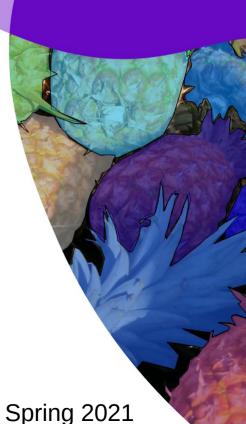


Deep Learning

Alfredo Canziani, Yann LeCun NYU - Courant Institute & Center for Data Science

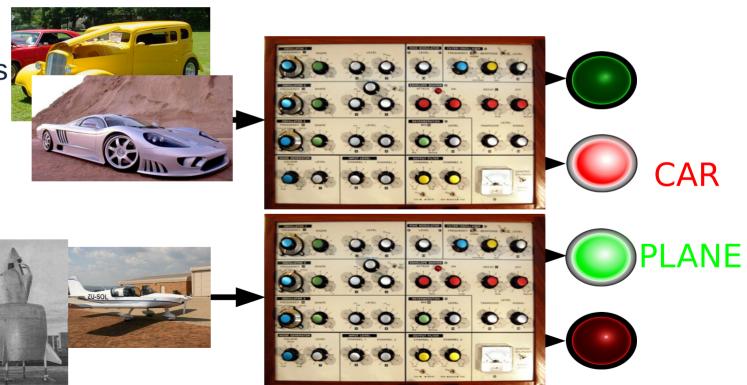


Deep Learning, NYU Spring 2021

Supervised Learning

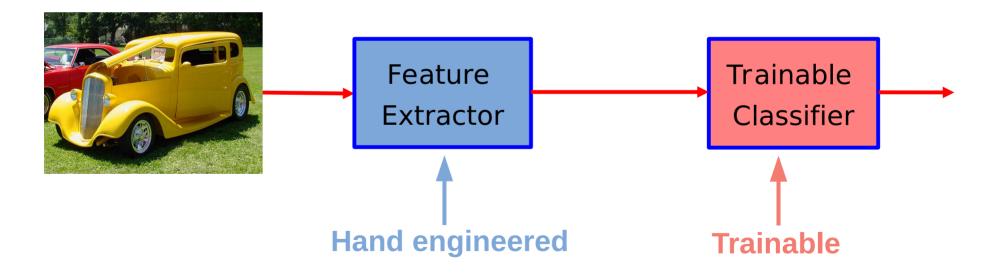
- Training a machine by showing examples instead of programming it
- When the output is wrong, tweak the parameters of the machine
- Works well for:
 - Speech → words
 - Image → categories
 - ▶ Portrait → name
 - Photo → caption
 - ► Text → topic





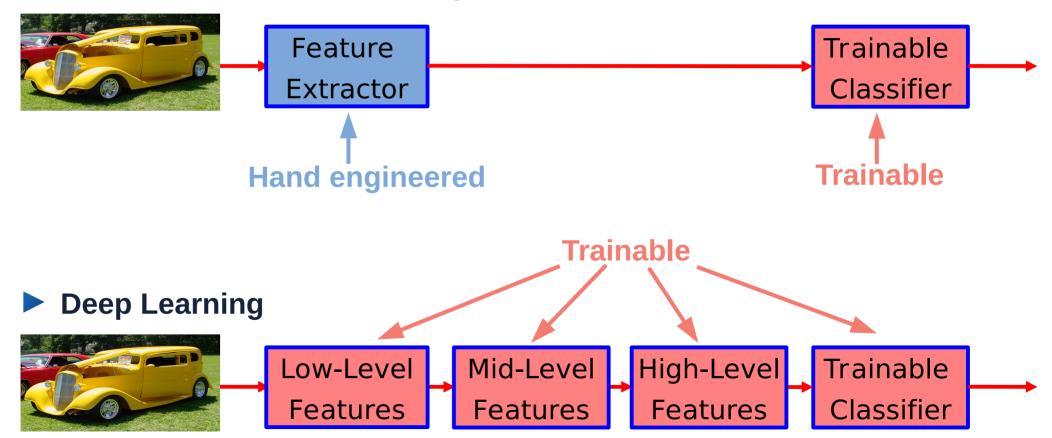
The Standard Paradigm of Pattern Recognition

- ...since the 1960s
- ...and "traditional" Machine Learning
 - ▶ until the "Deep Learning Revolution" (circa 2012)



Multilayer Neural Nets and Deep Learning

Traditional Machine Learning



Parameterized Model

Parameterized model

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

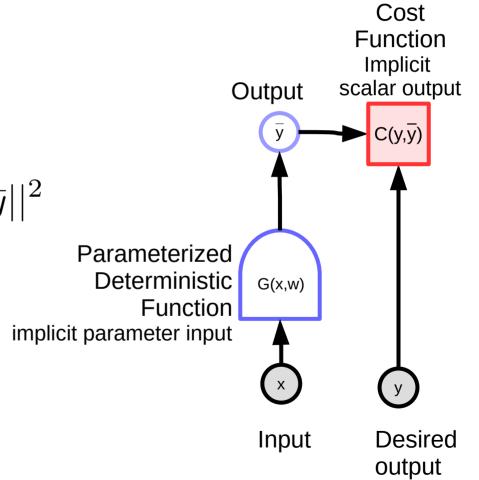
Example: linear regression

$$\bar{y} = \sum w_i x_i \quad C(y, \bar{y}) = ||y - \bar{y}||^2$$

Example: Nearest neighbor:

$$\bar{y} = \operatorname{argmin}_k ||x - w_{k,.}||^2$$

Computing function G may involve complicated algorithms



Block diagram notations for computation graphs





► Observed: input, desired output...



