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Representations, Deep Architectures & Backpropagation

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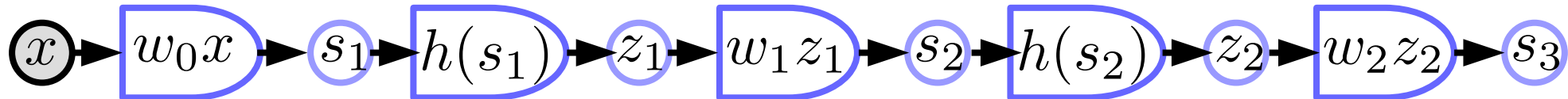
Facebook AI Research

Deep Learning, NYU Fall 2020

Block Diagram of a Traditional Neural Net

▶ linear blocks $s_{k+1} = w_k z_k$

▶ Non-linear blocks $z_k = h(s_k)$

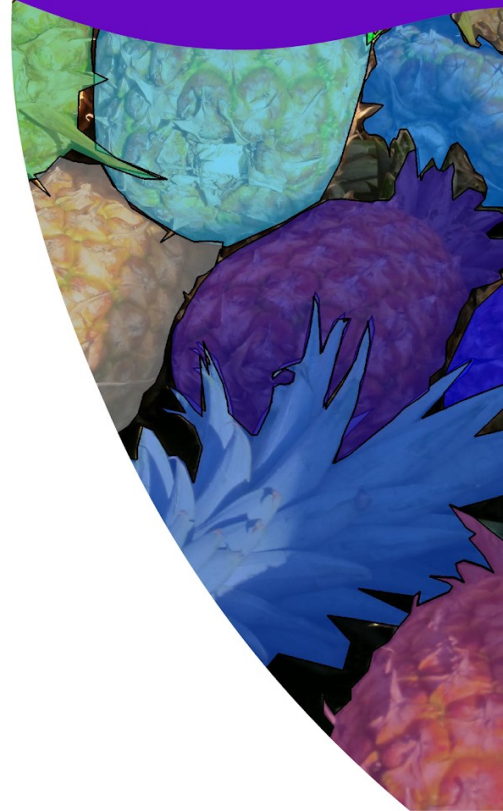




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What are Good Representations?

What are good features?



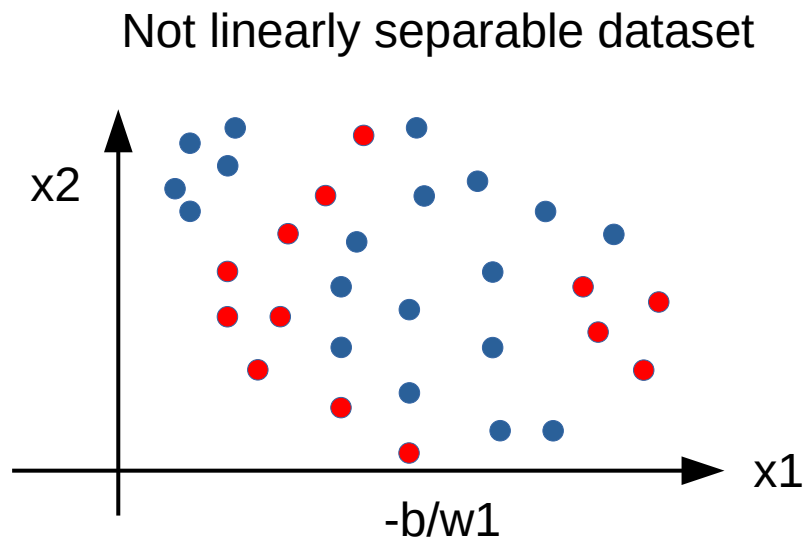
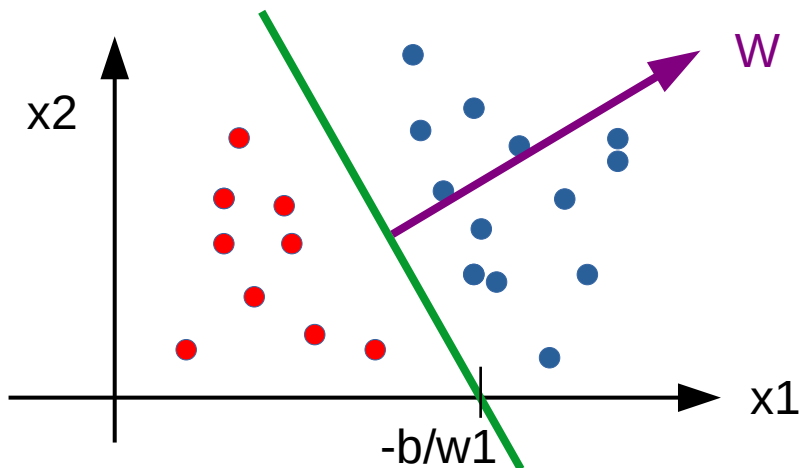
Linear Classifiers and their limitations

► Linear classifier

$$\bar{y} = \text{sign}\left(\sum_{i=1}^N w_i x_i + b\right)$$

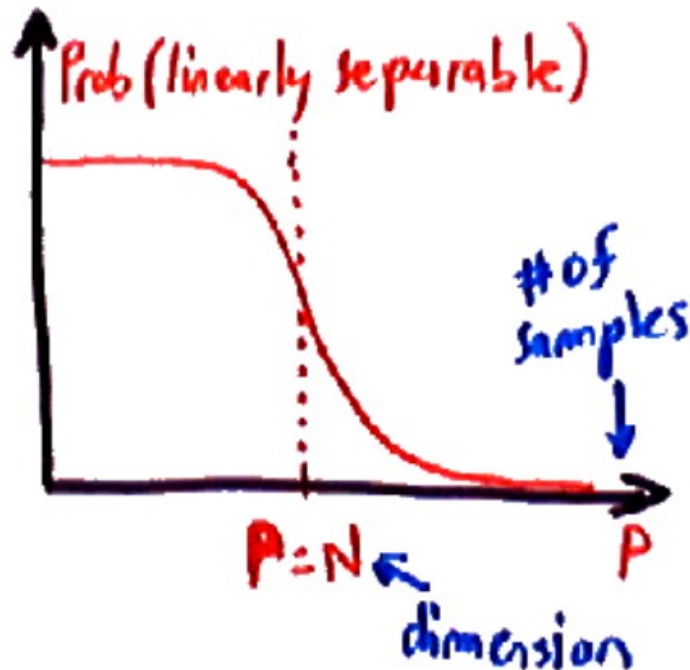
- Partitions the space into two half spaces separated by the hyperplane:

$$\sum_{i=1}^N w_i x_i + b = 0$$



Number of linearly separable dichotomies

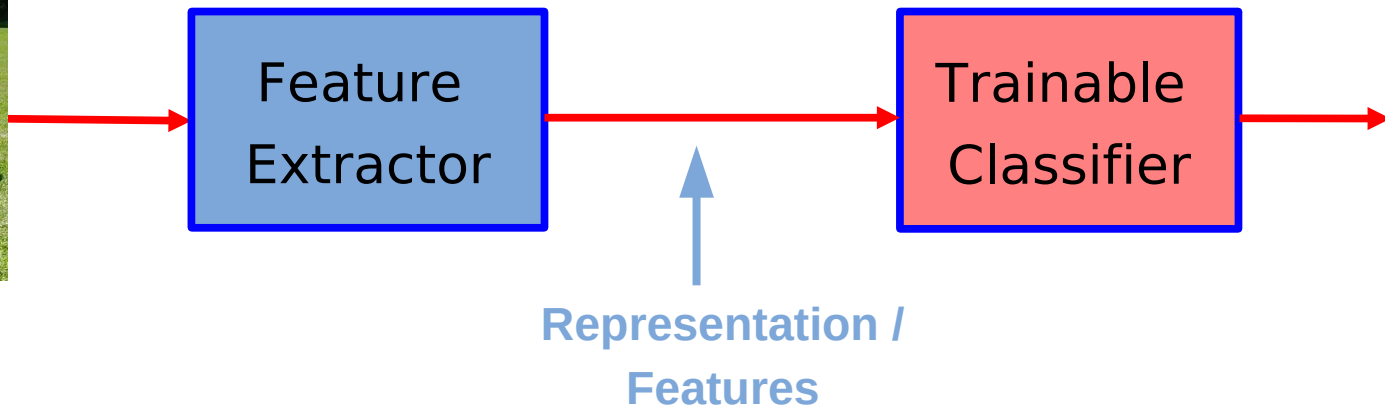
- ▶ The probability that a dichotomy over P points in N dimensions is linearly separable goes to zero as P gets larger than N
- ▶ [Cover's theorem 1966]



- Problem: there are 2^P possible dichotomies of P points.
- Only about N are linearly separable.
- If P is larger than N , the probability that a random dichotomy is linearly separable is very, very small.

