TTIC 31230, Fundamentals of Deep Learning

David McAllester, April 2019

Interpreting Deep Networks

The Black Box Problem

The Human Black Box — Perception

Introspection is notoriously inadequate for AI.

Explain how you know there are upside down glasses in this picture.



The Human Black Box — Inference

Certain facts are obvious.

A king on empty chess board can reach every square (obvious).

A knight on an empty chess board can reach every square (true but not obvious).

The Human Black Box — Inference

Consider a graph with colored nodes.

If every edge is between nodes of the same color, then any path connects nodes of the same color.

Consider a swiss chocolate bar of 3×5 little squares.

How many breaks does it take to reduce this to fifteen unconnected squares?

Dimensionality Reduction

Visualizing the representation

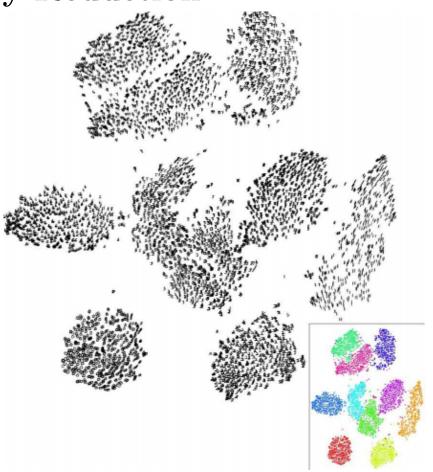
t-SNE visualization

[van der Maaten & Hinton]

Embed high-dimensional points so that locally, pairwise distances are conserved

i.e. similar things end up in similar places. dissimilar things end up wherever

Right: Example embedding of MNIST digits (0-9) in 2D



[Stanford CS231]

t-SNE

Consider high dimensional data x_1, \ldots, x_N with $x \in \mathbb{R}^d$.

$$P(j|i) = \frac{1}{Z_i} \exp\left(\frac{-||x_i - x_j||^2}{2\sigma_i^2}\right)$$

Set σ_i such that $H(P(j|i)) = \ln k$ (soft k nearest neighbors).

$$P(i,j) = P(i)P(j|i) = \frac{1}{N} P(j|i)$$

t-SNE

Let $Y = \{y_i, \dots, y_N\}$ be an assignment of a vector with $y_i \in \mathbb{R}^2$ to each high dimensional point x_i .

$$Q_Y(i,j) = \frac{1}{Z} \left(\frac{1}{1 + ||y_i - y_j||^2} \right)$$

$$Y^* = \underset{Y}{\operatorname{argmin}} \operatorname{KL}(P, Q_Y)$$

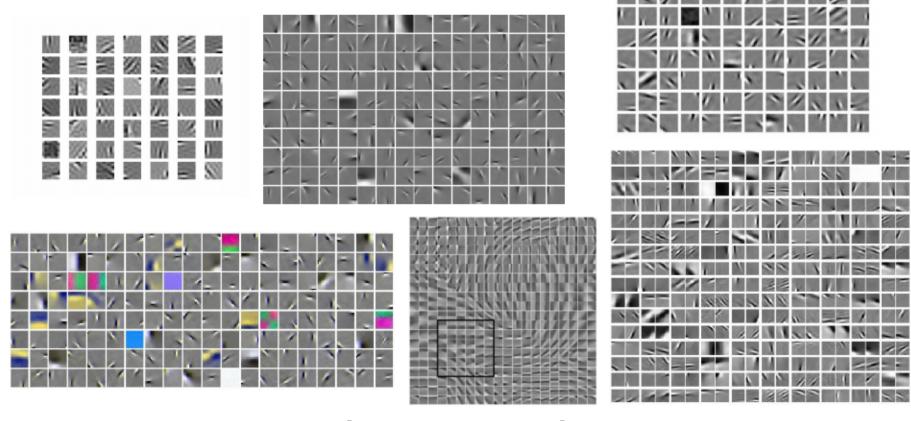
t-SNE vs. Projection Modeling

t-SNE — y(x) is defined by a table on the data points.