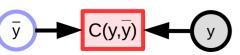
► Computed variable: outputs of deterministic functions

g(x,w) \overline{y}

Deterministic function

- ► Multiple inputs and outputs (tensors, scalars,....)
- ► Implicit parameter variable (here: w)

Scalar-valued function (implicit output)



- Single scalar output (implicit)
- used mostly for cost functions

Loss function, average loss.

▶ Simple per-sample loss function

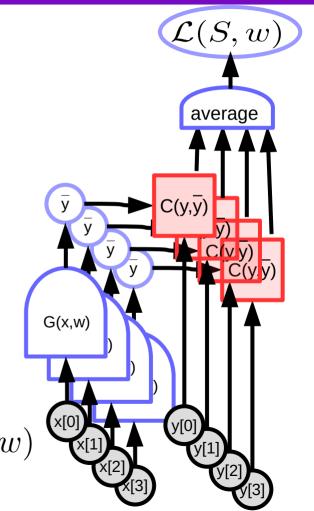
$$L(x, y, w) = C(y, G(x, w))$$

► A set of samples

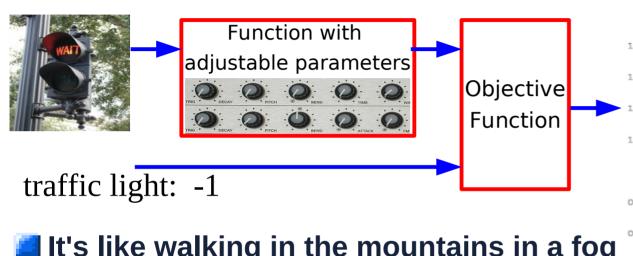
$$S = \{(x[p], y[p]) / p = 0 \dots P - 1\}$$

Average loss over the set

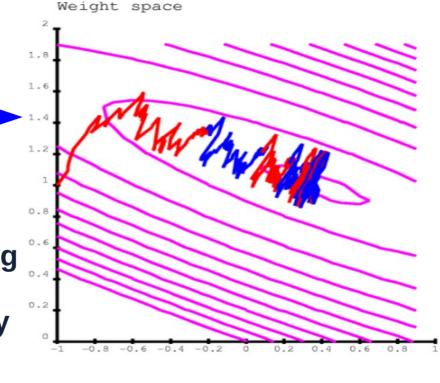
$$\mathcal{L}(S, w) = \frac{1}{P} \sum_{(x,y)} L(x, y, w) = \frac{1}{P} \sum_{p=0}^{P-1} L(x[p], y[p], w)$$



Supervised Machine Learning = Function Optimization



- It's like walking in the mountains in a fog and following the direction of steepest descent to reach the village in the valley
- But each sample gives us a noisy estimate of the direction. So our path is a bit random.



$$W_i \leftarrow W_i - \eta \frac{\partial L(W, X)}{\partial W_i}$$

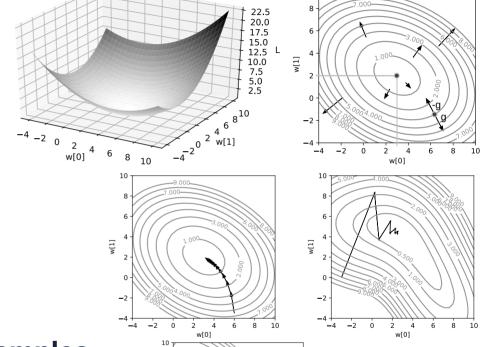
Gradient Descent

Full (batch) gradient

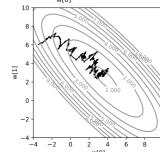
$$w \leftarrow w - \eta \frac{\partial \mathcal{L}(S, w)}{\partial w}$$

- Stochastic Gradient (SGD)
 - ► Pick a p in 0...P-1, then update w:

$$w \leftarrow w - \eta \frac{\partial L(x[p], y[p], w)}{\partial w}$$

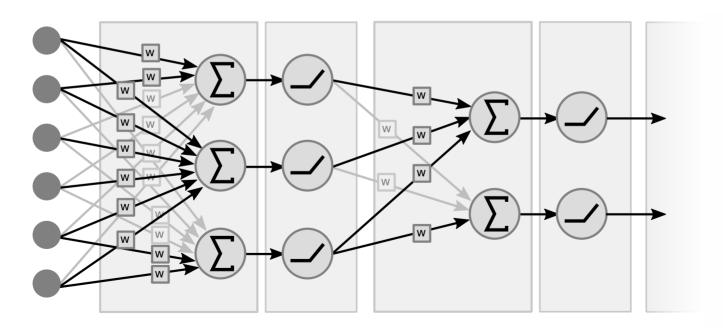


- SGD exploits the redundancy in the samples
 - ► It goes faster than full gradient in most cases
 - ▶ In practice, we use mini-batches for parallelization.



