGINEERING

Neural Network



Supervised Learning

$$\min_{\theta} \quad \mathbb{E}\left[\ell(f_\theta(X), Y)\right]$$

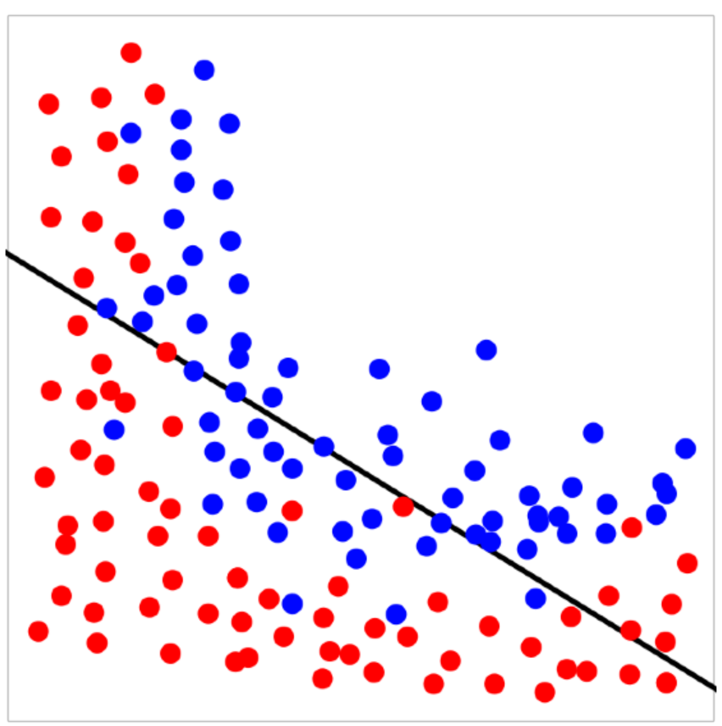
- Expectation over unseen examples
- ℓ is the loss function
- f_θ is the predictor (neural network) with parameters θ
- (X, Y) are random input/target variables

Training objective

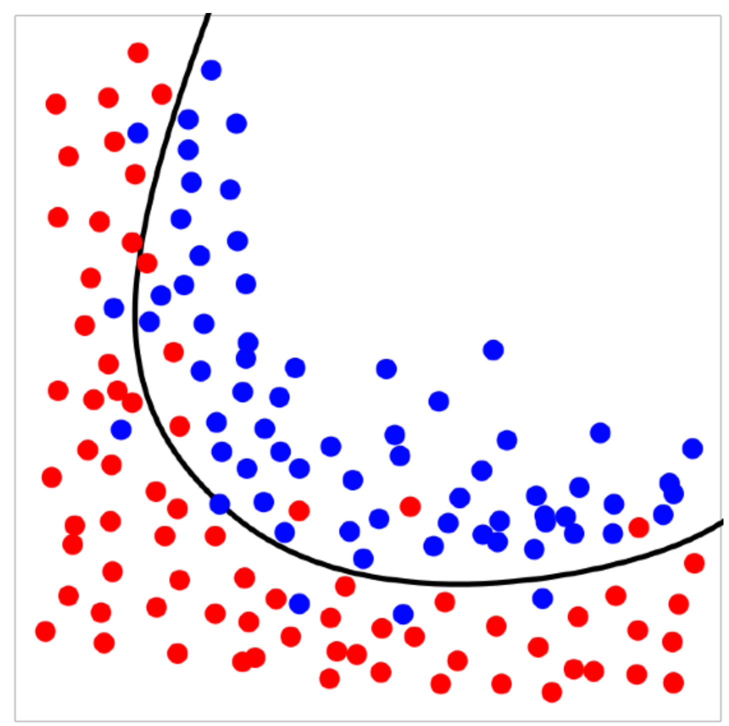
$$\min_{\theta} \quad \mathscr{L}(\theta) = \frac{1}{N} \sum_{i=1}^{N} \ell(f_\theta(x_i), y_i)$$

- N examples in the training set
- ℓ is the loss function (problem specific, *e.g.* MSE)
- f_θ is the predictor (neural network) with parameters θ
- (x_i, y_i) are the training examples