In PCA or Isomap we have $y_{\Phi}(x) \in \mathbb{R}^2$ for a parameterized function y_{Φ} .

Visualizing the Filters

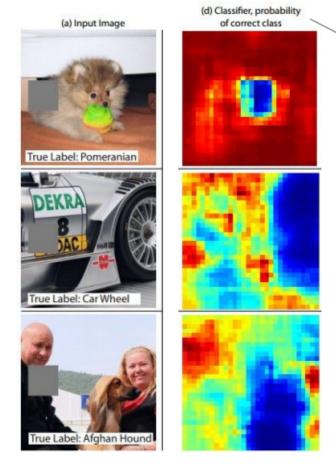
The gabor-like filters fatigue



[Stanford CS231]

Occlusion experiments

[Zeiler & Fergus 2013]

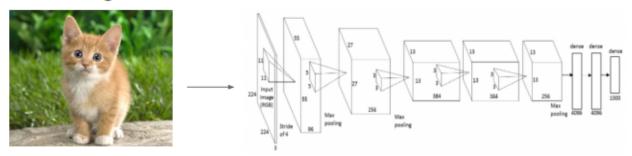


(as a function of the position of the square of zeros in the original image)

[Stanford CS231]

Backpropagation from Individual Neurons Deconv approaches

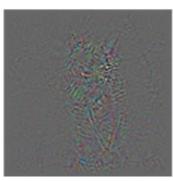
1. Feed image into net



2. Pick a layer, set the gradient there to be all zero except for one 1 for

some neuron of interest

3. Backprop to image:



"Guided backpropagation:" instead



[Stanford CS231]

Rather than $\partial \ell/\partial x$ we are interested in ∂ neuron/ ∂x .

We are interested in ∂ neuron/ ∂x where x in one color channel of one input pixel.

It turns out that ∂ neuron/ ∂x looks like image noise.

Instead we compute $x.\operatorname{ggrad}$ — a **guided** version of ∂ neuron $/\partial x$.

Guided backpropagation only considers computation paths that activate (as opposed to suppress) the neuron all along the activation path.

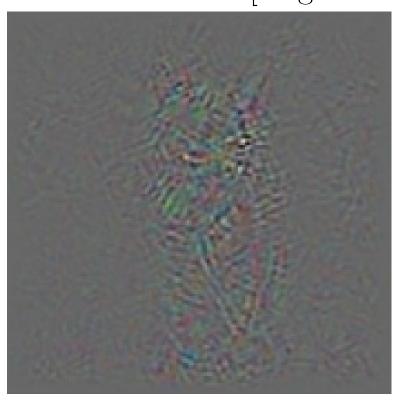
The backpropagation at activation functions is modified.

For a neuron y with y = s(x) for activation function s:

$$x.\text{ggrad} = \mathbf{1}[y.\text{ggrad} > 0] \ y.\text{ggrad} \ ds/dx$$



[Zeigler and Fergus 2013]





[Zeigler and Fergus 2013]

Neural Network Neuroscience

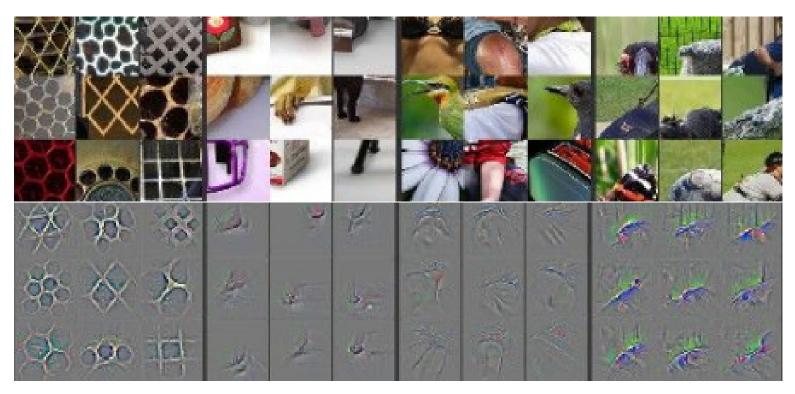
[Zeigler and Fergus 2013]

Take a neuron (linear threshold unit) and select the images causing the greatest response of that Neuron.