Solution: representations (a.k.a. features)

- ▶ Extracting relevant features from the raw input
- ▶ Computing good representations of the input
- ▶ **The feature extractor must be non-linear**
- ▶ Simple solution: expand the dimension non-linearly
 - ▶ But how?



Example: monomial features

- ▶ Feature extractor computes cross products of input variables
- ▶ A linear classifier on top computes a polynomial of input variables

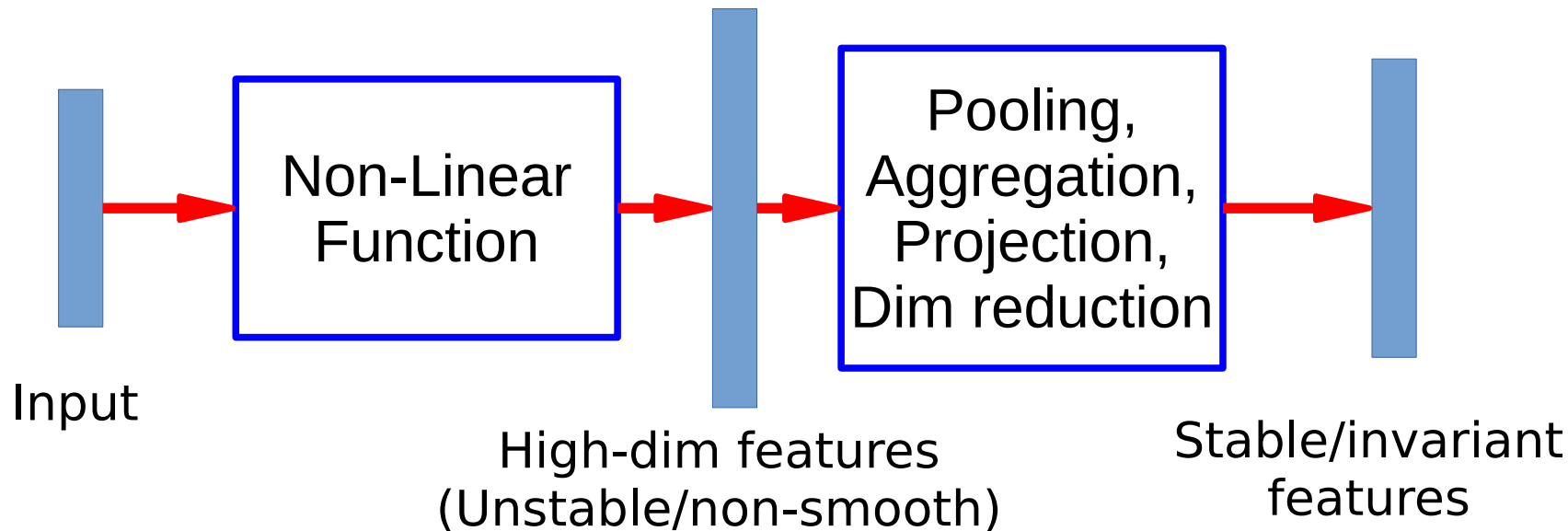
$$\Phi(x_1, x_2) = [1, x_1, x_2, x_1x_2, x_1^2, x_2^2]$$

- ▶ generalizable to degree d
- ▶ Unfortunately impractical for large d
- ▶ Number of features is d choose N , which grows like N^d
- ▶ But $d=2$ is used a lot in “attention” circuits.



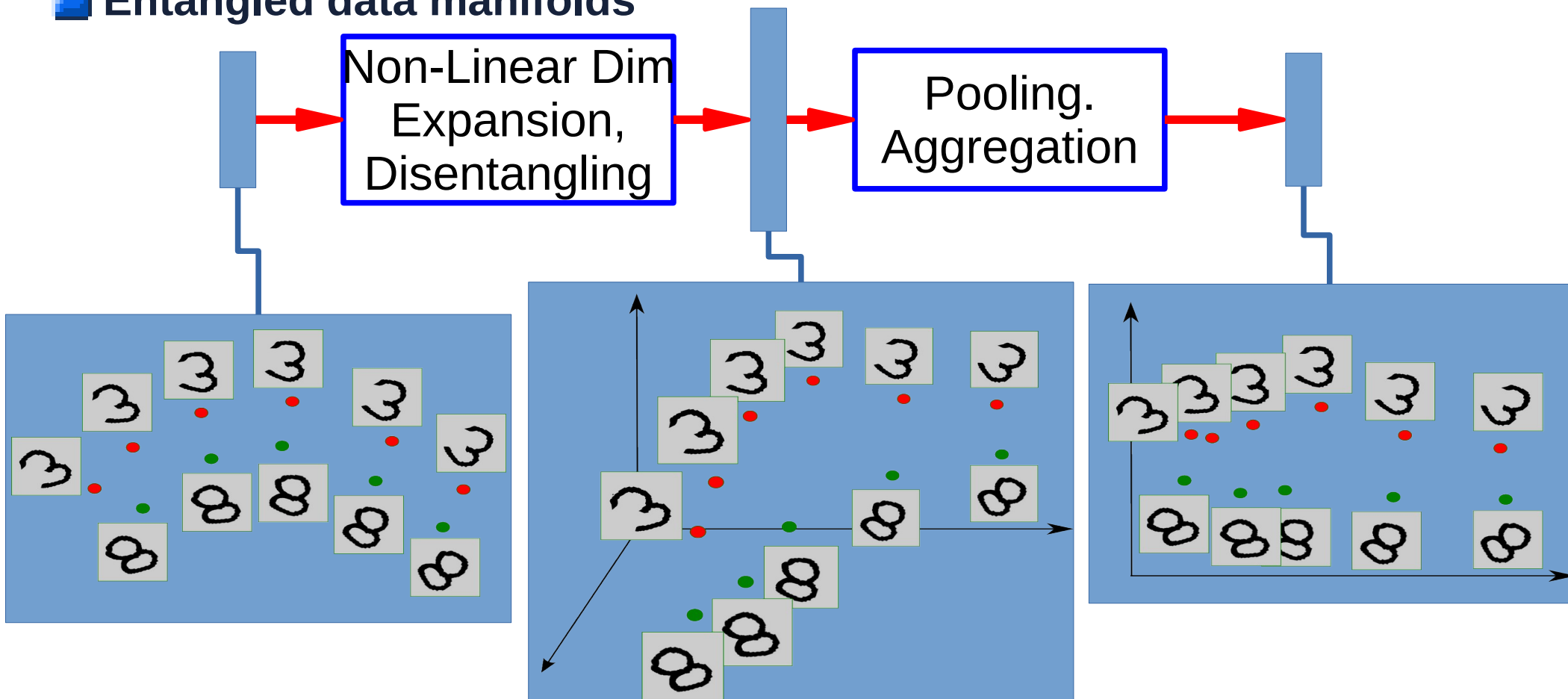
Basic Idea for Invariant Feature Learning

- Embed the input **non-linearly** into a high(er) dimensional space
 - ▶ In the new space, things that were non separable may become separable
- Pool regions of the new space together
 - ▶ Bringing together things that are semantically similar. Like pooling.



