PAIR
People + AI Research
Bringing Design Thinking and HCI to Machine Learning
google.ai/pair
Today’s Agenda

What is data visualization?
How does it work? What are some best practices?

How has visualization been applied to ML?
Overview of the landscape
Special case: high-dimensional data
Goals

Understand state of the art
Known best practices in visualization
Broad survey of existing applications to ML

Apply visualizations in your own situation
References to tools and libraries
References to literature
What is data visualization?

Transform data into visual encodings

What is it good for?
Data exploration
Scientific insight
Communication
Education

How to ensure it works well?
Engage the visual system in smart ways
Take advantage of pre-attentive processing
What is data visualization?

Transform data into visual marks

What is it good for?
Data exploration
Scientific insight
Communication
Education

How is it different from statistics?

Vis: no specific question necessary
Classic Stats: you investigate a specific question*
Vis & Stats: wonderful, complementary partners

How to ensure it works well?
Engage the visual system in smart ways
Take advantage of pre-attentive processing

*OK, maybe not in EDA, but visualization is the key technique there anyway!
Predates computers...
William Playfair (1786)

Line, bar, pie charts were all invented by the same person!

Aside from revolutionizing graphics, Playfair was an economist, engineer, and even a secret agent.
Florence Nightingale (1858)

These charts led to the adoption of better hygiene / sanitary practices in military medicine, saving millions of lives.

Arguably the most effective visualization ever!

This particular visualization technique would be frowned on today. Lesson: technique is less important than having the right data and right message.
W. E. B. Du Bois (1900)

For 1900 World’s Fair, a compendium of visualizations. Many new chart types!

Excellent example of visualization aimed at political change.

<table>
<thead>
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<th>Class of Annual Income</th>
<th>Actual Average</th>
<th>Rent</th>
<th>Food</th>
<th>Clothes</th>
<th>Direct Taxes</th>
<th>Other Expenses and Savings</th>
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<td>43%</td>
<td>28%</td>
<td>8.9%</td>
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<td>18%</td>
<td>37%</td>
<td>15%</td>
<td>5.5%</td>
<td>24.5%</td>
</tr>
</tbody>
</table>

(Quartz)
What do these have in common?

Using special properties of the visual system to help us think.
What do these have in common?

Using special properties of the visual system to help us think.

Our visual system is like a GPU
- Incredibly good at a few special tasks
- With work, can be repurposed for more general situations
What do these have in common?

Using special properties of the visual system to help us think.

Our visual system is like a GPU

- Incredibly good at a few special tasks
- With work, can be repurposed for more general situations

All visualizations are made from a series of compromises.
How do visualizations work?
How do visualizations work?

Find visual encodings that

- Guide viewer’s attention
- Communicate data to the viewer
- Let viewer calculate with data

On computer

- Interactive exploration
How do visualizations work?

Find visual encodings that

- Guide viewer’s attention
- Communicate data to the viewer
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On computer

- Interactive exploration
Encodings: some examples

Comparison A (2012): US Wind Map

Comparison B (2013): Earth.nullschool
Encodings: some theory

From perceptual psychology:
different encodings have different properties.
Encodings: some theory

Good for communicating exact values...
Encodings: some theory

Good for communicating ratios...
Encodings: some theory

Good for drawing attention...
Special case: color scales

Intensively studied for decades...
Rogowitz & Treinish (1996)

Web article:
“Why Should Engineers and Scientists Be Worried About Color?”

Conclusions:
- Rainbow scales: bad
- There is no “best” scale
Practically speaking...

When in doubt, use the "Color Brewer" site:
http://colorbrewer2.org

(Built by Cynthia Brewer, a cartographer)
And study continues to this day...