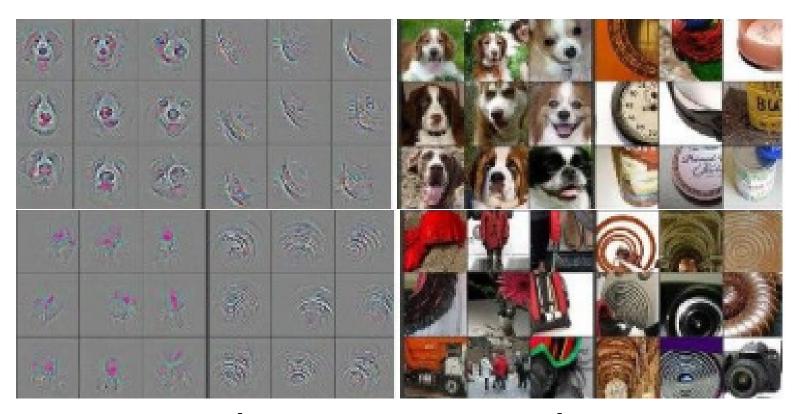
Do guided backpropagation from that neuron onto the image.



[Zeigler and Fergus 2013]



[Zeigler and Fergus 2013]



[Zeigler and Fergus 2013]



[Zeigler and Fergus 2013]

A Wheel or Face Detector

The nine strongest stimulators of the "wheel or face cell" are the following.





[Zeigler and Fergus 2013]

it's like "vodka & potato" classifier!

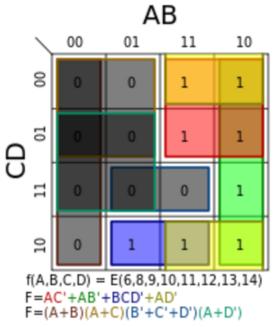


[Alyosho Efros]

The Kaurnaugh Model of DNNs

The Karnaugh map, also known as the K-map, is a method to simplify boolean algebra expressions.

Truth table of a function					
	A	В	C	D	f(A, B, C, D)
0	0	0	0	0	0
1	0	0	0	1	0
2	0	0	1	0	0
3	0	0	1	1	0
4	0	1	0	0	0
5	0	1	0	1	0
6	0	1	1	0	1
7	0	1	1	1	0
8	1	0	0	0	1
9	1	0	0	1	1
10	1	0	1	0	1
11	1	0	1	1	1
12	1	1	0	0	1
13	1	1	0	1	1
14	1	1	1	0	1
15	1	1	1	1	0



$$F(A, B, C, D) = AC' + AB' + BCD' + AD'$$

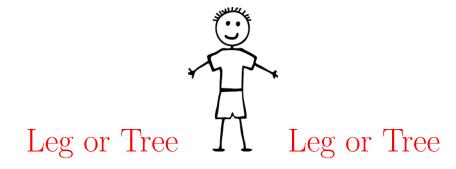
= $(A + B)(A + C)(B' + C' + D')(A + D')$

A Kaurnaugh Person Detector

Wheel or Face

Hand or Flower

Hand or Flower



The set of locally minimal models (circuits) could be vast (exponential) without damaging performance.

Is a Boolean circuit a distributed representation?

The Glass Model of SGD

Pysical glass (ordinary silica glass) is a metastable state — the ground state is quartz crystal.

As molten glass cools there is a temperature T_g (± 1 degrees C) at which it "solidifies" (the viscosity becomes huge).

This soldification process is very repeatable with a well defined final energy.

However, the local optimum achieved is presumably very different for each instance of cooling.