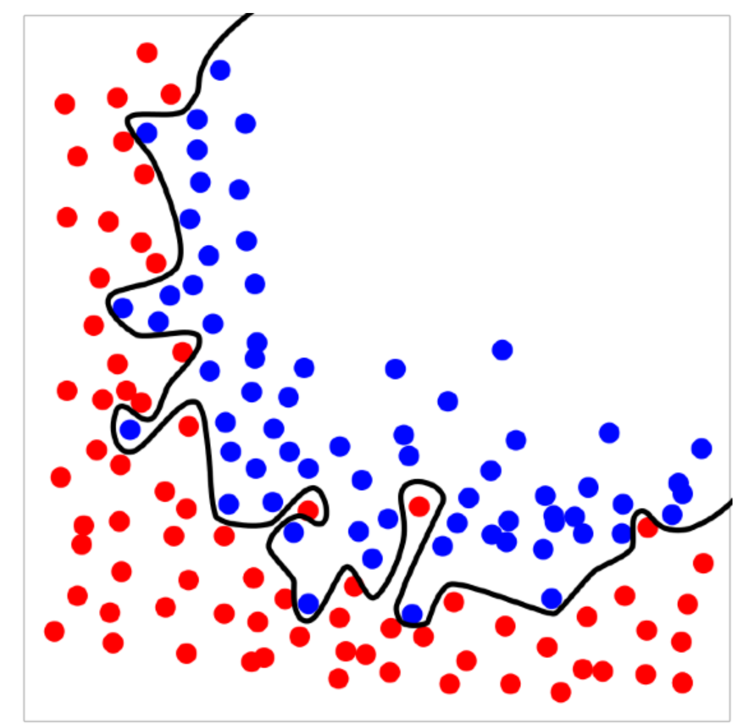
Goodness of Fit



Underfit

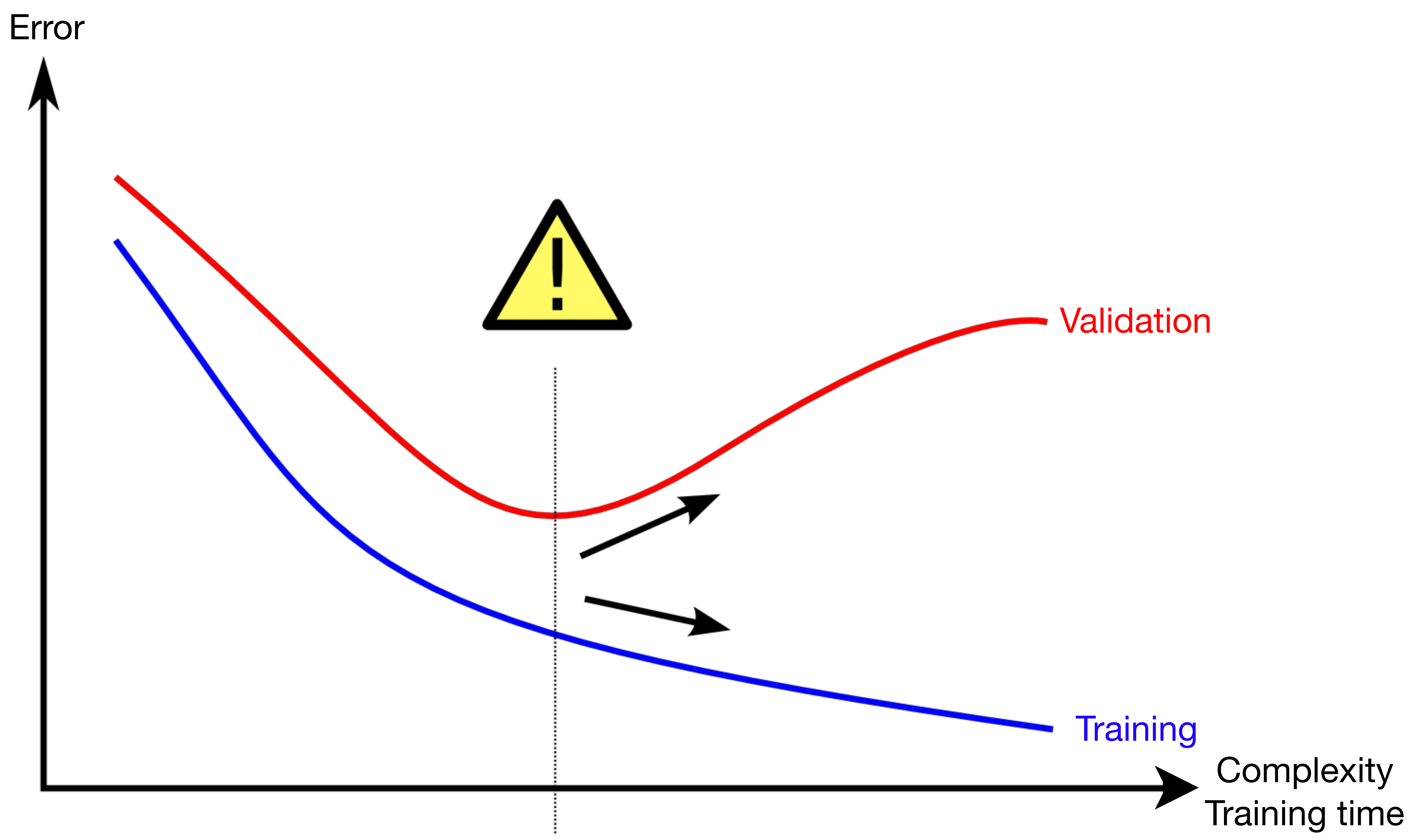


Good fit



Overfit

Goodness of Fit



Data Layout

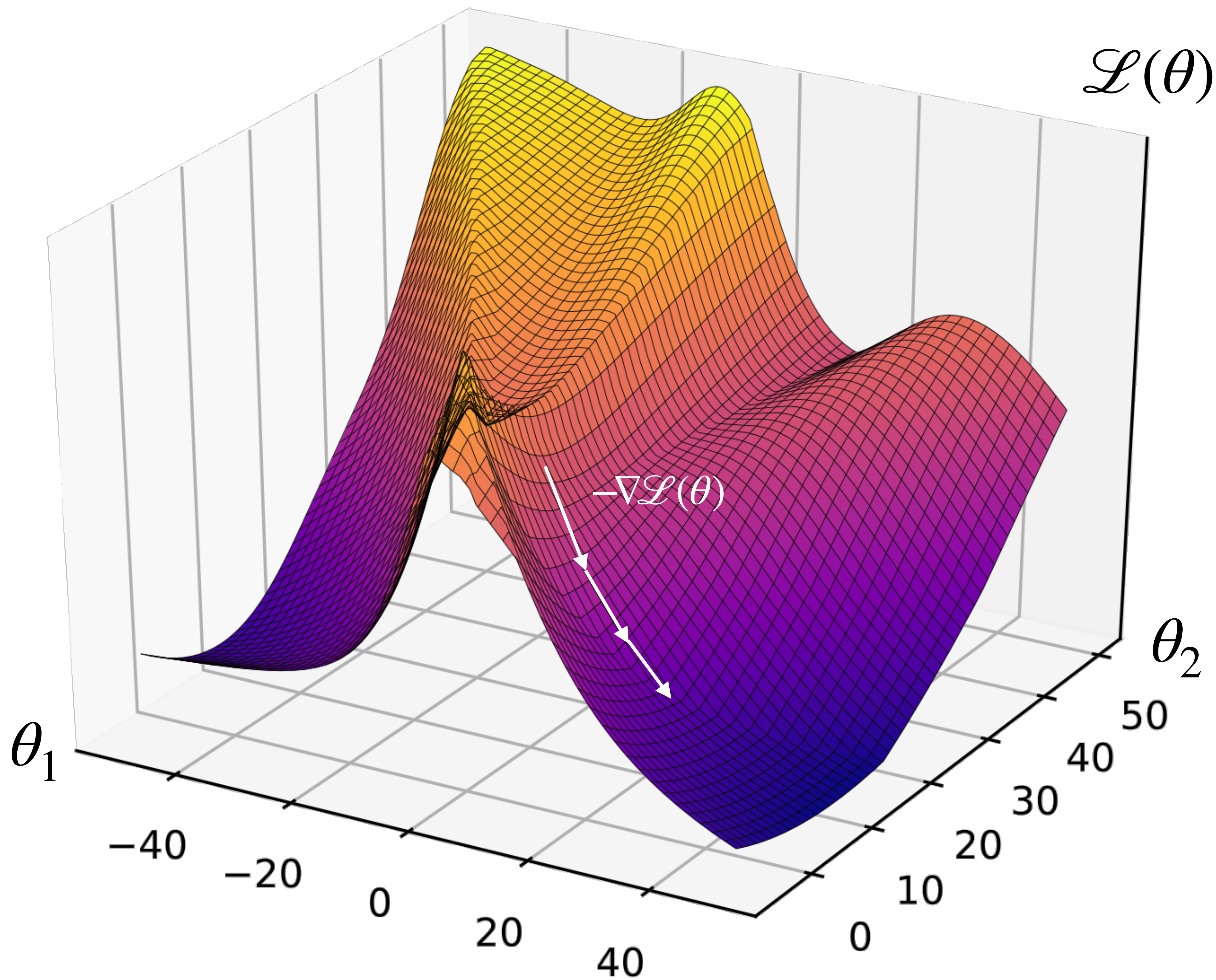
k^{th} feature

i^{th} example

```
tensor([[0.6376, 0.9057, 0.6846, 0.7117, 0.8487, 0.0744, 0.9518],
        [0.2923, 0.7165, 0.1973, 0.2397, 0.5771, 0.5638, 0.9993],
        [0.2369, 0.9512, 0.7222, 0.2426, 0.1483, 0.6278, 0.7791],
        [0.2237, 0.5489, 0.9370, 0.8457, 0.9986, 0.7233, 0.7889],
        [0.8468, 0.2340, 0.0911, 0.4262, 0.1687, 0.6305, 0.7508],
        [0.3378, 0.1670, 0.3443, 0.0444, 0.2323, 0.8563, 0.0130],
        [0.5080, 0.7051, 0.8770, 0.3361, 0.6279, 0.9214, 0.7670],
        [0.5072, 0.1404, 0.3881, 0.9701, 0.6215, 0.1271, 0.5980],
        [0.6257, 0.4641, 0.3438, 0.8921, 0.8798, 0.0657, 0.1461],
        [0.9679, 0.6459, 0.8980, 0.2363, 0.9688, 0.4283, 0.2100],
        [0.4895, 0.4566, 0.3123, 0.2635, 0.5453, 0.0066, 0.5287],
        [0.1535, 0.0807, 0.5558, 0.9945, 0.2332, 0.8090, 0.1357],
        [0.7637, 0.5319, 0.8635, 0.8072, 0.5585, 0.1226, 0.3948],
        [0.5267, 0.1512, 0.0959, 0.0583, 0.1057, 0.5622, 0.5102],
        [0.3715, 0.4426, 0.4319, 0.9708, 0.4003, 0.6172, 0.8253],
        [0.5909, 0.8879, 0.1540, 0.9327, 0.9577, 0.8344, 0.8575],
        [0.4352, 0.2752, 0.2222, 0.6507, 0.8302, 0.9882, 0.1323],
        [0.3817, 0.9683, 0.0256, 0.8480, 0.9195, 0.5951, 0.1267],
        [0.9772, 0.1110, 0.4525, 0.2388, 0.3032, 0.4890, 0.2888],
        [0.1775, 0.7266, 0.9099, 0.8389, 0.5672, 0.2913, 0.8584],
        [0.2952, 0.0455, 0.5989, 0.9106, 0.6178, 0.6184, 0.6094],
        [0.2643, 0.0340, 0.7447, 0.2637, 0.2932, 0.7452, 0.6972],