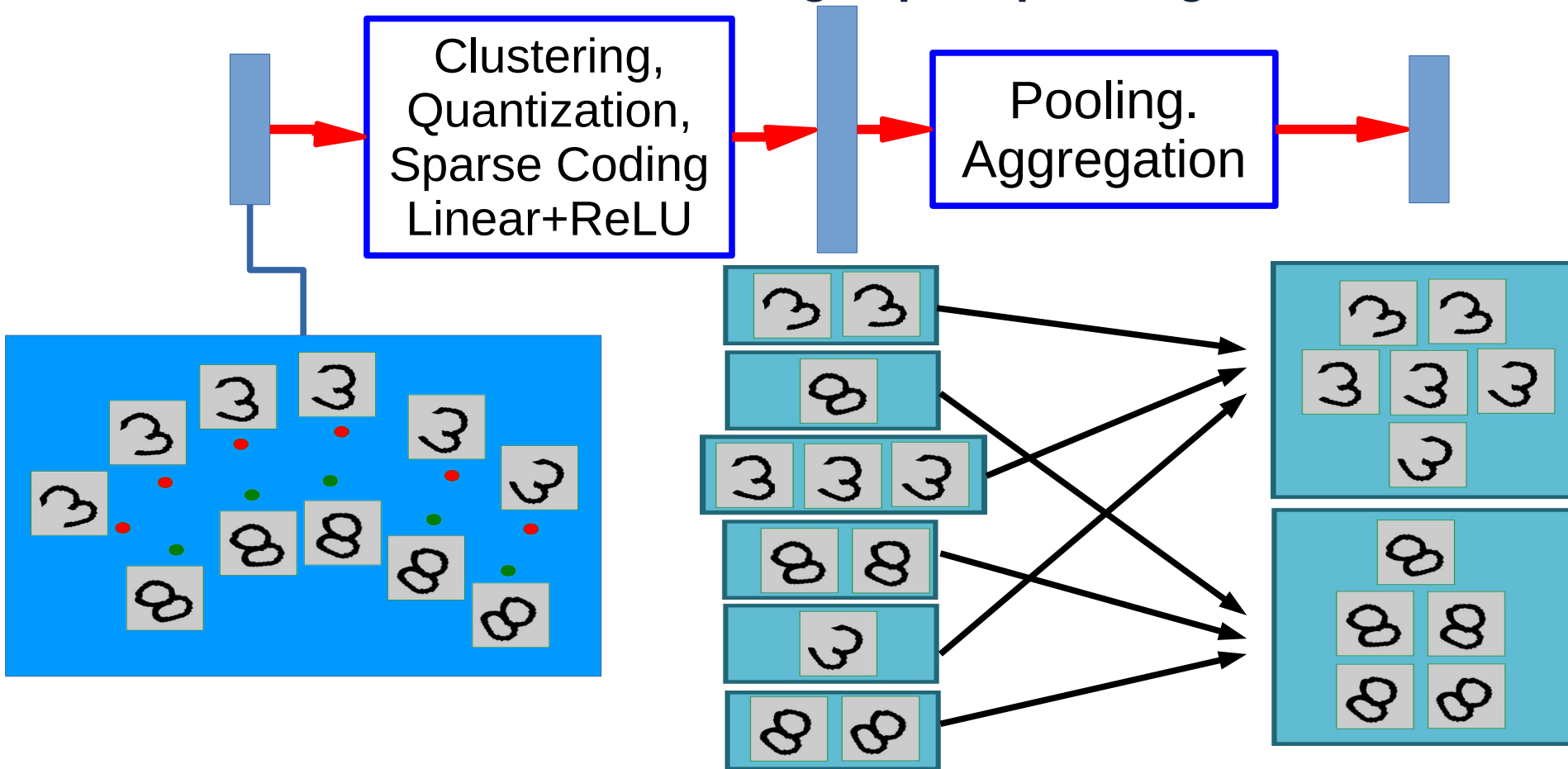
Non-Linear Expansion → Pooling

Entangled data manifolds



Sparse Non-Linear Expansion → Pooling

■ Use non-linear fn to break things apart, pool together similar things



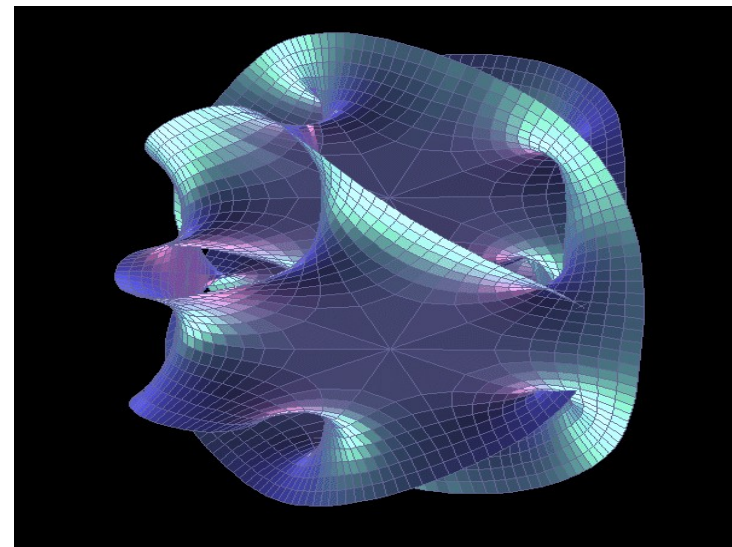
Discovering the Hidden Structure in High-Dimensional Data: The manifold hypothesis

■ Learning Representations of Data:

- ▶ Discovering & disentangling the independent explanatory factors

■ The Manifold Hypothesis:

- ▶ Natural data lives in a low-dimensional (non-linear) manifold
- ▶ Because variables in natural data are mutually dependent



Discovering the Hidden Structure in High-Dimensional Data

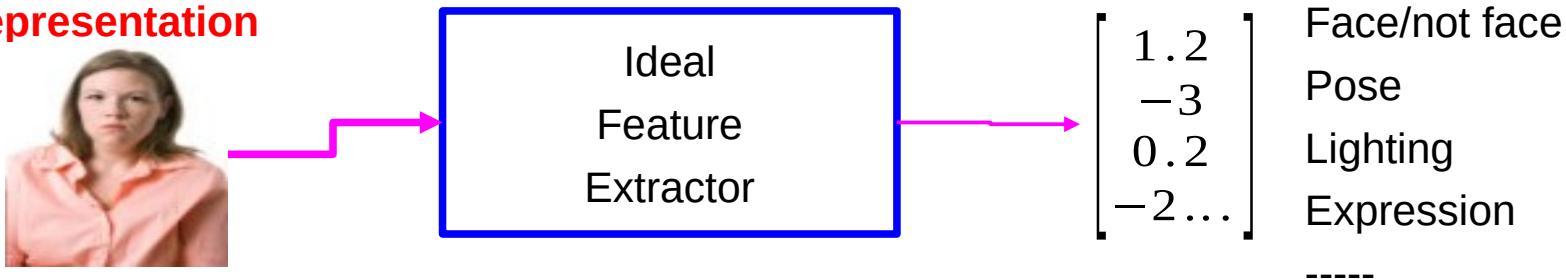
■ Example: all face images of a person

- ▶ 1000x1000 pixels = 1,000,000 dimensions
- ▶ But the face has 3 Cartesian coordinates and 3 Euler angles
- ▶ And humans have less than about 50 muscles in the face
- ▶ Hence the manifold of face images for a person has <56 dimensions

