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Note. code examples torch.nn.

Let  $f: \mathbb{X} \longrightarrow \mathbb{Y}$  be a function we want to learn from observations  $\mathcal{D} \in \mathbb{X} \times \mathbb{Y}$ 

| $\mathcal{X}$   | $y \simeq f(x)$ |
|-----------------|-----------------|
| $x_1$           | $y_1$           |
| •               | •               |
| $\mathcal{X}_n$ | $y_n$           |

The function f can be learned from (noisy) observations  $\mathcal{D}$  by optimization if

- 1. we have a suitably expressive function class  $\mathcal{F} := \{f(x;\theta) | \theta \in \Theta\}$  such that  $f(x) \simeq f(x; \theta^*)$  for some parameter (vector)  $\theta^*$  and some quality criterion " $\simeq$ ".
- 2. we have a practicable algorithm  $A: (\mathcal{D}, \mathcal{F}, \mathcal{H}) \longrightarrow \theta^*$ .
  - → rich model class, quality criterion and practical inference algorithm ←

rich model class. (deep) feedforward neural networks

quality criterion. low test error: empirical risk minimization + regularization

learning algorithm. descent along gradients calculated by backpropagation

Feedforward neural networks became useful function approximators with concurrent, often interdependent improvements in

- expressivity (depth, conv/pool layers)
- regularization (dropout, early stopping, explicit cost penalties...)
- inference speed/stability (activations, gradient rules, backpropagation...).

networks. graphical expression of function composition

feedforward. no cycles – network is a DAG

**neural.** each node calculates  $h_i = g(x^T W_{:,i} + c_i)$ . The linear combination followed by nonlinear threshold/saturation function resembles a *very* stylized neuron

deep. more layers facilitate training of very expressive networks

```
torch.nn.[Conv2d|Linear|Dropout2d|...],
torch.nn.functional.[max_pool2d, |relu|...]
```

**Note:** H = g(XW + c) batch matrix multiplication  $\rightarrow$  leverage GPU acceleration

```
torch.[.cuda].Tensor, a_tensor.to_device(<dev>)
```

As our functions are parameterised, we turn this into an optimisation problem:

$$\theta^* = \operatorname{argmin}_{\theta} \operatorname{cost}(f(x; \theta), y)$$

Two terms contribute to the cost:

- i. loss: penalizes bad predictions, i.e. some idea of training error
- ii. regularization: penalizes complex f, leading to generalization error
  - $\rightarrow$  this is the difference between pure optimization (fit = minimize training error) and a machine *learning* algorithm.

torch.nn.\*loss

- Find how the cost J depends on each of the parameters  $\theta_i$ 
  - → find gradients, (reverse) differentiation → backpropagation
- and adjust the parameters to minimize it
  - → use gradients, learning rule

$$\theta^{[k]} = \theta^{[k-1]} - \eta \nabla_{\theta} J(\theta), \quad \eta \in \mathbb{R}^+$$

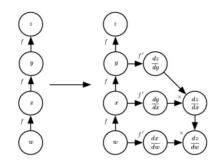
- only local minima but some of these surprisinly useful in NNs
- since *J* usually additive on samples, i.e.  $J = J_i$  we can perform gradient updates with fixed batch size  $\ll$  dataset size  $\rightarrow$  *minibatches* (uniform sampling)
- Adadelta, Adagrad, Adam, momentum, RMSprop...

```
torch.optim.*
```

• gradient descent may need or benefit from learning rate adaptation

```
torch.optim.lr_scheduler.*
```

Where do the gradients come from?



```
torch.Tensor(..., require_grad=True)
```

a\_tensor.backward()

torch.autograd.

## Engineering

- dynamic computation graphs vs. declaration/execution phases
- distributed, multimachine training → torch.distributed
- C++ model serving → tensorflow.serving
- checkpointing → torch.utils.checkpoint
- monitoring / debugging / optimizing → tensorflow.tensorboard
- model porting (to production / other frameworks) → ONNX
- fast forward mode embedded / mobile → tensorflow lite

- caffe 2 (production, mobile) → PyTorch 1.0
- tensorflow: docs, community, tensorboard, serving, lite
- keras (tf, cntk, theano): prototyping, spark,
- mxnet: language agnostic
- cntk: spark, azure