        [0.7966, 0.0639, 0.8146, 0.7864, 0.0794, 0.7675, 0.1843],
        [0.7056, 0.3377, 0.9615, 0.6633, 0.0111, 0.3464, 0.8024],
        [0.7954, 0.2537, 0.7292, 0.9774, 0.9494, 0.5149, 0.1547],
        [0.0217, 0.0160, 0.0199, 0.2547, 0.5276, 0.8306, 0.3736],
        [0.2487, 0.7770, 0.7682, 0.0269, 0.9355, 0.1020, 0.3830],
        [0.8083, 0.5732, 0.6287, 0.1231, 0.1675, 0.4726, 0.3766],
        [0.1188, 0.6217, 0.7025, 0.4512, 0.1456, 0.7578, 0.8339],
        [0.1987, 0.6446, 0.3461, 0.8246, 0.7431, 0.9381, 0.0073],
        [0.2910, 0.9862, 0.8221, 0.2347, 0.2430, 0.3811, 0.2865],
        [0.3573, 0.9250, 0.0106, 0.6855, 0.7090, 0.5050, 0.6747],
        [0.3651, 0.5485, 0.5214, 0.4207, 0.1140, 0.3645, 0.1332],
        [0.4607, 0.0735, 0.3656, 0.2844, 0.7690, 0.8687, 0.8679],
```

Data Layout

Gradient Descent



Gradient Descent

$$\theta \leftarrow \theta - \lambda \nabla \mathscr{L}(\theta)$$

- θ parameters of the models (weights)
- $\nabla \mathscr{L}(\theta)$ gradient of the loss with regard to the parameters
- λ learning rate

Stochastic Gradient

```
tensor([[0.6376, 0.9057, 0.6846, 0.7117, 0.8487, 0.0744, 0.9518],
        [0.2923, 0.7165, 0.1973, 0.2397, 0.5771, 0.5638, 0.9993],
        [0.2369, 0.9512, 0.7222, 0.2426, 0.1483, 0.6278, 0.7791],
        [0.2237, 0.5489, 0.9370, 0.8457, 0.9986, 0.7233, 0.7889],
        [0.8468, 0.2340, 0.0911, 0.4262, 0.1687, 0.6305, 0.7508],
        [0.3378, 0.1670, 0.3443, 0.0444, 0.2323, 0.8563, 0.0130],
        [0.5080, 0.7051, 0.8770, 0.3361, 0.6279, 0.9214, 0.7670],
        [0.5072, 0.1404, 0.3881, 0.9701, 0.6215, 0.1271, 0.5980],
        [0.6257, 0.4641, 0.3438, 0.8921, 0.8798, 0.0657, 0.1461],