Identifying Channel Correspondences

Convergent Learning: Do Different Neural Networks Learn The Same Representations?, Li eta al., ICLR 2016.

Train Alexnet twice with different initializations to get net1 and net2.

For each convolution layer, each channel i of net1, and each channel j of net2, compute their correlation.

$$\rho_{i,j} = E\left[\frac{(u_i - \mu_i)(u_j - \mu_j)}{\sigma_i \sigma_j}\right]$$

Semi-matching and Bipartite matching

Semi-matching: for each i in net1 find the best j in net2:

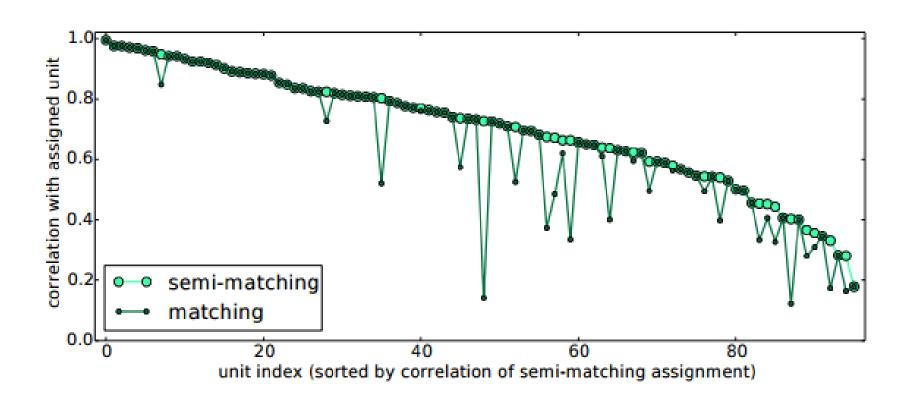
$$\hat{j}(i) = \operatorname*{argmax}_{j} \rho_{i,j}$$

Biparetitie Matching: Find the best one-to-one correspondence.

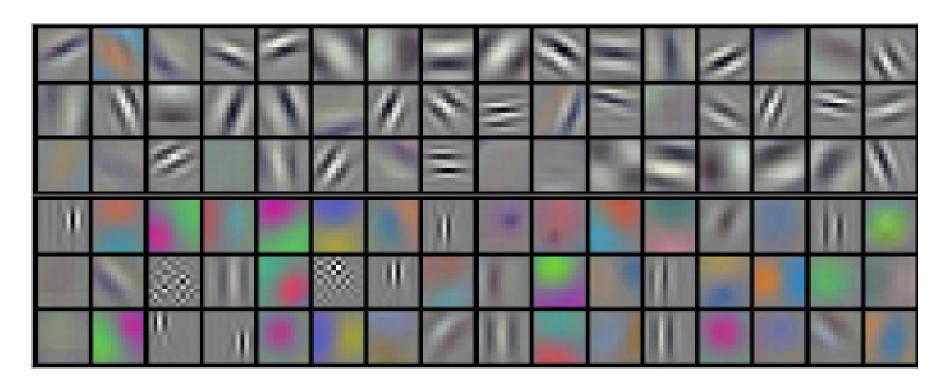
$$\hat{j} = \underset{\hat{j} \text{ a bijection}}{\operatorname{argmax}} \sum_{i} \rho_{i,\hat{j}(i)}$$

Bipartite matching can be solved by a classical algorithm [Hopcroft and Karp, 1973]. John Hopcroft (age 77) is an author on this ICLR paper.