A dive into a very recent paper (CHI 2018)

Somewhere Over the Rainbow: An Empirical Assessment of Quantitative Colormaps

Yang Liu
University of Washington
Seattle, WA, USA
yliu0@cs.washington.edu

Jeffrey Heer
University of Washington
Seattle, WA, USA
jheer@uw.edu
Color scales

Figure 1: **Colormaps under study.** We evaluate four single-hue, three perceptually-uniform multi-hue, a diverging, and a rainbow colormap(s). We divide them into (a) assorted, (b) single-hue and (c) multi-hue groups, with two colormaps repeated across groups for replication.

Figure 2: **Experiment interface.** Participants see a reference stimulus along with two choices, and pick which of these alternatives is closer in distance to the reference.
Color scales

(a) Assorted Colormaps

(b) Single-Hue Colormaps

(c) Multi-Hue Colormaps
Uh oh, colorblindness... (very common!)

Guiding attention
Pre-attentive processing
Count the 5s

987349790275647902894728624092406037070570279072
803208029007302501270237008374082078720272007083
247802602703793775709707377970667462097094702780
927979709723097230979592750927279798734972608027
Count the 5s
Theory: attention

Pre-attentive processing / “popout”

Under the right circumstances, visual search can be parallel, rather than serial.

Time to find target does not increase as number of distractors increases.

(Colin Ware, Visual Thinking for Design)
Pre-Attentive Processing

Color

Shape
Layering & separation after Tufte
Layering & separation

after Tufte
Theory: calculation
Calculation

Example: we naturally average sizes.

Calculation

We can do weighted averages, too!

Example
Calculation

Hertzsprung-Russell diagram (via Wikipedia)

Your eye is doing something like kernel density estimation...

How do visualizations work - on computers?
How do visualizations work - on computers?

Beyond static representations

- Interaction
- Conversation and collaboration
Theory: interaction

Shneiderman “mantra”:
(1996: “The Eyes Have It: A Task by Data Type Taxonomy for Information Visualizations”)

- Overview first
- Zoom and filter
- Details on demand
Theory: interaction

Shneiderman “mantra”:
(1996: “The Eyes Have It: A Task by Data Type Taxonomy for Information Visualizations”)

- Overview first
- Zoom and filter
- Details on demand

Example: dot maps

There are many visual design guidelines but the basic principle might be summarized as the Visual Information Seeking Mantra:

Overview first, zoom and filter, then details-on-demand
Overview first, zoom and filter, then details-on-demand
Overview first, zoom and filter, then details-on-demand
Overview first, zoom and filter, then details-on-demand
Overview first, zoom and filter, then details-on-demand
Overview first, zoom and filter, then details-on-demand
Overview first, zoom and filter, then details-on-demand
Overview first, zoom and filter, then details-on-demand

Each line represents one project in which I found myself rediscovering this principle and therefore wrote it down it as a reminder.
The Racial Dot Map: One Dot Per Person for the Entire U.S.
demographics.virginia.edu/DotMap/
Recap: How do visualizations work?

Find visual encodings that
● Guide viewer’s attention
● Communicate data to the viewer
● Let viewer calculate with data

On computer
● Interactive exploration
Some common techniques
That could help in the ML context...

From the simple...
Case study: the humble table

We’ve talked to many, many ML teams

Every one of them displayed data in tables

Good design can make a huge difference
Design thinking in action, a little movie:

Remove to improve data tables
Joey Cherdarchuk
DarkHorse Analytics
Key points

- Structure & hierarchy
- Alignment
- Typography
- Color

These all apply to more complicated visualizations!
Some common techniques
That could help in the ML context...
Data density: small multiples

Drought’s Footprint
Haeyoun Park, Kevin Quealy
NY Times
Across U.S. Companies, Tax Rates Vary Greatly

M. Bostock, M. Ericson, D. Leonhardt, B. Marsh

NY Times
Back to machine learning!
Opportunities for Vis

Source: Yannick Assogba
Framework: visualization uses in ML

1. Training Data
2. Model Performance
3. Interpretability + model inspection
4. High-dimensional data
5. Education and communication
1. Visualizing training data
The CIFAR-10 dataset consists of 60000 32x32 colour images in 10 classes, with 6000 images per class. There are 50000 training images and 10000 test images.