Traditional Neural Net

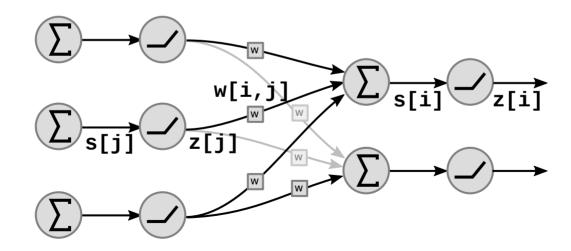
- Stacked linear and non-linear functional blocks
 - Weighted sums, matrix-vector product
 - ► Point-wise non-linearities (e.g. ReLu, tanh,)



Traditional Neural Net

Stacked linear and non-linear functional blocks

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



Backprop through a non-linear function

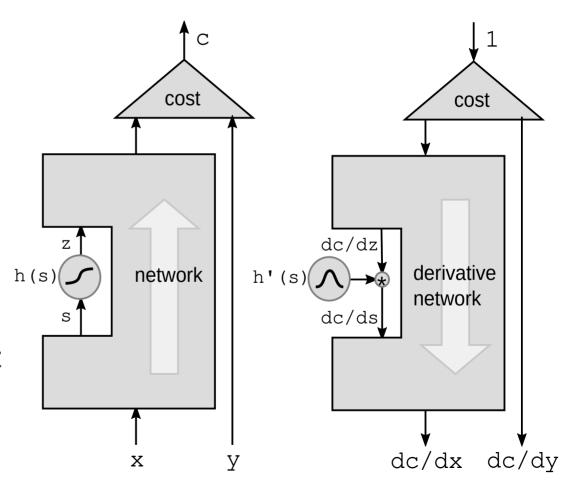
Chain rule:

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

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

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



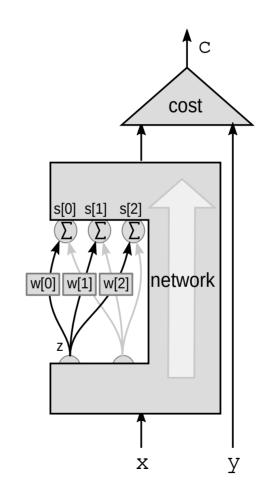
Backprop through a weighted sum

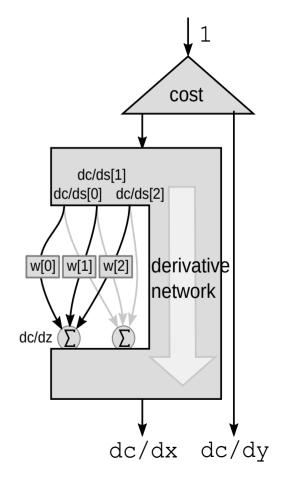
Perturbations:

- 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

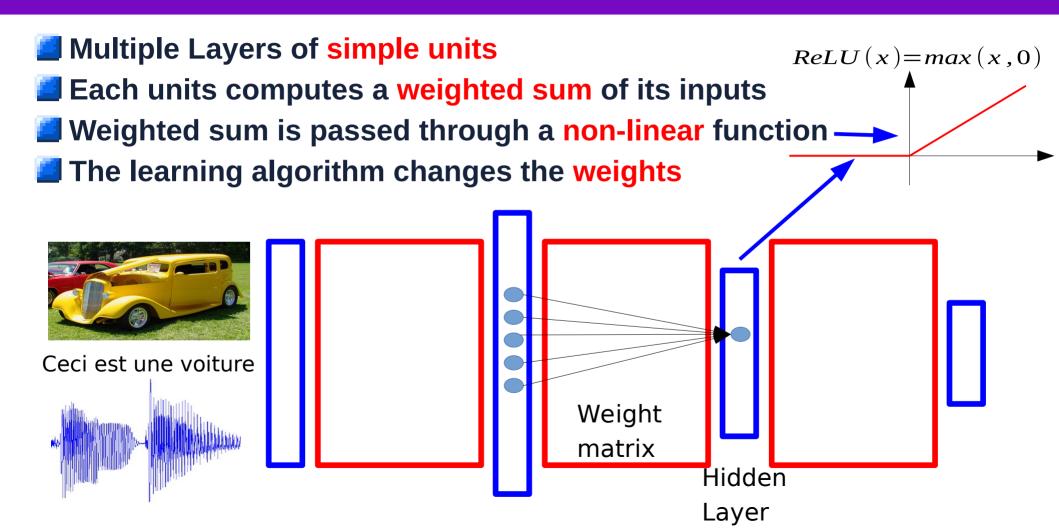
```
dc = ds[0]*dc/ds[0]+
ds[1]*dc/ds[1]+
ds[2]*dc/ds[2]
```