        [0.9679, 0.6459, 0.8980, 0.2363, 0.9688, 0.4283, 0.2100],
        [0.4895, 0.4566, 0.3123, 0.2635, 0.5453, 0.0066, 0.5287],
        [0.1535, 0.0807, 0.5558, 0.9945, 0.2332, 0.8090, 0.1357],
        [0.7637, 0.5319, 0.8635, 0.8072, 0.5585, 0.1226, 0.3948],
        [0.5267, 0.1512, 0.0959, 0.0583, 0.1057, 0.5622, 0.5102],
        [0.3715, 0.4426, 0.4319, 0.9708, 0.4003, 0.6172, 0.8253],
        [0.5909, 0.8879, 0.1540, 0.9327, 0.9577, 0.8344, 0.8575],
        [0.4352, 0.2752, 0.2222, 0.6507, 0.8302, 0.9882, 0.1323],
        [0.3817, 0.9683, 0.0256, 0.8480, 0.9195, 0.5951, 0.1267],
        [0.9772, 0.1110, 0.4525, 0.2388, 0.3032, 0.4890, 0.2888],
        [0.1775, 0.7266, 0.9099, 0.8389, 0.5672, 0.2913, 0.8584],
        [0.2952, 0.0455, 0.5989, 0.9106, 0.6178, 0.6184, 0.6094],
        [0.2643, 0.0340, 0.7447, 0.2637, 0.2932, 0.7452, 0.6972],
        [0.7966, 0.0639, 0.8146, 0.7864, 0.0794, 0.7675, 0.1843],
        [0.7056, 0.3377, 0.9615, 0.6633, 0.0111, 0.3464, 0.8024],
        [0.7954, 0.2537, 0.7292, 0.9774, 0.9494, 0.5149, 0.1547],
        [0.0217, 0.0160, 0.0199, 0.2547, 0.5276, 0.8306, 0.3736],
        [0.2487, 0.7770, 0.7682, 0.0269, 0.9355, 0.1020, 0.3830],
        [0.8083, 0.5732, 0.6287, 0.1231, 0.1675, 0.4726, 0.3766],
        [0.1188, 0.6217, 0.7025, 0.4512, 0.1456, 0.7578, 0.8339],
        [0.1987, 0.6446, 0.3461, 0.8246, 0.7431, 0.9381, 0.0073],
        [0.2910, 0.9862, 0.8221, 0.2347, 0.2430, 0.3811, 0.2865],
        [0.3573, 0.9250, 0.0106, 0.6855, 0.7090, 0.5050, 0.6747],
        [0.3651, 0.5485, 0.5214, 0.4207, 0.1140, 0.3645, 0.1332],
        [0.4607, 0.0735, 0.3656, 0.2844, 0.7690, 0.8687, 0.8679],
```