■ The perfect representations of a face image:

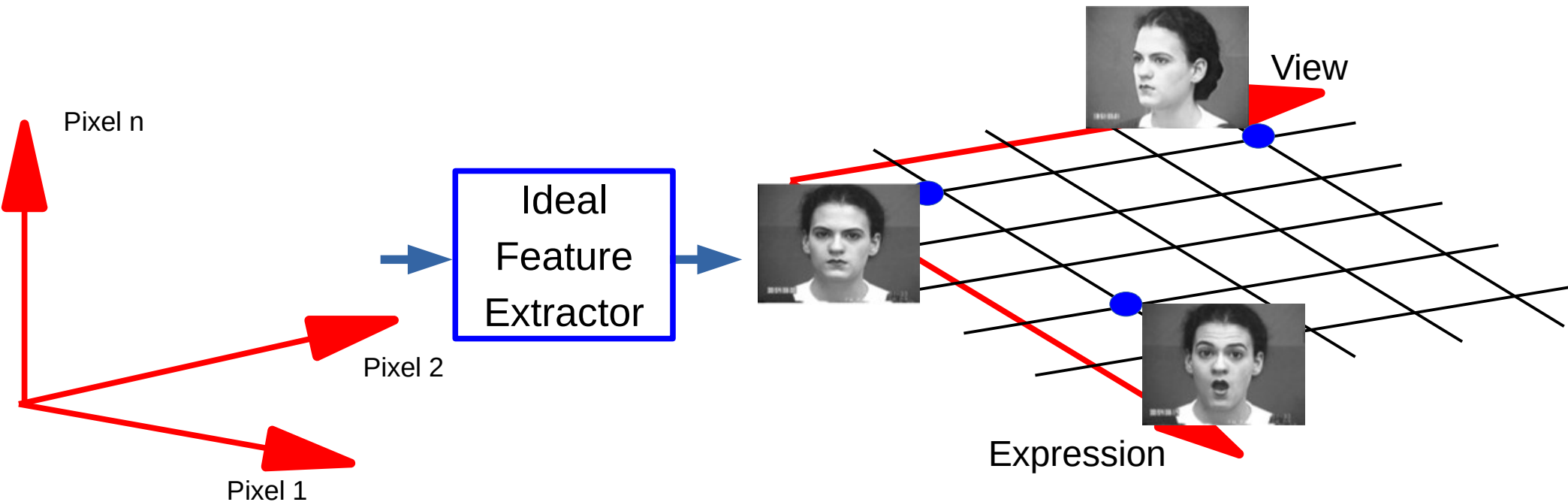
- ▶ Its coordinates on the face manifold
- ▶ Its coordinates away from the manifold

■ We do not have good and general methods to learn functions that turns an image into this kind of representation