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





(Deep) Multi-Layer Neural Nets



Block Diagram of a Traditional Neural Net

- ullet linear blocks $\,s_{k+1}=w_kz_k\,$
- $lacksymbol{ ine}$ Non-linear blocks $z_k=h(s_k)$

$$w_0x$$
 b_1 $h(s_1)$ b_2 b_3 b_4 b_5 b_6 b_6 b_7 b_8 b_8

PyTorch definition

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

```
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)
```

import torch

Backprop through a functional module

Using chain rule for vector functions

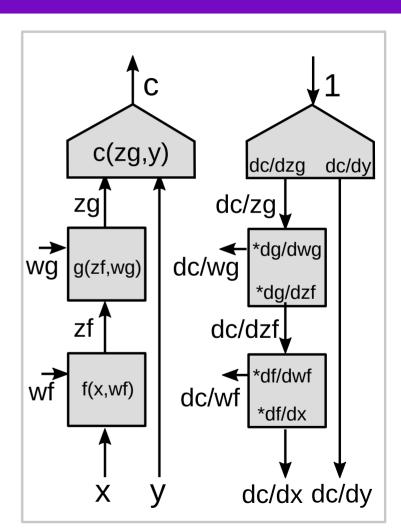
$$z_g:[d_g\times 1]\ z_f:[d_f\times 1]$$

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

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

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

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



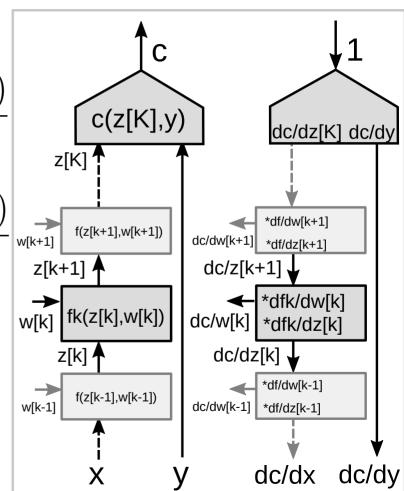
Backprop through a multi-stage graph

Using chain rule for vector functions

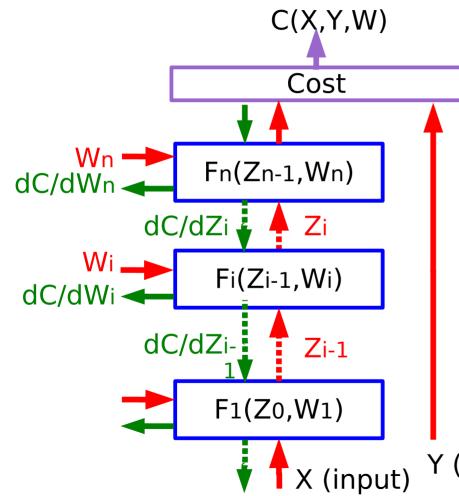
$$\frac{\partial c}{\partial z_k} = \frac{\partial c}{\partial z_{k+1}} \frac{\partial z_{k+1}}{\partial z_k} = \frac{\partial c}{\partial z_{k+1}} \frac{\partial f_k(z_k, w_k)}{\partial z_k}$$

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

- **▶** Two Jacobian matrices for the module:
 - ► One with respect to z[k]
 - One with respect to w[k]



Computing Gradients by Back-Propagation



- A practical Application of Chain Rule
- Backprop for the state gradients:
- $dC/dZ_{i-1} = dC/dZ_{i-1} dZ_{i}/dZ_{i-1}$
- $dC/dZ_{i-1} = dC/dZ_i \cdot dF_i(Z_{i-1},W_i)/dZ_{i-1}$
- Backprop for the weight gradients:
- dC/dWi = dC/dZi . dZi/dWi
- dC/dWi = dC/dZi . dFi(Zi-1,Wi)/dWi
- Much more on this later......