Examples used to compute average loss on 2nd mini-batch

Batch size

Stochastic Gradient

```
tensor([[0.6376, 0.9057, 0.6846, 0.7117, 0.8487, 0.0744, 0.9518],
        [0.2923, 0.7165, 0.1973, 0.2397, 0.5771, 0.5638, 0.9993],
        [0.2369, 0.9512, 0.7222, 0.2426, 0.1483, 0.6278, 0.7791],
        [0.2237, 0.5489, 0.9370, 0.8457, 0.9986, 0.7233, 0.7889],
        [0.8468, 0.2340, 0.0911, 0.4262, 0.1687, 0.6305, 0.7508],
        [0.3378, 0.1670, 0.3443, 0.0444, 0.2323, 0.8563, 0.0130],
        [0.5080, 0.7051, 0.8770, 0.3361, 0.6279, 0.9214, 0.7670],
        [0.5072, 0.1404, 0.3881, 0.9701, 0.6215, 0.1271, 0.5980],
        [0.6257, 0.4641, 0.3438, 0.8921, 0.8798, 0.0657, 0.1461],
        [0.9679, 0.6459, 0.8980, 0.2363, 0.9688, 0.4283, 0.2100],
        [0.4895, 0.4566, 0.3123, 0.2635, 0.5453, 0.0066, 0.5287],
        [0.1535, 0.0807, 0.5558, 0.9945, 0.2332, 0.8090, 0.1357],
        [0.7637, 0.5319, 0.8635, 0.8072, 0.5585, 0.1226, 0.3948],
        [0.5267, 0.1512, 0.0959, 0.0583, 0.1057, 0.5622, 0.5102],
        [0.3715, 0.4426, 0.4319, 0.9708, 0.4003, 0.6172, 0.8253],
        [0.5909, 0.8879, 0.1540, 0.9327, 0.9577, 0.8344, 0.8575],
        [0.4352, 0.2752, 0.2222, 0.6507, 0.8302, 0.9882, 0.1323],
        [0.3817, 0.9683, 0.0256, 0.8480, 0.9195, 0.5951, 0.1267],
        [0.9772, 0.1110, 0.4525, 0.2388, 0.3032, 0.4890, 0.2888],
        [0.1775, 0.7266, 0.9099, 0.8389, 0.5672, 0.2913, 0.8584],
        [0.2952, 0.0455, 0.5989, 0.9106, 0.6178, 0.6184, 0.6094],
        [0.2643, 0.0340, 0.7447, 0.2637, 0.2932, 0.7452, 0.6972],
        [0.7966, 0.0639, 0.8146, 0.7864, 0.0794, 0.7675, 0.1843],
        [0.7056, 0.3377, 0.9615, 0.6633, 0.0111, 0.3464, 0.8024],
        [0.7954, 0.2537, 0.7292, 0.9774, 0.9494, 0.5149, 0.1547],
        [0.0217, 0.0160, 0.0199, 0.2547, 0.5276, 0.8306, 0.3736],
        [0.2487, 0.7770, 0.7682, 0.0269, 0.9355, 0.1020, 0.3830],
        [0.8083, 0.5732, 0.6287, 0.1231, 0.1675, 0.4726, 0.3766],
        [0.1188, 0.6217, 0.7025, 0.4512, 0.1456, 0.7578, 0.8339],
        [0.1987, 0.6446, 0.3461, 0.8246, 0.7431, 0.9381, 0.0073],
        [0.2910, 0.9862, 0.8221, 0.2347, 0.2430, 0.3811, 0.2865],
        [0.3573, 0.9250, 0.0106, 0.6855, 0.7090, 0.5050, 0.6747],
        [0.3651, 0.5485, 0.5214, 0.4207, 0.1140, 0.3645, 0.1332],
        [0.4607, 0.0735, 0.3656, 0.2844, 0.7690, 0.8687, 0.8679],
```