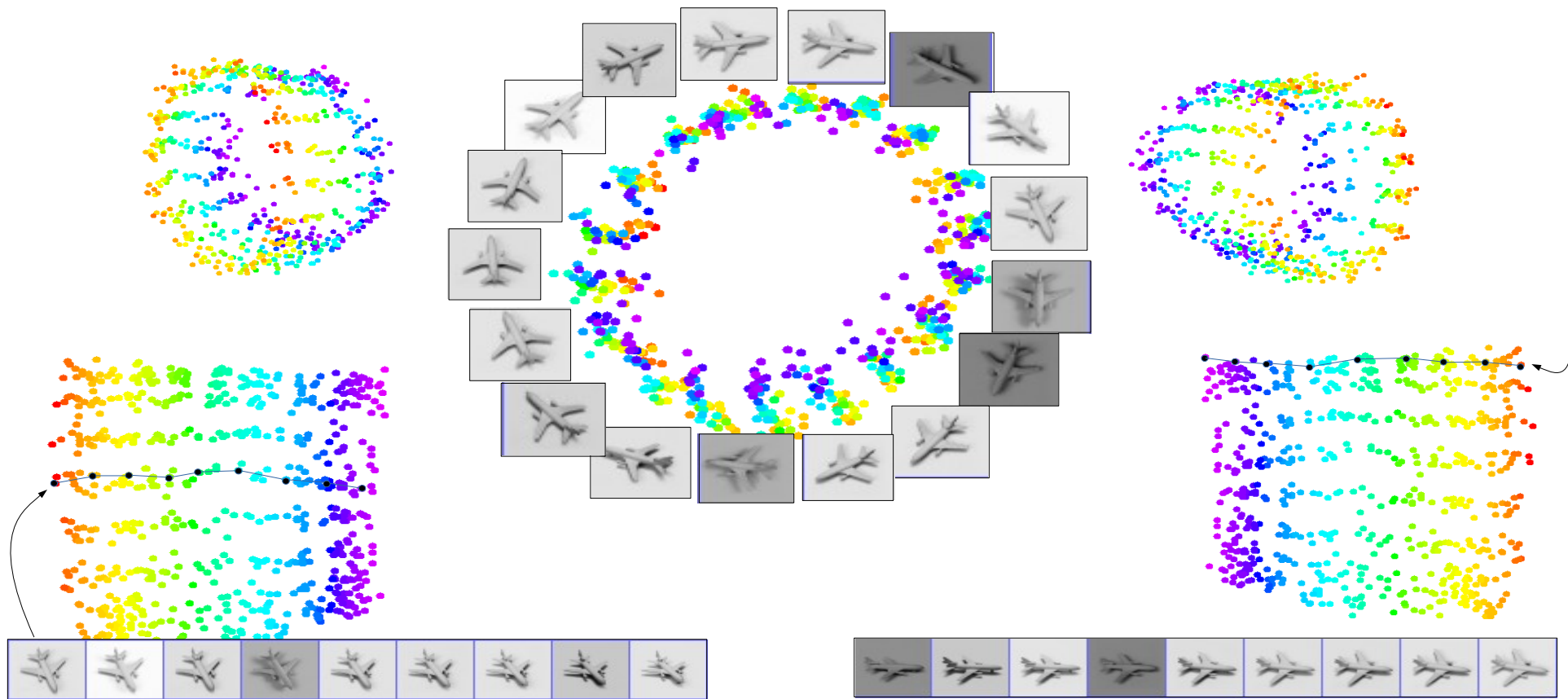
Disentangling factors of variation

The Ideal Disentangling Feature Extractor



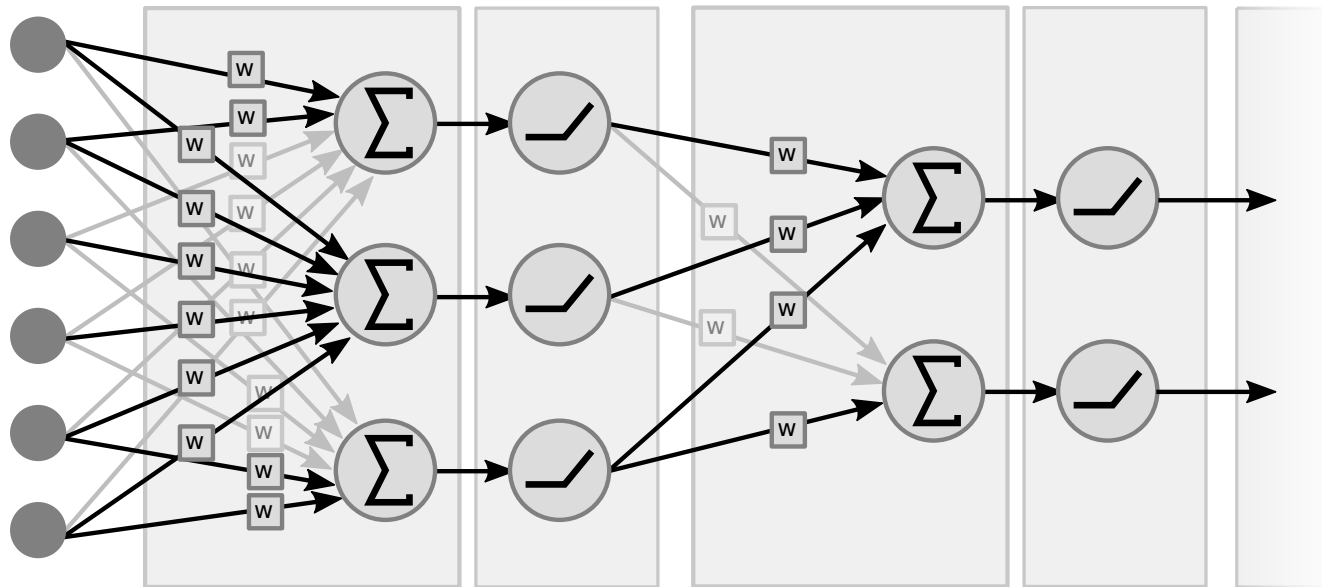
Data Manifold

[Hadsell et al. CVPR 2006]



Traditional Neural Net

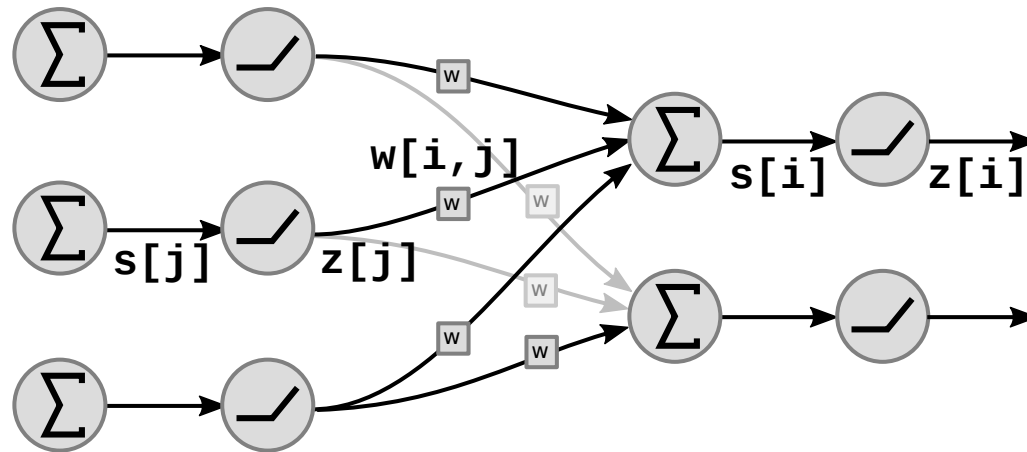
- ▶ **Stacked linear and non-linear functional blocks**
 - ▶ Weighted sums, matrix-vector product
 - ▶ Point-wise non-linearities (e.g. ReLu, tanh,)



Traditional Neural Net

► Stacked linear and non-linear functional blocks

$$s[i] = \sum_{j \in \text{UP}(i)} w[i, j] \cdot z[j] \quad z[i] = f(s[i])$$



Backprop through a non-linear function

► Chain rule:

$$g(h(s))' = g'(h(s)).h'(s)$$

$$dc/ds = dc/dz * dz/ds$$

$$dc/ds = dc/dz * h'(s)$$

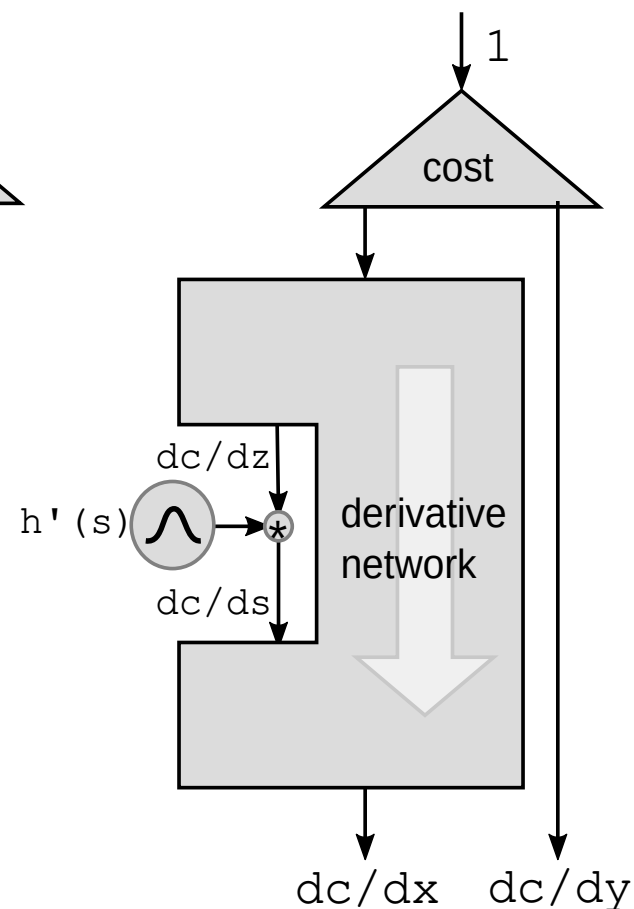
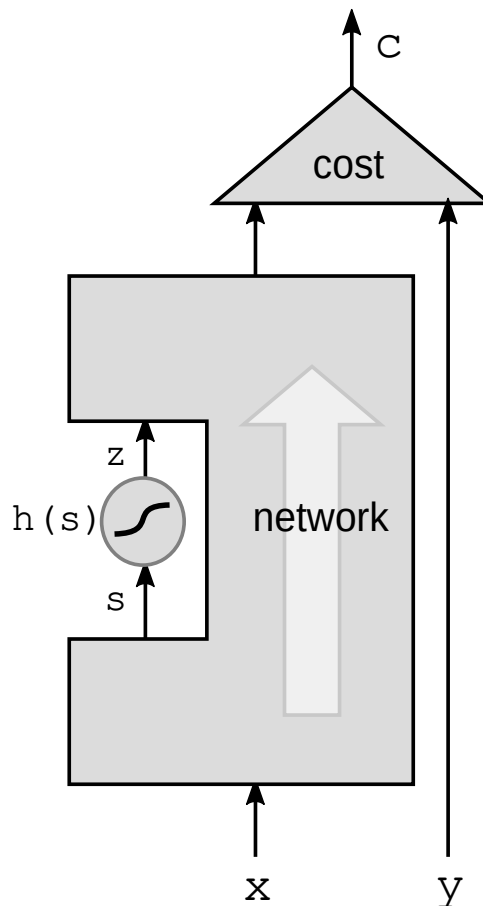
► Perturbations:

- Perturbing s by ds will perturb z by: $dz = ds * h'(s)$

- This will perturb c by

$$dc = dz * dc/dz = ds * h'(s) * dc/dz$$

- Hence: $dc/ds = dc/dz * h'(s)$

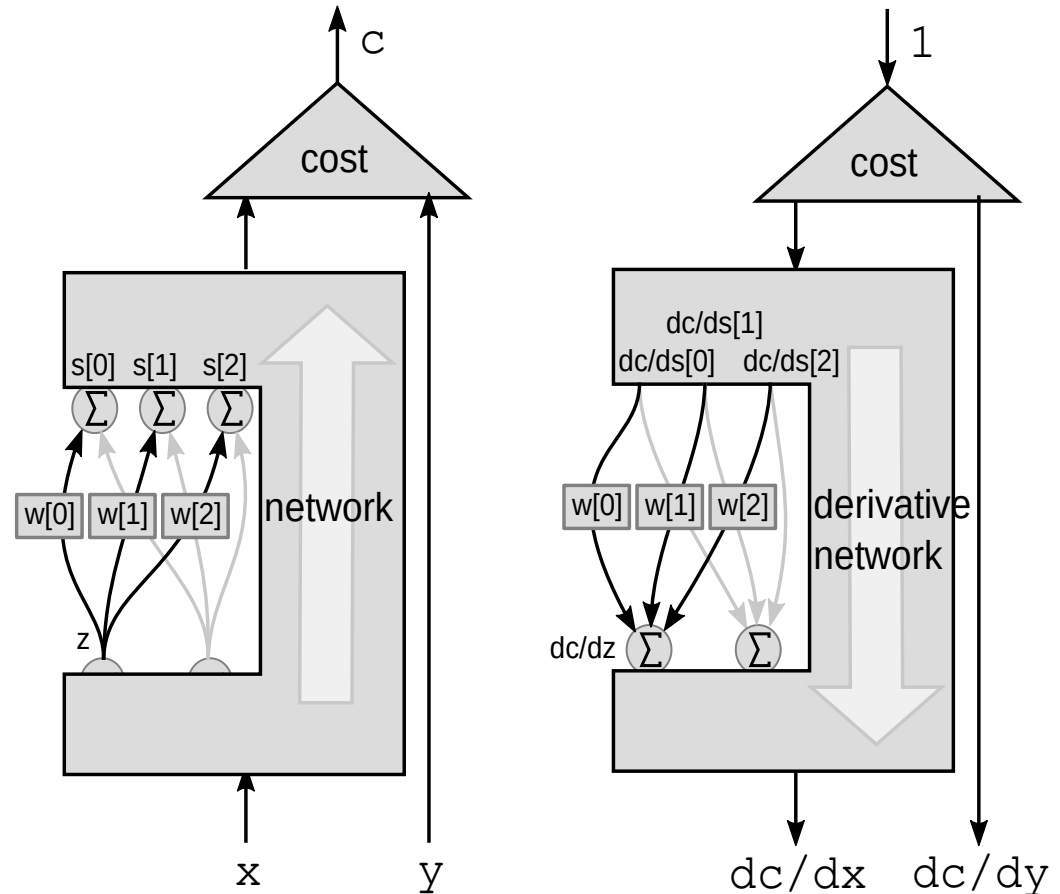


Backprop through a weighted sum

► Perturbations:

- Perturbing z by dz will perturb $s[0], s[1], s[2]$ by $ds[0]=w[0]*dz$, $ds[1]=w[1]*dz$, $ds[2]=w[2]*dz$
- This will perturb c by

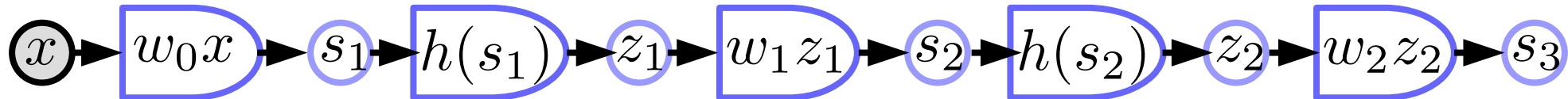
$$dc = ds[0]*dc/ds[0] + ds[1]*dc/ds[1] + ds[2]*dc/ds[2]$$
- Hence: $dc/dz = dc/ds[0]*w[0] + dc/ds[1]*w[1] + dc/ds[2]*w[2] +$



Block Diagram of a Traditional Neural Net

► linear blocks $s_{k+1} = w_k z_k$

► Non-linear blocks $z_k = h(s_k)$



PyTorch definition

► Object-oriented version

- Uses predefined nn.Linear class, (which includes a bias vector)
- Uses torch.relu function
- State variables are temporary

```
import torch
```

```
from torch import nn
```

```
image = torch.randn(3, 10, 20)
```

```
d0 = image.nelement()
```

```
class mynet(nn.Module):
```

```
    def __init__(self, d0,d1,d2,d3):
```

```
        super().__init__()
```

```
        self.m0 = nn.Linear(d0, d1)
```

```
        self.m1 = nn.Linear(d1, d2)
```

```
        self.m2 = nn.Linear(d2, d3)
```

```
    def forward(self, x):
```

```
        z0 = x.view(-1)  ## flatten input tensor
```

```
        s1 = self.m0(x)
```

```
        z1 = torch.relu(s1)
```

```
        s2 = self.m1(z1)
```

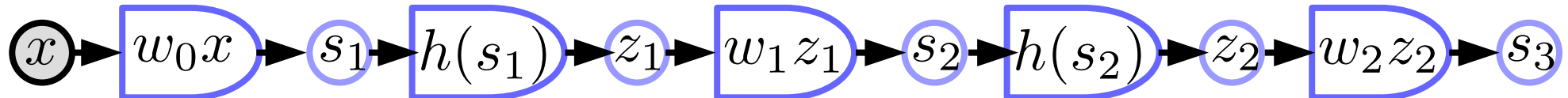
```
        z2 = torch.relu(s2)
```

```
        s3 = self.m2(z2)
```

```
        return s3
```

```
model = mynet(d0,60,40,10)
```

```
out = model(image)
```



Backprop through a functional module

► Using chain rule for vector functions

$$z_g : [d_g \times 1] \quad z_f : [d_f \times 1]$$

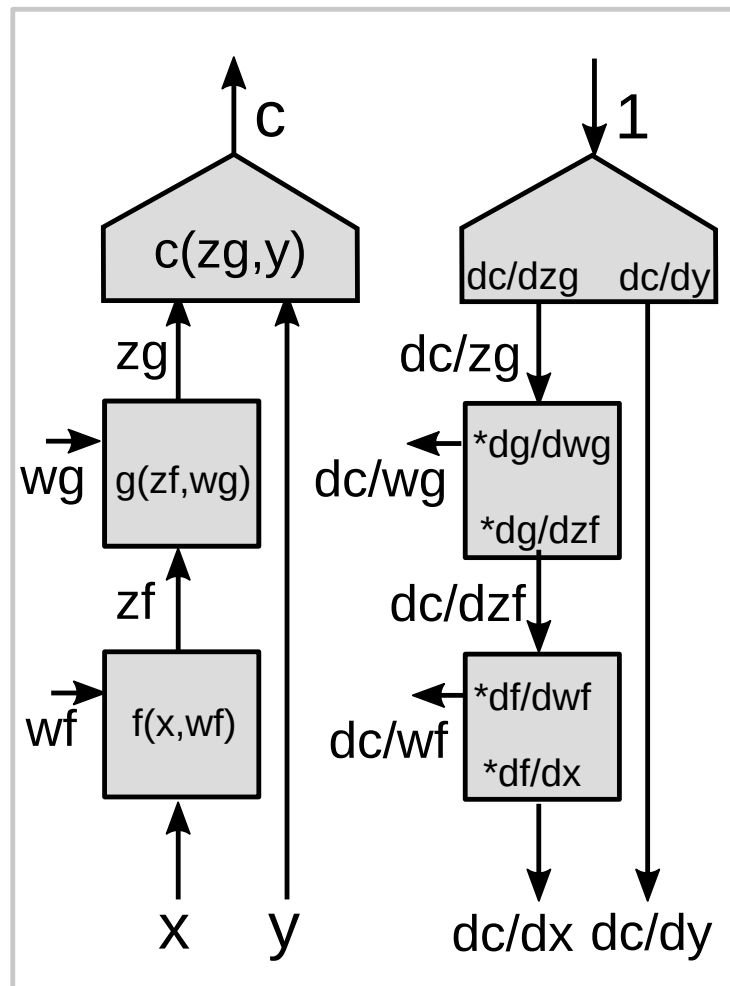
$$\frac{\partial c}{\partial z_f} = \frac{\partial c}{\partial z_g} \frac{\partial z_g}{\partial z_f}$$

$$[1 \times d_f] = [1 \times d_g] * [d_g \times d_f]$$

► Jacobian matrix

► Partial derivative of i-th output w.r.t. j-th input

$$\left(\frac{\partial z_g}{\partial z_f} \right)_{ij} = \frac{(\partial z_g)_i}{(\partial z_f)_j}$$