The dataset is divided into five training batches and one test batch, each with 10000 images. The test batch contains exactly 1000 randomly-selected images from each class. The training batches contain the remaining images in random order, but some training batches may contain more images from one class than another. Between them, the training batches contain exactly 50000 images from each class.

Here are the classes in the dataset, as well as 10 random images from each:

- airplane
- automobile
- bird
- cat
- deer
- dog
- frog
- horse
- ship
- truck

The classes are completely mutually exclusive. There is no overlap between automobiles and trucks. "Automobile" includes sedans, SUVs, things of that sort. "Truck" includes only big trucks. Neither includes pickup trucks.
CIFAR-10 Facets Demo
Facets
Open-source visualization
pair-code.github.io/facets
Quick Draw, the data.

https://quickdraw.withgoogle.com/data.
When things look alike across cultures

Machine Learning for Visualization
Let’s Explore the Cutest Big Dataset
Ian Johnson
And when they don’t

Visual Averages by Country
Kyle McDonald
Outlets

Visual Averages by Country
Kyle McDonald
Finding nemo: small multiples

Visual Averages by Country
Kyle McDonald
2. Performance monitoring (very briefly!)
Monitoring dashboards - apply standard visualization tools!

TensorBoard

Visdom

Two examples among many...
3. Interpretability + model inspection
Convolutional NNs
Image classification: interpretability petri dish

Image classifiers are effective in practice

Exactly what they’re doing is somewhat mysterious
- And their failures (e.g. adversarial examples) add to mystery

**But**: Way easier to inspect what’s going on in artificial classifiers than in human classifiers ;-) 

Since these are visual systems, it’s natural to use visualization to inspect them
- What features are these networks really using?
- Do individual units have meaning?
- What roles are played by different layers?
- How are high-level concepts built from low-level ones?
Saliency maps - examples

More comparisons: https://pair-code.github.io/saliency/
Saliency maps
(a.k.a. "Sensitivity maps")

Idea: consider sensitivity of class to each pixel
i.e. $\text{grad}(f)$, where $f$ is function from pixels to class score.

Many ways to extend basic idea!
- Layer-wise relevance propagation (Binder et al.)
- Integrated gradients (Sundararajan et al.)
- Guided backprop (Springenberg et al.)
- etc.

Yet interpretation is slippery (Adebayo et al., Kindermans et al.)
- Tend to be visually noisy. Are these sometimes Rorschach tests?
- Are some of these methods essentially edge detectors?
Visualizing arbitrary neurons along the way to the top...

Gray: trying to maximize neural response. Colorful squares: maximal examples from an image data set

Visualizing and Understanding Convolutional Networks
Zeiler & Fergus, 2013
Understanding Neural Networks Through Deep Visualization
Yosinski et al., 2015
http://yosinski.com/deepvis
Combining these interpretability ideas to create new visualizations.
Going From Visualization to Interpretation

Interpreting Deep Visual Representations
Bau, Khosla, Oliva, Torralba
RNNs
The sole importance of the crossing of the Berezina lies in the fact that it plainly and indubitably proved the fallacy of all the plans for cutting off the enemy's retreat and the soundness of the only possible line of action--the one Kutuzov and the general mass of the army demanded--namely, simply to follow the enemy up. The French crowd fled at a continually increasing speed and all its energy was directed to reaching its goal. It fled like a wounded animal and it was impossible to block its path. This was shown not so much by the arrangements it made for crossing as by what took place at the bridges. When the bridges broke down, unarmed soldiers, people from Moscow and women with children who were with the French transport, all--carried on by vis inertiae--pressed forward into boats and into the ice-covered water and did not surrender.