Random draw
Without replacement

Chain Rule

$$h : x \mapsto g(f(x))$$

$$h' : x \mapsto g'(f(x)) \times f'(x)$$

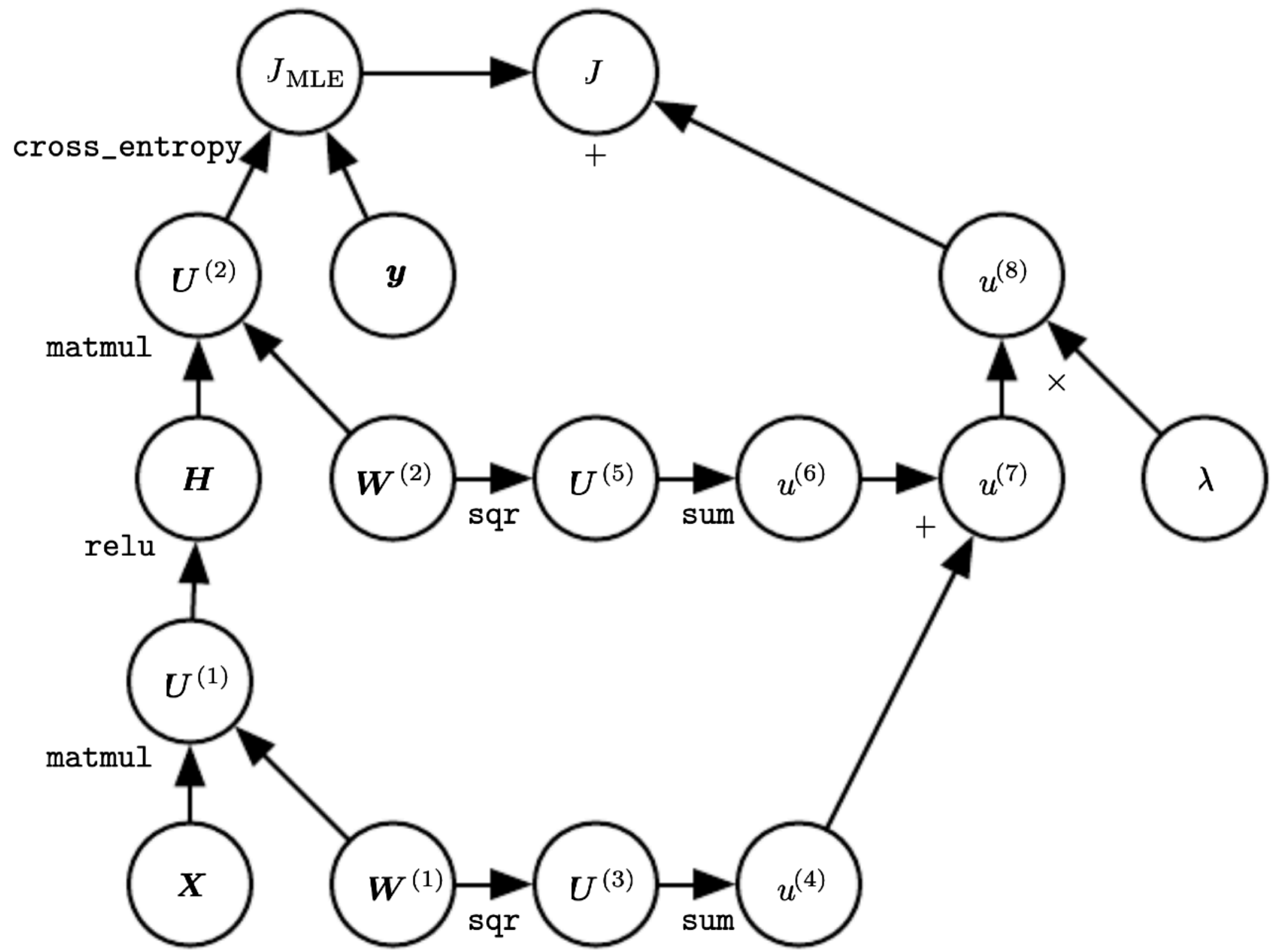
$$y = f(x) \qquad z = g(f(x))$$

$$\frac{\mathrm{d}z}{\mathrm{d}x} = \frac{\mathrm{d}z}{\mathrm{d}y}\frac{\mathrm{d}y}{\mathrm{d}x}$$