Y (desired output)

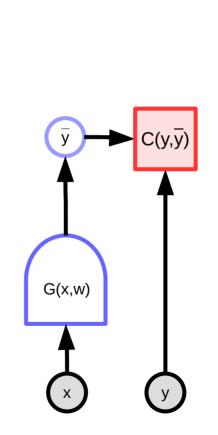
Backprop = propagation through a transformed graph

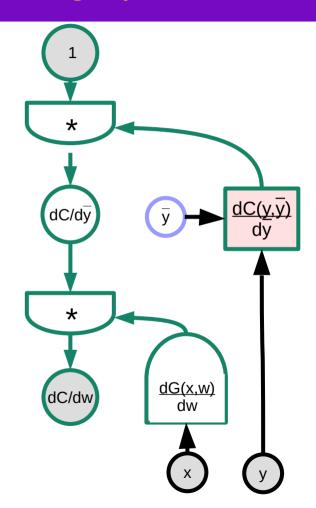
Derivative of composed functions

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

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

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





Gradient, Jacobian,

Dimensions:

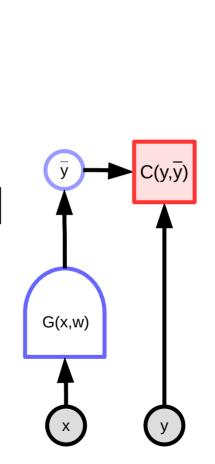
$$y, \bar{y}: [M \times 1] \quad w: [N \times 1]$$

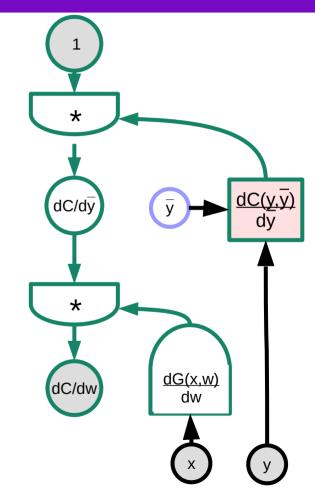
$$\frac{\partial C(y,\bar{y})}{\partial w} = \frac{\partial C(y,\bar{y})}{\partial \bar{y}} \frac{\partial \bar{y}}{\partial w} \\ [1 \times N] = [1 \times M] \cdot [M \times N]$$

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; dC/dX = W^T. dC/dY; dC/dW = X dC/dY