"You mean to imply that I have nothing to eat out of.... On the contrary, I can supply you with everything even if you want to give dinner parties," warmly replied Chichagov, who tried by every word he spoke to prove his own rectitude and therefore imagined Kutuzov to be animated by the same desire.

Kutuzov, shrugging his shoulders, replied with his subtle penetrating smile: "I meant merely to say what I said."
Cell that robustly activates inside if statements:

```c
static int __dequeue_signal(struct sigpending *pending, sigset_t *mask, siginfo_t *info)
{
    int sig = next_signal(pending, mask);
    if (sig) {
        if (current->notifier) {
            if (sigismember(current->notifier_mask, sig)) {
                if (!((current->notifier)(current->notifier_data))) {
                    clear_thread_flag(TIF_SIGPENDING);
                    return 0;
                }
            }
        }
        collect_signal(sig, pending, info);
    }
    return sig;
}
```
Seq2Seq-Vis: Visual Debugging Tool for Sequence-to-Sequence Models
Strobelt, 2018

Examine model decisions
Connect decisions to previous examples
Test alternative decisions
Linking multiple views...

DQNViz: A Visual Analytics Approach to Understand Deep Q-Networks

Wang et al., VAST 2018.

Fig. 1. DQNViz: (a) the Statistics view presents the overall training statistics with line charts and stacked area charts; (b) the Epoch view shows epoch-level statistics with pie charts and stacked bar charts; (c) the Trajectory view reveals the movement and reward patterns of the DQN agent in different episodes; (d) the Segment view reveals what the agent really sees from a selected segment.
4. High-dimensional data
Why high-dimensional data?

Vectors spaces are the lingua franca of much of ML these days
- Data such as images, audio, video is naturally high-dimensional
- Dense representations of discrete data (e.g. word embeddings) have had major successes
Why is it hard? Because it’s impossible
Why is it hard? Because it’s impossible

See Every Map Projection, Bostock.
Main approaches

Linear
- Principal Component Analysis
- Visualization of Labeled Data Using Linear Transformations (Koren & Carmel)

Non-linear (just a few of many)
- Multidimensional scaling
- Sammon mapping
- Isomap
- t-SNE
- UMAP
Main approaches

**Linear**
- Principal Component Analysis *(show as much variation in data as possible)*
- Visualization of Labeled Data Using Linear Transformations *(clusters match labels)*

**Non-linear** *(just a few of many)*
- Multidimensional scaling
- Sammon mapping
- Isomap
- t-SNE
- UMAP

Minimize distortion, according to some metric
t-SNE

Visualizing Data using t-SNE

Laurens van der Maaten
TiCC
Tilburg University
P.O. Box 90153, 5000 LE Tilburg, The Netherlands

Geoffrey Hinton
Department of Computer Science
University of Toronto
6 King’s College Road, M5S 3G4 Toronto, ON, Canada

LVDMAATEN@GMAIL.COM
HINTON@CS.TORONTO.EDU
t-SNE

Fairly complex non-linear technique

Uses an adaptive sense of "distance." Translates well between geometry of high- and low-dimensional space

Has become a standard tool, so we’ll spend some time discussing how to read it.
Demo: MNIST visualization

Embedding Projector
Open Source visualization tool
Also available on Tensorboard
projector.tensorflow.org/
"Close reading" a visualization technique

What's the right way to understand a "magic" visualization technique?

See Distill article
"Close reading" a visualization technique

What's the right way to understand a "magic" visualization technique?

More visualization, of course!
Those hyperparameters really matter
Those hyperparameters really matter
Cluster sizes in a t-SNE plot mean nothing
Cluster sizes in a t-SNE plot mean nothing
Distances between clusters may not mean much.
Distances between clusters may not mean much.
You can see some shapes, sometimes
You can see some shapes, sometimes
Let’s try this out with MNIST
Stopping too soon yields weird artifacts.
The 4’s may not be separated into two clusters.