Correlations at Layer 1 (Wavelet Layer)

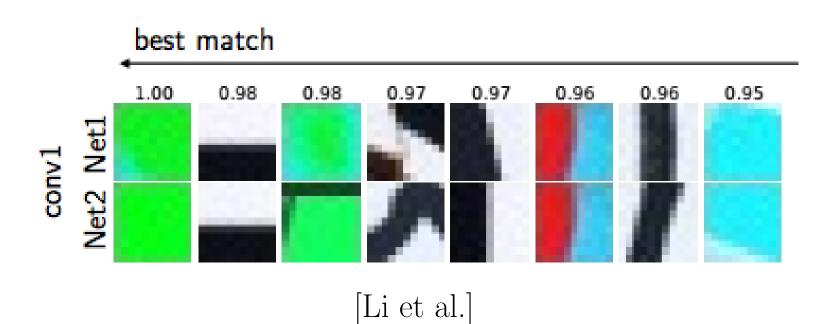


Alexnet Layer 1

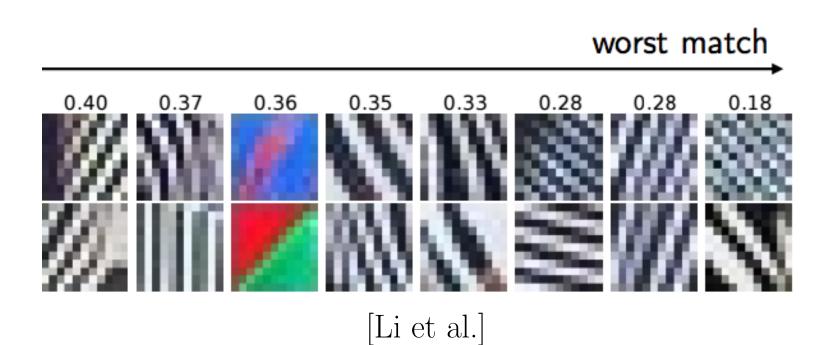


[Krizhevsky et al.]

Best Matches in Layer 1 semi-matching

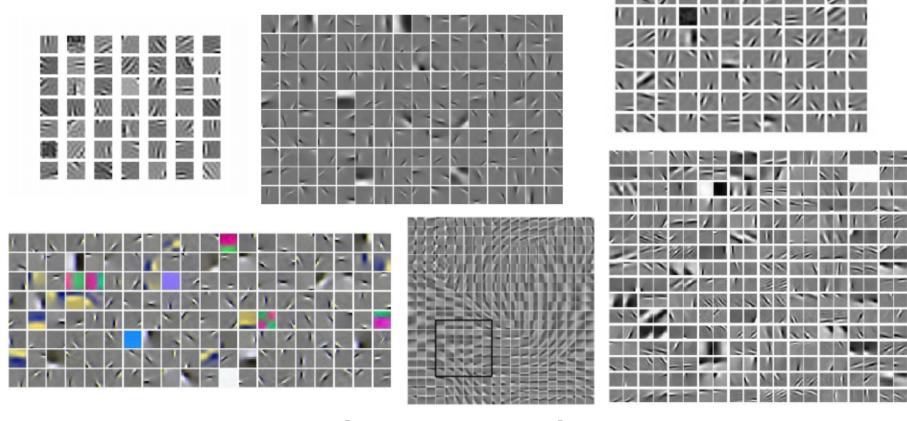


Worst Matches in Layer 1 semi-matching



Layer 1 in Other Networks

The gabor-like filters fatigue



[Stanford CS231]

Regression Between Networks at Layer 1

Model each channel of net1 as a linear combination of channels of net2 using least squares regression.

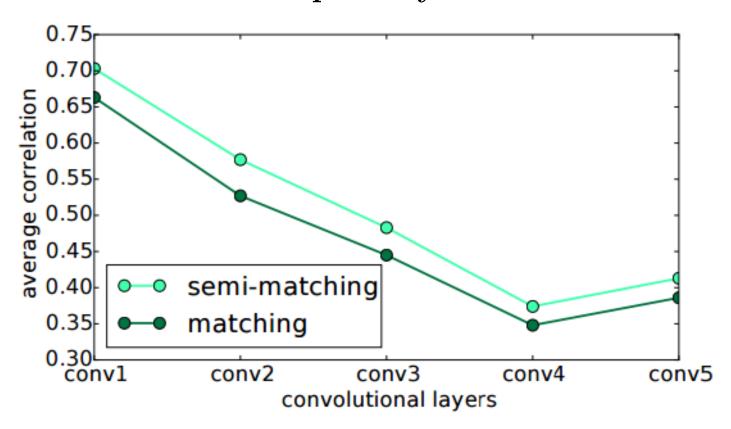
Before the regression each channel is normalized to have zero mean and channel variance.