ReLU y = ReLU(x); if (x<0) dC/dx = 0 else dC/dx = dC/dy

Duplicate Y1 = X, Y2 = X; dC/dX = dC/dY1 + dC/dY2

Add Y = X1 + X2; dC/dX1 = dC/dY; dC/dX2 = dC/dY

Max y = max(x1,x2); if (x1>x2) dC/dx1 = dC/dy else dC/dx1=0

LogSoftMax Yi = Xi - log[\sum_i exp(Xj)]; .....???
```

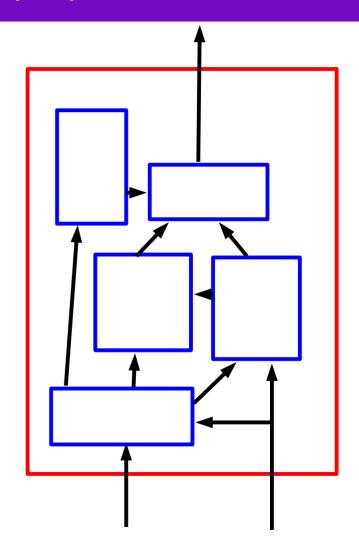
Non-Linear functions and Loss functions in PyTorch

- 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 backprop through time



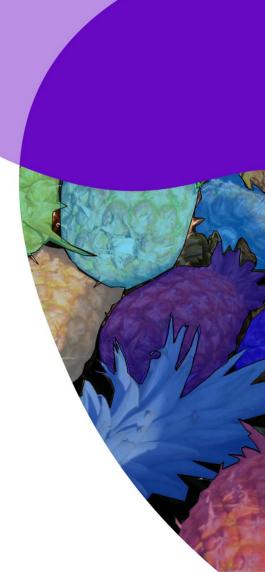
Backprop in Practice

- 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.



Learning Representations

What are good representations? Why do networks need to be deep?



Linear Classifiers and their limitations

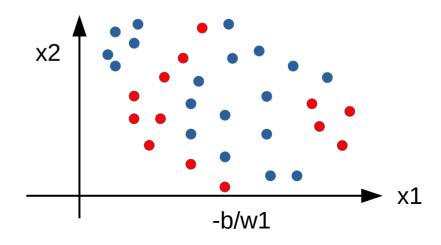
Linear classifier

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

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

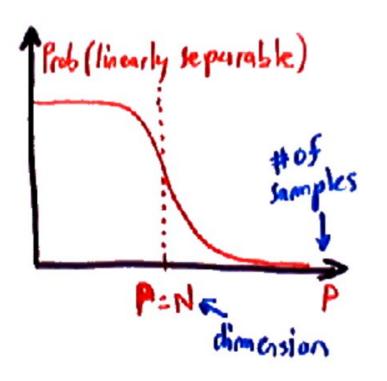
$$\sum_{i=1}^{N} w_i x_i + b = 0$$

Not linearly separable dataset



Number of linearly separable dichotomies

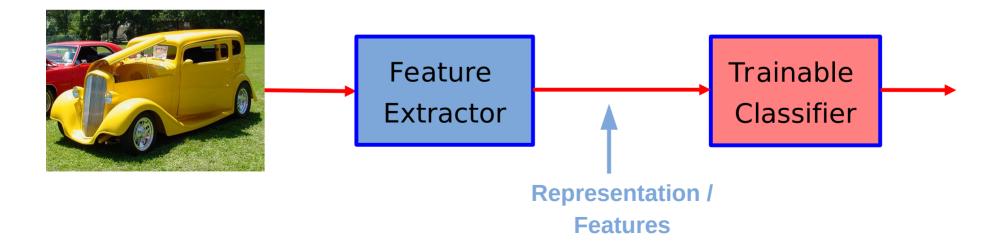
- ► The probability that a dichotomy over P points in N dimensions is linearly separable goes to zero as P gets larger than N
 - [Cover's theorem 1966]



- 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?



Ideas for "generic" feature extraction

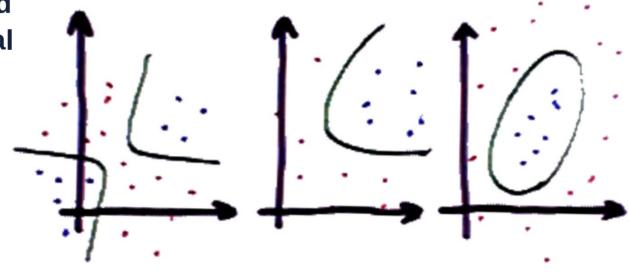
- Basic principle:
 - expanding the dimension of the representation so that things are more likely to become linearly separable.
- space tiling
- random projections
- polynomial classifier (feature cross-products)
- radial basis functions
- kernel machines

Example: monomial features

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

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

- 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.



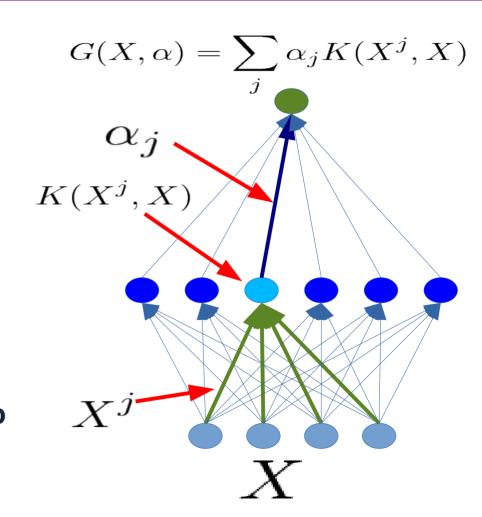