Clusters seem about equally far apart in 3D; may not actually be.
The clusters of 1's probably is long and thin.
UMAP: New kid on the block

UMAP: Uniform Manifold Approximation and Projection for Dimension Reduction

Leland McInnes and John Healy
Tutte Institute for Mathematics and Computing
leland.mcinnes@gmail.com  jchealy@gmail.com

February 13, 2018
UMAP: New kid on the block

Practical value
- Faster than t-SNE
- Can efficiently embed into high dimensions (i.e. useful not just for visualization)
- Often seems to capture global structure better
UMAP: New kid on the block

Practical value
- Faster than t-SNE
- Can efficiently embed into high dimensions (i.e. useful not just for visualization)
- Often seems to capture global structure better

Theory
- Roughly: manifold learning combined with explicit topology
- In detail: I don’t completely understand the theory!
  - This note does an amazing job of extracting key bits of UMAP paper: https://www.math.upenn.edu/~jhansen/2018/05/04/UMAP/
UMAP: New kid on the block

Comparison of UMAP (left) and t-SNE (right) from McInnes & Healy.

Global structure does seem to emerge more in UMAP.

For more
Let’s compare in real-time on an audio data set!
[Comparative Audio Analysis With Wavenet, MFCCs, UMAP, t-SNE and PCA](#)
(Leon Fedden)
Putting this together

The Beginner’s Guide to Dimensionality Reduction
Matthew Conlen and Fred Hohman

https://idyll.pub/post/dimensionality-reduction-293e465c2a3443e8941b016d/
(just Google "Beginner’s Guide to Dimensionality Reduction")
Pitfalls of high-dimensional space

Geometry of high-dimensional space holds many surprises...
Be careful about interpreting visualizations!

Adding "usually," "most," and "approximately" where appropriate:

- Two random vectors are perpendicular
- A standard Gaussian distribution is just a uniform distribution on a sphere
- A random matrix is a scalar multiple of an orthogonal matrix
- Random walks all have the same shape
Example: PCA of gradient descent trajectories

Lorch, Visualizing Deep Network Training Trajectories, 2017

Li et al, Visualizing the Loss Landscape of Neural Nets, 2018
How to interpret? Compare random walks

It turns out that principal components of a random walk in a high-dimensional space are (probably, approximately) cosines of various frequencies! (Antognini, Sohl-Dickstein)

Can also see this via Karhunen-Loeve theorem for Brownian motion.

**Important:** This doesn’t invalidate work that uses PCA to look at SGD trajectories. But it changes how we read the visualizations: the interesting parts are differences from Lissajous patterns, not similarities.

Antognini, Sohl-Dickstein. 2018
Lesson

If you see something interesting in high-dimensional space...

compare to a random baseline!
Model interpretability example

Multi-lingual translation

What does the language embedding space look like?

https://arxiv.org/abs/1611.04558
Google’s Multilingual Neural Machine Translation System: Enabling Zero-Shot Translation

Melvin Johnson, Mike Schuster, Quoc V. Le, Maxim Krikun, Yonghui Wu, Zhifeng Chen, Nikhil Thorat, Fernanda Viégas, Martin Wattenberg, Greg Corrado, Macduff Hughes, Jeffrey Dean
Training:

English ↔ → Japanese

English ↔ → Korean

Japanese ↔ → Korean (zero shot)
Visualize internal representation ("embedding space")
Research question
What does the multi language embedding space look like?

Note: not real data
What does a sentence look like in embedding space?
(points in 1024-dim space: the data that the decoder receives)

E.g. “The stratosphere extends from 10km to 50km in altitude”
What does a sentence look like in embedding space?

Note: simplification of real situation!
What does a sentence look like in embedding space?
What do parallel sentences look like in embedding space? (same meaning, different language)

like this?
What do parallel sentences look like in embedding space? (same meaning, different language)

or like this?
Interlingua?
Sentences with the same meaning mapped to similar regions regardless of language!
Distance between bridge / non-bridge sentences is inversely related to translation quality.

