# TTIC 31230, Fundamentals of Deep Learning

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## 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 $3 \times 5$ little squares.

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

# Dimensionality Reduction

[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 $\sigma_i$ 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 $x_i$.

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

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

# 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 $y_\Phi$.

# Visualizing the Filters

[Stanford CS231]

[Stanford CS231]

# Backpropagation from Individual Neurons

[Stanford CS231]

# Guided Backpropagation

Rather than $\partial\ell/\partial x$ we are interested in $\partial\text{neuron}/\partial x$.

We are interested in $\partial\text{neuron}/\partial x$ where $x$ in one color channel of one input pixel.

It turns out that $\partial\text{neuron}/\partial x$ looks like image noise.

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

# Guided Backpropagation

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 $s$:

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

# Guided Backpropagation

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[Zeigler and Fergus 2013]

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# 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.

# Guided Backpropagation Layer 2

[Zeigler and Fergus 2013]

# Guided Backpropagation Layer 3

[Zeigler and Fergus 2013]

# Guided Backpropagation Layer 4

[Zeigler and Fergus 2013]

# Guided Backpropagation Layer 5

[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]

[Alyosho Efros]

# The Kaurnaugh Model of DNNs

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

$$
\begin{aligned}
F(A, B, C, D) &= AC' + AB' + BCD' + AD' \\
&= (A + B)(A + C)(B' + C' + D')(A + D')
\end{aligned}
$$

# A Kaurnaugh Person Detector

Wheel or Face

Hand or Flower                    Hand or Flower

Leg or Tree  Leg or Tree

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

Is a Boolean circuit a distributed representation?

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# 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 $T_g$ ($\pm 1$ 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.

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

# Semi-matching and Bipartite matching

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

$$\hat{j}(i) = \underset{j}{\mathrm{argmax}}\, \rho_{i,j}$$

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

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

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

[Li et al.]

# Worst Matches in Layer 1 semi-matching

[Li et al.]

# Layer 1 in Other Networks

[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 <span style="color:red">square loss of 1.000</span>.

No regularization gives a <span style="color:red">square loss of 0.170</span> and uses <span style="color:red">96 channels</span> in each prediction.

L1 regularization gives a <span style="color:red">square loss of 0.235</span> and uses <span style="color:red">4.7 channels</span> 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

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

# 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

Xu et al. ICML 2015

# Interpretation from Domain Correspondence

Kushner verliert den Zugang zu streng geheimen Informationen.

$$\Rightarrow$$

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,
.....

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