Shallow networks are universal approximators!

SVMs and Kernel methods

- Layer1: kernels; layer2: linear
- The first layer is "trained" with the simplest unsupervised method ever devised: using the samples as templates for the kernel functions.

2-layer neural nets

- Layer1: dot products + non-linear function; Layer2: linear
- But few useful functions can be efficiently represented with only two layers of reasonable size.



Do we really need deep architectures?

Theoretician's dilemma: "We can approximate any function as close as we want with shallow architecture. Why would we need deep ones?"

$$y = \sum_{i=1}^{P} \alpha_i K(X, X^i)$$
 $y = F(W^1.F(W^0.X))$

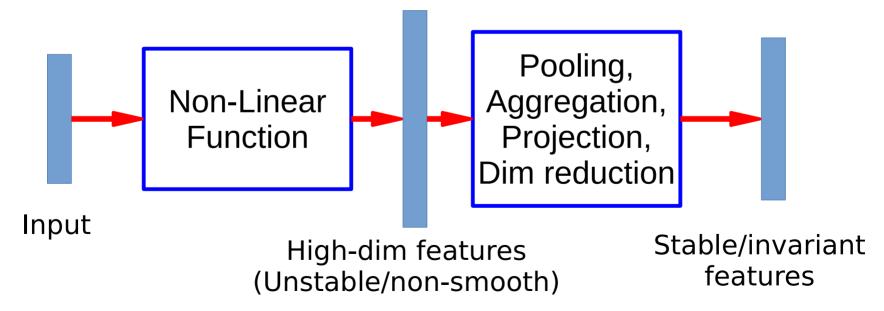
- kernel machines (and 2-layer neural nets) are "universal".
- Deep learning machines

$$y = F(W^K.F(W^{K-1}.F(....F(W^0.X)...)))$$

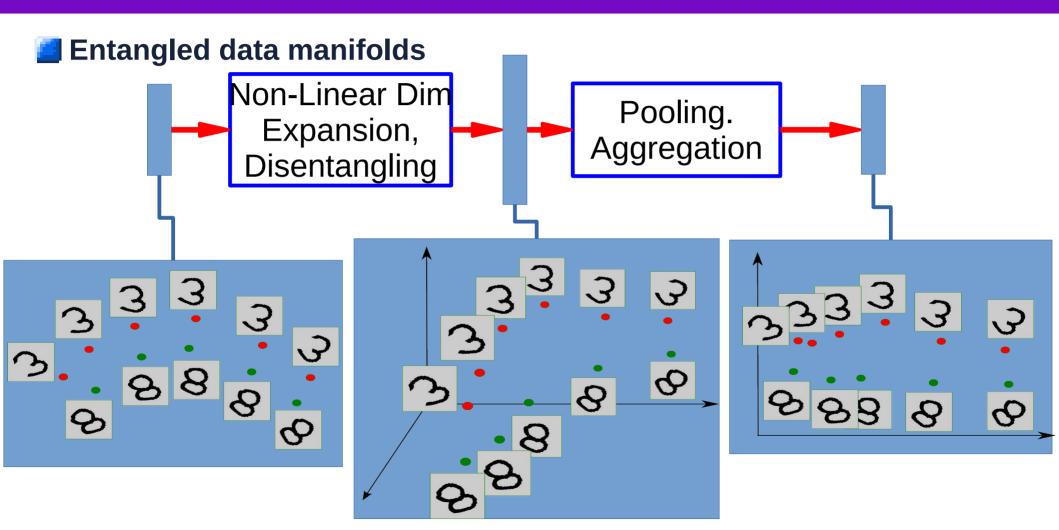
- Deep machines are more efficient for representing certain classes of functions, particularly those involved in visual recognition
 - they can represent more complex functions with less "hardware"
- We need an efficient parameterization of the class of functions that are useful for "AI" tasks (vision, audition, NLP...)

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



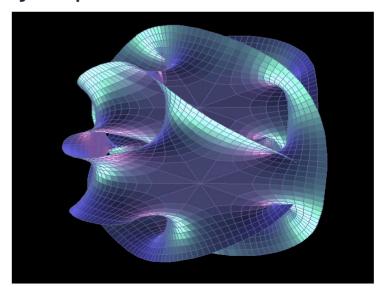
Sparse Non-Linear Expansion → Pooling

Use non-linear fn to break things apart, pool together similar things Clustering, Pooling. Quantization, Aggregation **Sparse Coding** Linear+ReLU

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





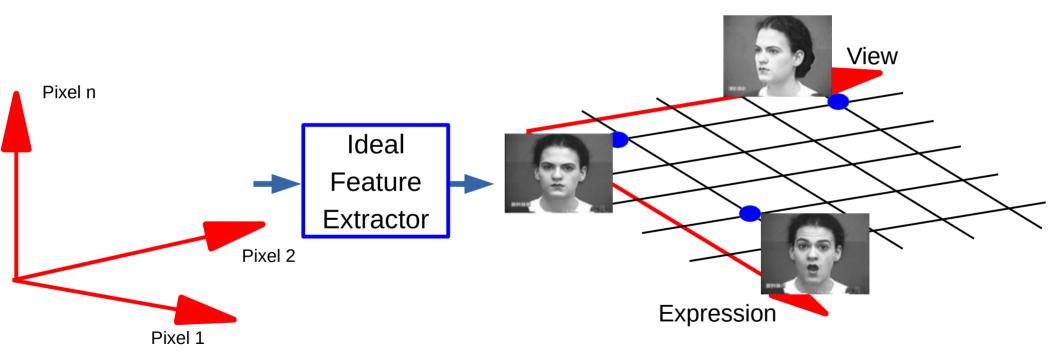
Discovering the Hidden Structure in High-Dimensional Data

- 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</p>
- 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

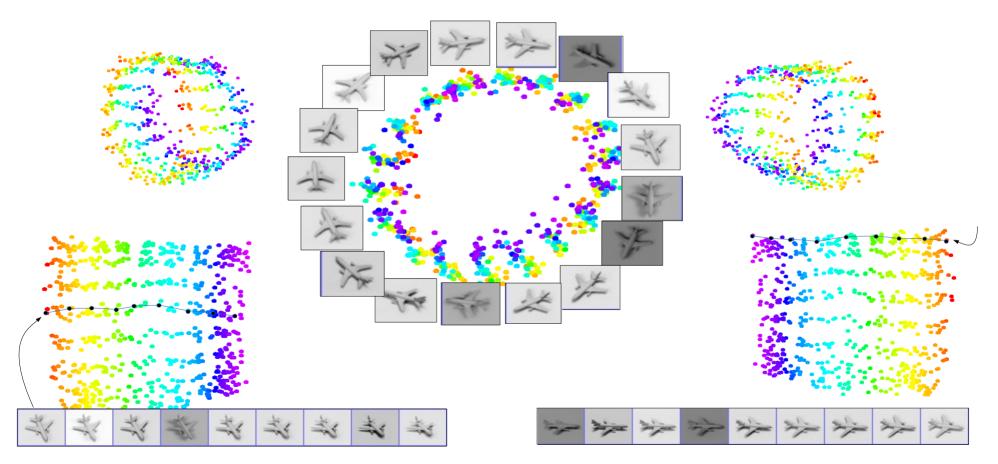
Disentangling factors of variation