Chain Rule

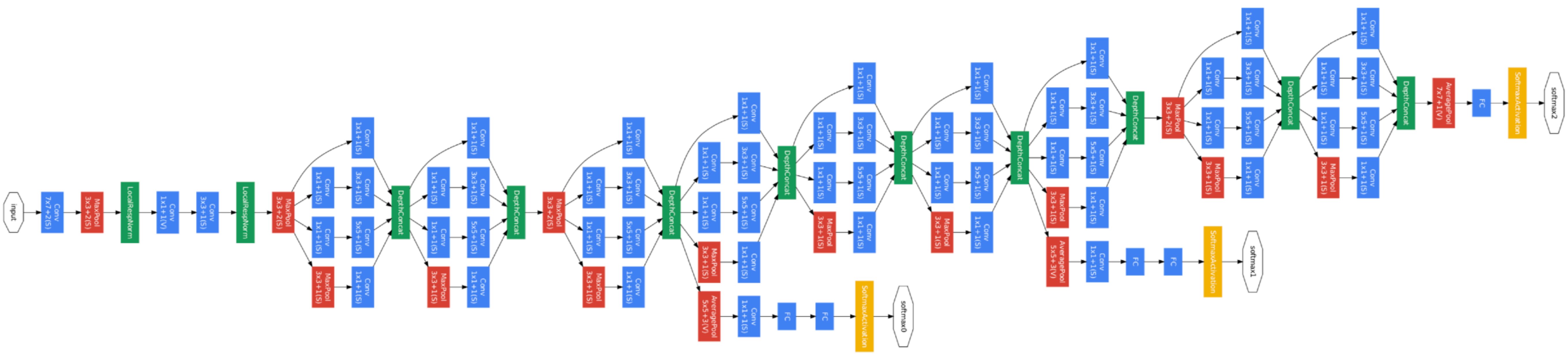
$$\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_i}$$

Compute Graph



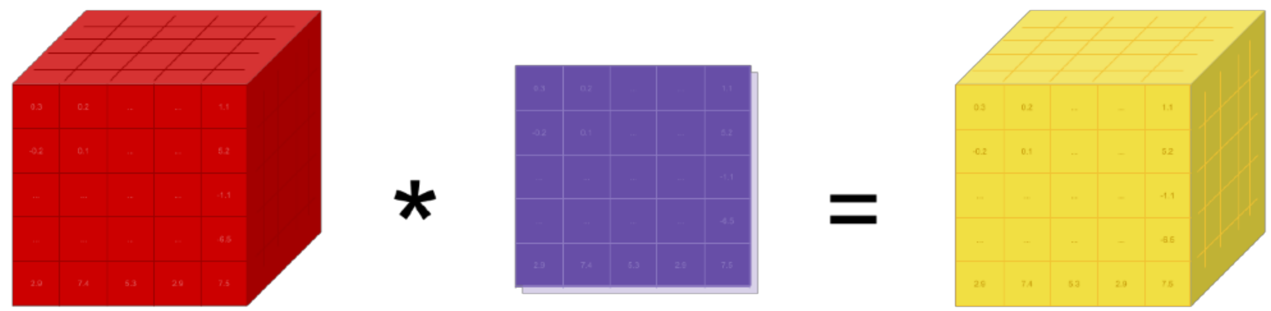
Compute graph for a MLP (Goodfellow et al.)

Compute Graph in Practice



GoogLeNet (2015)