Figure 3: (a) A bird’s-eye view of a t-SNE projection of an embedding of the model trained on Portuguese→English (blue) and English→Spanish (yellow) examples with a Portuguese→Spanish zero-shot bridge (red). The large red region on the left primarily contains the zero-shot Portuguese→Spanish translations. (b) A scatter plot of BLEU scores of zero-shot translations versus the average point-wise distance between the zero-shot translation and a non-bridged translation. The Pearson correlation coefficient is $-0.42$. 
5. Education and communication
Education & communication for technical audiences
Distill Update 2018
An Update from the Editorial Team

July 26, 2018
Differentiable Image Parameterizations
A powerful, under-explored tool for neural network visualizations and art.

July 9, 2018
Feature-wise transformations
A simple and surprisingly effective family of conditioning mechanisms.

March 6, 2018
The Building Blocks of Interpretability
Interpretability techniques are normally studied in isolation. We explore the powerful interfaces that arise when you combine them—and the rich structure of this combinatorial space.

Dec. 4, 2017
Using Artificial Intelligence to Augment Human Intelligence
By creating user interfaces which let us work with the...
A Visual Exploration of Gaussian Processes

How to turn a collection of small building blocks into a versatile tool for solving regression problems.

Regression is used to find a function (line) that represents a set of data points as closely as possible.

A Gaussian process is a probabilistic method that gives a confidence (shaded) for the predicted function.
Education & communication for non-technical audiences
Attacking discrimination with smarter machine learning

Research into attacking discrimination in machine learning

Transform math into a visual, interactive simulation that can be used by a broader set of stakeholders such as policymakers and regulators.

Wattenberg, Viegas, Hardt. 2016
On Quickdraw, users draw common objects (e.g. avocado), then see if the algorithm has correctly recognized the object.

You were asked to draw avocado, and the neural net did not recognize it.
After users see the recognition result, Quickdraw shows **visual examples** to help users understand the algorithm’s reasoning.

For example, it shows examples of what typical avocados look like.
It also shows a **visual diff** between the user’s drawing and the most-similar drawings from alternative classes.
You were asked to draw bee

You drew this, and the neural net didn't recognize it.

It thought your drawing looked more like these:

- Closest match: sea turtle
- 2nd closest match: mouse
- 3rd closest match: shark

Compare user input to classes system thought were closest
What does it think bee looks like?
It learned by looking at these examples drawn by other people.

Show examples of what the system expected for the class in question

Illustrate latent space to users
Visual Analytics in Deep Learning: An Interrogative Survey for the Next Frontiers
Hohman, Kahng, Pienta, Chau

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<th>HOW</th>
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Abadi, et al., 2016 [27]  | arXiv  |  |
Bau, et al., 2017 [28]  | CVPR  |  |
Bilal, et al., 2017 [29]  | TVCG  |  |
Bruckner, 2014 [31]  | MS Thesis  |  |
Cashman, et al., 2017 [33]  | VADL  |  |
Chae, et al., 2017 [34]  | VADL  |  |
Chung, et al., 2016 [35]  | FILM  |  |
Harley, 2015 [37]  | ISVC  |  |
Hohman, et al., 2017 [38]  | CHI  |  |
Kahng, et al., 2018 [39]  | TVCG  |  |
Karpathy, et al., 2015 [40]  | arXiv  |  |
Li, et al., 2015 [41]  | arXiv  |  |
Liu, et al., 2017 [42]  | TVCG  |  |
Liu, et al., 2018 [42]  | TVCG  |  |
Ming, et al., 2017 [43]  | VAST  |  |
Norton & Qi, 2017 [44]  | VisSec  |  |
Olaf, et al., 2018 [46]  | Distill  |  |
Pezzotti, et al., 2017 [47]  | TVCG  |  |
## Resources

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