No correlation would yield a square loss of 1.000.

No regularization gives a square loss of 0.170 and uses 96 channels in each prediction.

L1 regularization gives a square loss of 0.235 and uses 4.7 channels in each prediction.

Deeper Layers



In the regression experiment squared error was not significantly reduced at layers 3 through 5 even without regularization.

SVCCA Analysis Raghu et al., November 2017

Consider a matrix W[i,j] used in some model as

$$y[i] = \sigma \left(\sum_{j} W[i, j] x[j] + b[i] \right)$$

We want to understand the meaning of the matrix W[i, j] and the vector y[I].

SVCCA

$$y[i] = \sigma \left(\sum_{j} W[i, j] x[j] + b[i] \right)$$

We can collect a set y[t, I] of vectors y computed from x[t, J]

$$y[t, i] = \sigma \left(\sum_{j} W[i, j] x[t, j] + b[i] \right)$$

Here t can range over different inputs to the entire network, or different image locations where the filter W is used, or different times with a single RNN execution.

PCA on the matrix outputs

We can then perform PCA over the vectors y[t, I] to find a a reduced set of covariance eigenvectors B[k, I]. and represent y by its projection on the eigenvectors.

$$\tilde{y}[t,k] = B[k,I]^{\top}(y[t,I] - \mu[I])$$

PCA can be defined by

$$B^* = \underset{B}{\operatorname{argmin}} \sum_{t} \left\| y[t, I] - \mu[I] + \sum_{j} \tilde{y}[t, k] B[k, I] \right\|^2$$

PCA reduction

Now consider a layer that uses y[I] and the tensor **before the** nonlinearity.

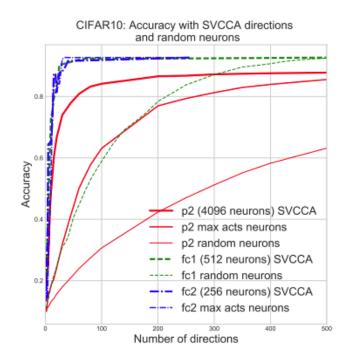
$$z[t, v] = \sum_{i} W'[v, i]y[i] + B'[v]$$

This layer can now be redefined to use the \tilde{y}

$$z[t,v] = \sum_{i} W''[v,k]\tilde{y}[t,k] + B''[v]$$

$$W''[v, k] = \sum_{i} W'[v, i]B[k, i]$$

Reduction



Attention as Explanation



A woman is throwing a frisbee in a park.



A little <u>girl</u> sitting on a bed with a teddy bear.

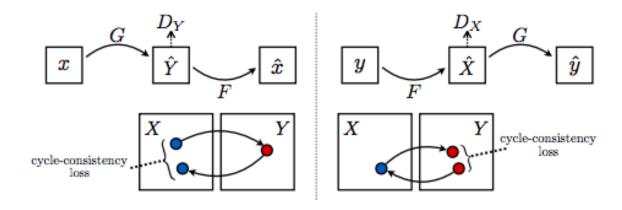
Xu et al. ICML 2015

Interpretation from Domain Correspondence

Kushner verliert den Zugang zu streng geheimen Informationen.



Kushner loses access to top-secret intelligence.



Causal Models are Explicitly Interpretable

Flu causes symptoms x, y z.

Strep causes symptoms x, y, u.

For the given information on the patient, the prior probability for flu is . . .

Can Alpha Zero Explain Chess Moves?

I did x because if I did y they would do z and, in that case, \dots

\mathbf{END}