PyTorch

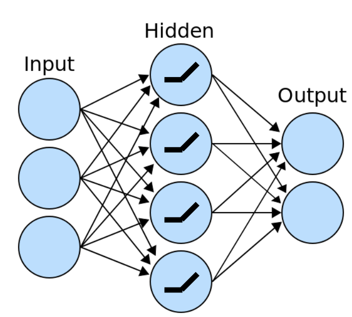


+

+

$$\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_i}$$

+



Playing Along with Others

ONNX

Google Cloud Platform

colab

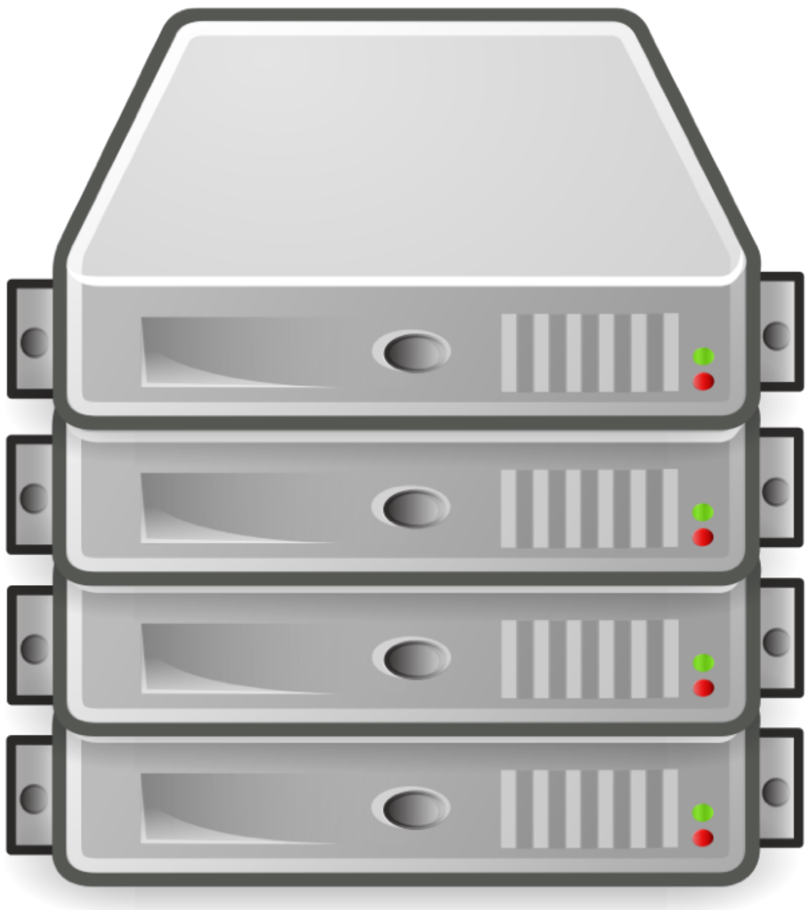
amazon web services™

Azure

Frontends

`@torch.jit.script`

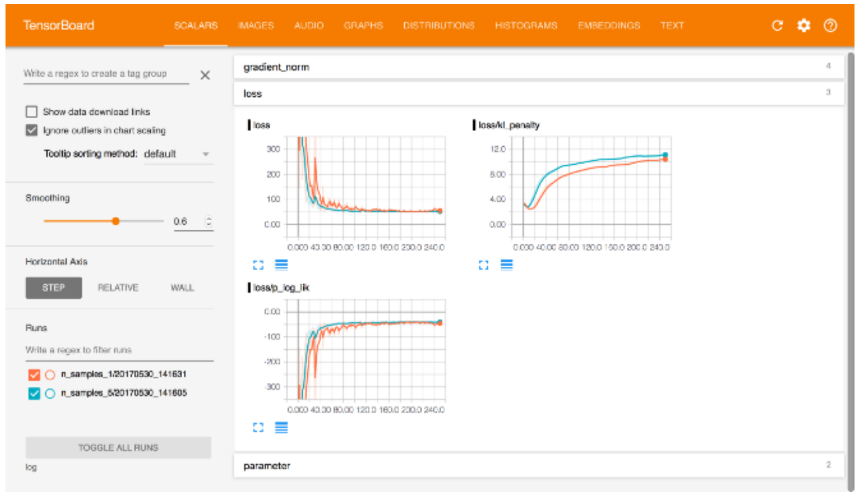
Distributed



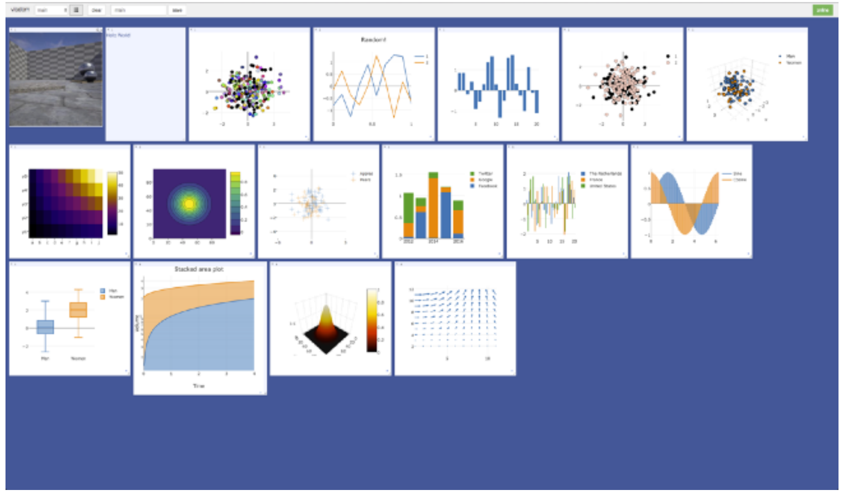
HOROVOD

Visualization

Not PyTorch strongest suit but compatibility is increasing



TensorboardX



Visdom

Comet.ml (service)

Ecosystem

flair

fast.ai

Ignite

AllenNLP

PyTorch geometric

And many more…

PyTorch or TensorFlow ?

Both have great ecosystems and can implement all models.

- Dynamic graph by design
- Great streamlined user interface
- Easier to use / debug

- Static graph by designed
- Messier API
- Better Tensorboard integration
- Easier to put in production
- TF Lite / TF Hub / TF.js

But TF is getting eager and PyTorch C++ frontend / JIT

They are converging