The Ideal Disentangling Feature Extractor



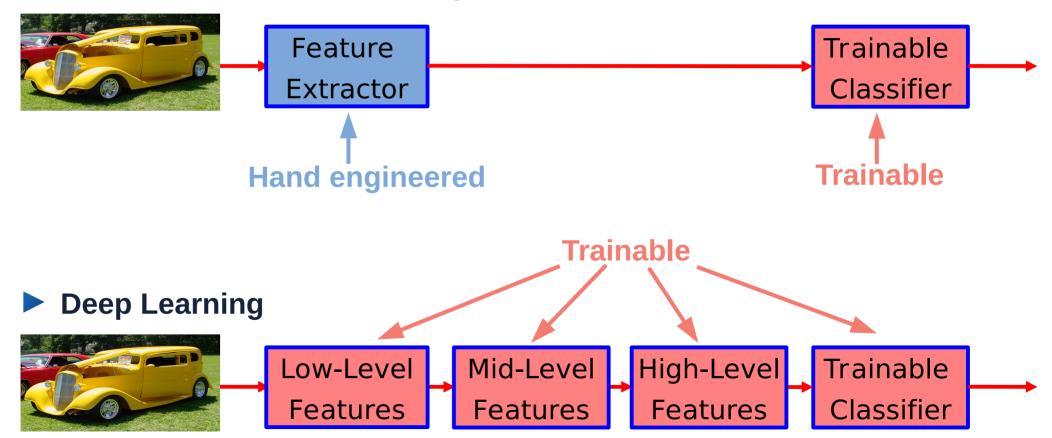
Data Manifold

[Hadsell et al. CVPR 2006]



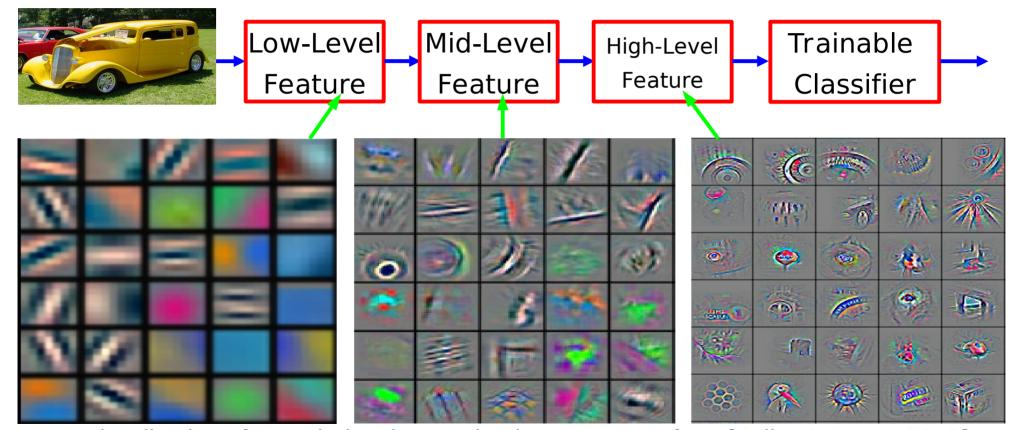
Deep Learning = Learning Hierarchical Representations

Traditional Machine Learning



Multilayer Architectures == Compositional Structure of Data

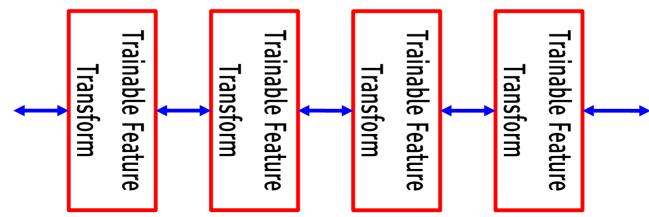
Natural is data is compositional => it is efficiently representable hierarchically



Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

Multilayer Architecture == Hierarchical representation

- Hierarchy of representations with increasing level of abstraction
- Each stage is a kind of trainable feature transform
- Image recognition
 - \triangleright Pixel \rightarrow edge \rightarrow texton \rightarrow motif \rightarrow part \rightarrow object
- Text
 - Character → word → word group → clause → sentence → story
- Speech
 - \triangleright Sample → spectral band → sound → ... → phone → phoneme → word



Why would deep architectures be more efficient?

[Bengio & LeCun 2007 "Scaling Learning Algorithms Towards AI"]

- A deep architecture trades space for time (or breadth for depth)
 - more layers (more sequential computation),
 - but less hardware (less parallel computation).
- Example1: N-bit parity
 - requires N-1 XOR gates in a tree of depth log(N).
 - Even easier if we use threshold gates
 - requires an exponential number of gates of we restrict ourselves to 2 layers (DNF) formula with exponential number of minterms).
- Example2: circuit for addition of 2 N-bit binary numbers
 - Requires O(N) gates, and O(N) layers using N one-bit adders with ripple carry propagation.
 - Requires lots of gates (some polynomial in N) if we restrict ourselves to two layers (e.g. Disjunctive Normal Form).
 - Bad news: almost all boolean functions have a DNF formula with an exponential number of minterms O(2^N).....