Backprop through a multi-stage graph

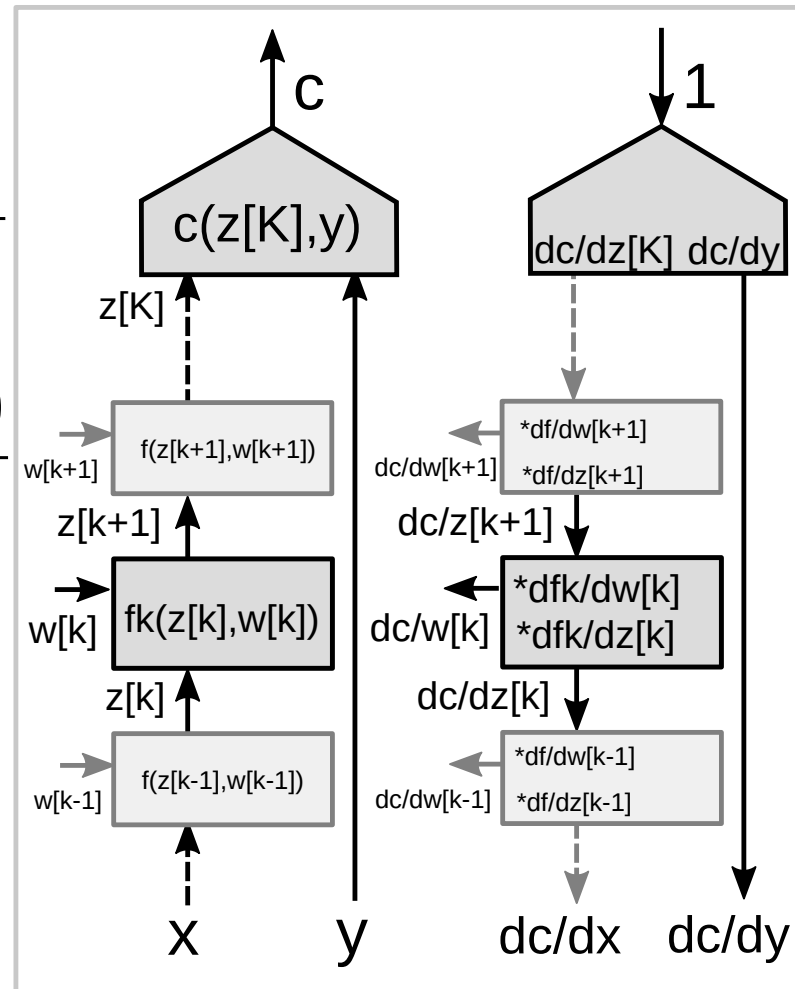
► Using chain rule for vector functions

$$\frac{\partial c}{\partial z_k} = \frac{\partial c}{\partial z_{k+1}} \frac{\partial z_{k+1}}{\partial z_k} = \frac{\partial c}{\partial z_{k+1}} \frac{\partial f_k(z_k, w_k)}{\partial z_k}$$

$$\frac{\partial c}{\partial w_k} = \frac{\partial c}{\partial z_{k+1}} \frac{\partial z_{k+1}}{\partial w_k} = \frac{\partial c}{\partial z_{k+1}} \frac{\partial f_k(z_k, w_k)}{\partial w_k}$$

► Two Jacobian matrices for the module:

- One with respect to $z[k]$
- One with respect to $w[k]$



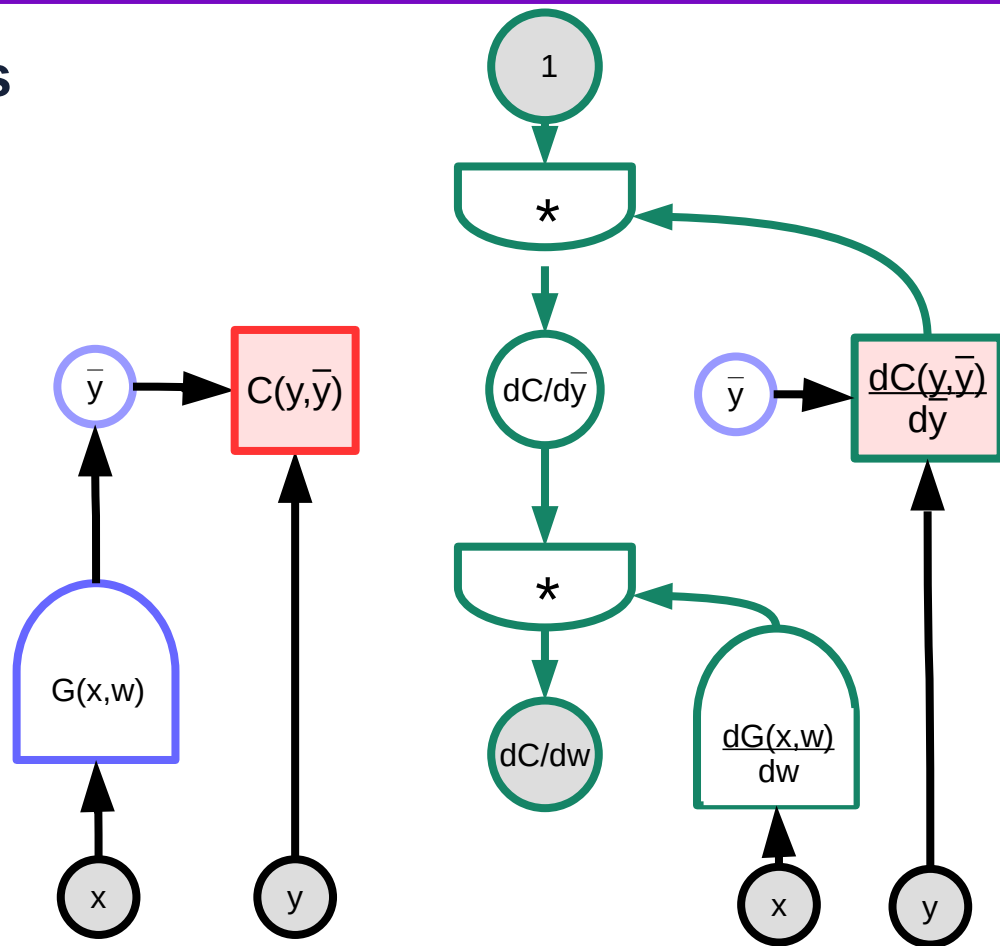
Backprop = propagation through a transformed graph

► Derivative of composed functions

$$C(G(w))' = C'(G(w))G'(w)$$

$$\frac{\partial C(y, \bar{y})}{\partial w} = \frac{\partial C(y, \bar{y})}{\partial \bar{y}} \frac{\partial \bar{y}}{\partial w}$$

$$\frac{\partial C(y, \bar{y})}{\partial w} = \frac{\partial C(y, \bar{y})}{\partial \bar{y}} \frac{\partial G(x, w)}{\partial w}$$



Gradient, Jacobian,

► Dimensions:

$$y, \bar{y} : [M \times 1] \quad w : [N \times 1]$$

$$\frac{\partial C(y, \bar{y})}{\partial w} = \frac{\partial C(y, \bar{y})}{\partial \bar{y}} \frac{\partial \bar{y}}{\partial w}$$

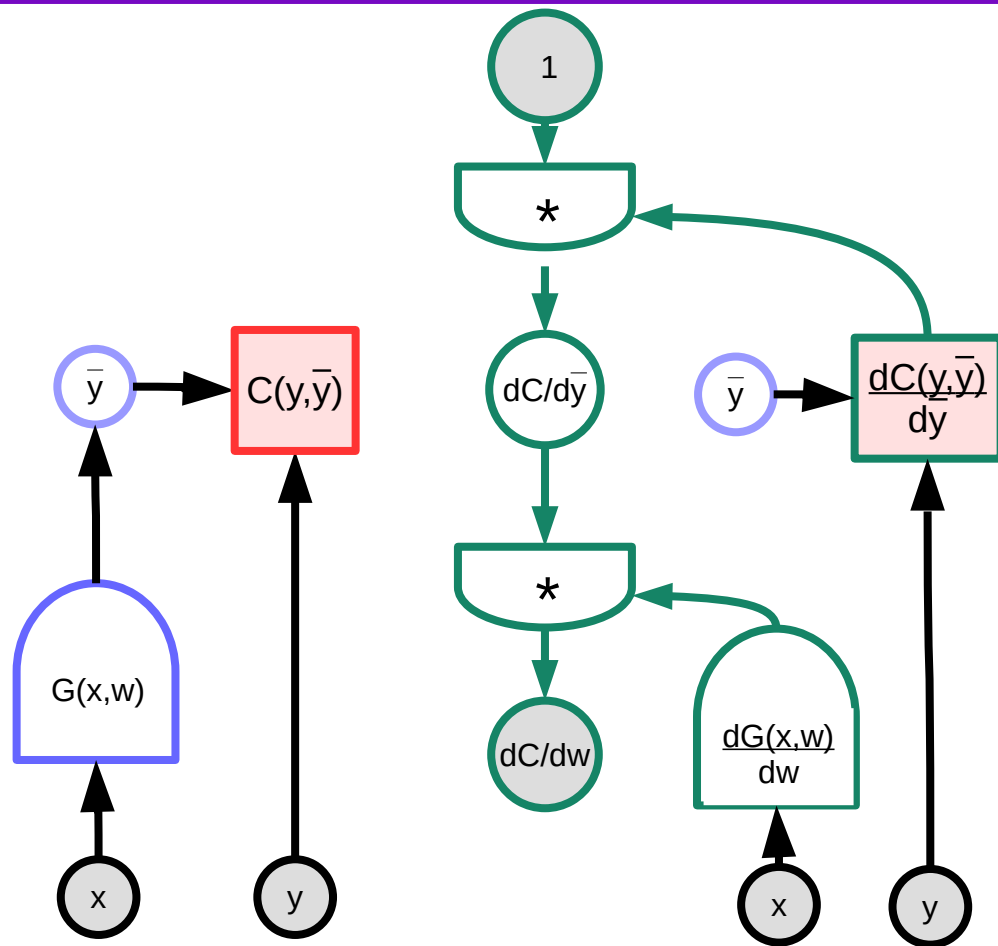
$$[1 \times N] = [1 \times M] \cdot [M \times N]$$

► Row vector = row vector . matrix

$$\frac{\partial C(y, \bar{y})}{\partial w} = \frac{\partial C(y, \bar{y})}{\partial \bar{y}} \frac{\partial G(x, w)}{\partial w}$$

$$[1 \times N] = [1 \times M] \cdot [M \times N]$$

► Gradient = gradient . Jacobian



Basic Modules

Linear

$$Y = W.X \quad ; \quad dC/dX = W^T \cdot dC/dY \quad ; \quad dC/dW = X \, dC/dY$$

ReLU

$$y = \text{ReLU}(x) \quad ; \quad \text{if } (x < 0) \, dC/dx = 0 \, \text{ else } \, dC/dx = dC/dy$$

Duplicate

$$Y1 = X, Y2 = X \quad ; \quad dC/dX = dC/dY1 + dC/dY2$$

Add

$$Y = X1 + X2 \quad ; \quad dC/dX1 = dC/dY \quad ; \quad dC/dX2 = dC/dY$$

Max

$$y = \max(x1, x2) \quad ; \quad \text{if } (x1 > x2) \, dC/dx1 = dC/dy \, \text{ else } \, dC/dx1 = 0$$

LogSoftMax

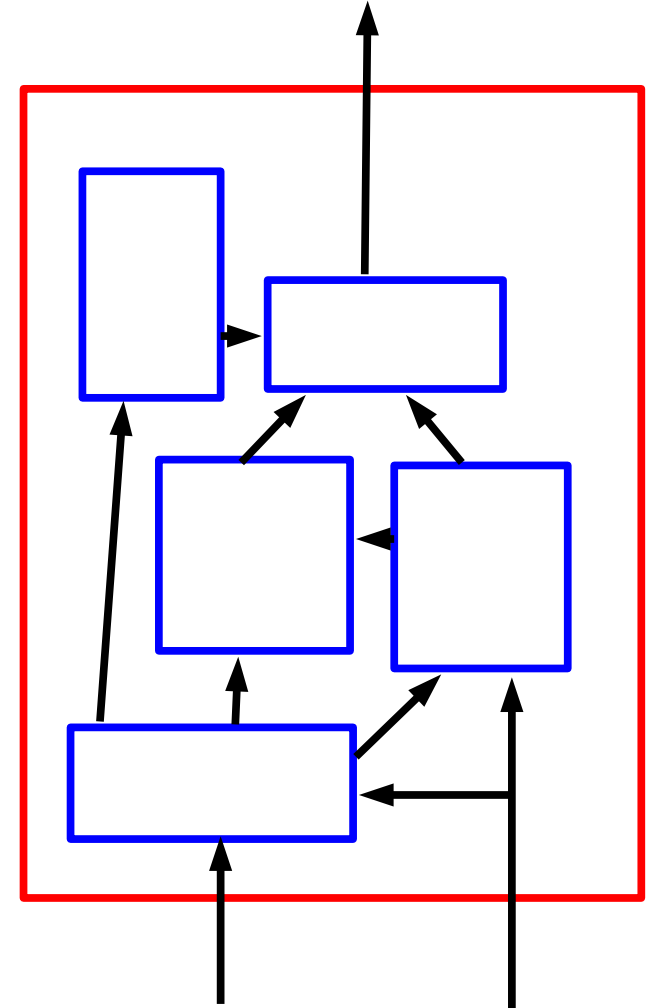
$$Y_i = X_i - \log[\sum_j \exp(X_j)] \quad ; \quad \dots???$$

Non-Linear functions and Loss functions in PyTorch

- ▶ **ReLu, sigmoids and variations**
- ▶ **Squared error, cross-entropy, hinge, ranking loss and variants**

Any directed acyclic graph is OK for backprop

- ▶ As long as there exist a partial order on the modules
- ▶ If the graph has loops, we need to “unroll” them.
 - ▶ Recurrent networks and bakprop through time



Backprop in Practice

- Use ReLU non-linearities (tanh and logistic are falling out of favor)
- Initialize the weights properly
- Use cross-entropy loss for classification
- Use Stochastic Gradient Descent on minibatches
- Shuffle the training samples
- Normalize the input variables (zero mean, unit variance)
- Schedule to decrease the learning rate
- Use a bit of L1 or L2 regularization on the weights (or a combination)
 - ▶ But it's best to turn it on after a couple of epochs
- Use “dropout” for regularization
 - ▶ Hinton et al 2012 <http://arxiv.org/abs/1207.0580>
- Lots more in [LeCun et al. “Efficient Backprop” 1998]
- Lots, lots more in recent papers.