A Sketch of a Theory of Visualization

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Abstract: A picture results from a possibly multi-layer transformation of data to a visual vocabulary in which humans can draw inferences about the original data. The goal of this visualization process is to expose relationships amongst the data that are otherwise difficult to find, or only emerge by the process of the transformation. In case of the former kind of inference (confirming a relationship that did exist but was not obvious), visualization provides a kind of inferential amplifying effect. In the case of the latter (exposing new data relationships), visualization provides an inductive mechanism to create hypotheses not manifest in the original data. In this regard, the creation of pictures from data is about data compression, which is naturally a kind of machine learning. Just as statistical concepts like average and standard deviation provide a measure on properties of a set of numbers, so too does visualization provide a kind of "measure" on data compressed to a visual vocabulary presented as a picture. Our position is that visualization is about the (potentially multi-step, multilayered) transformation of data to pictures, and that ever such transformation must make choices about what kinds of relations to preserve, and what kinds of data artifacts to avoid in each such transformation. Like a chain of formal inference, conclusions following from the end result (the picture) are determined by what each transformation in the inference chain is intended to accomplish. We argue that the visualization of large data sets, too large to inspect directly, requires a rigorous theory of how to transform data to pictures, so that the scientists as observers can be assured that inferences drawn from the pictures are either confirmable in the detailed data, or at least plausible hypotheses which can be further pursued by seeking further data (evidence).

1 INTRODUCTION

The process of visualization is about transforming data into pictures. As Stuart Card has written, "The purpose of information visualization is to amplify cognitive performance, not just to create interesting pictures. Information visualizations should do for the mind what automobiles do for the feet.¹" There are, of course, an incredibly large number of ways in which one could transform some arbitrary collection of data into a picture. But it is sensible to first consider those transformations that expose data relationships not easily revealed, either because of data complexity or data volume.

The real practical challenge of visualization is making choices: how should one select within the data to focus the quest for implicit relationships, and what kind of visual vocabulary should those data be mapped to? Neither question can be addressed well without some way of evaluating which kind of data selection and picture transformation is "best." If the the overall motivation of visualization is to expose implicit data relationships, then visualization evaluation needs to be able to determine which methods provide the best support for inferences drawn from the pictures created from the selected data.

There is no existing theory of visualization which can be used to guide the decisions about how to compress large data sets and transform them into pictures. There is, of course, some strong even compelling arguments that the foundation of any visualization theory must be based on the cognitive processes of human perception (e.g., (Patterson et al., 2013)). And there is also computational scaffolding that provides a computational perspective on a potential pipeline of picture production (Card et al., 1999). Furthermore, it is clear that a number of researchers have noted the relationship between visualization manipulation and analytics (e.g., (May et al., 2010)), and it is clear that the effectiveness of amplifying human inference on

¹(Card, 2012), page 539.

pictures is improved by interaction. Our position here is *not* to argue against the role of human cognition in a theory of visualization, nor to suggest picture manipulation is not important. Instead, our goal is to sketch a set of what we view as necessary and complementary components of a visualization theory, based on machine learning coupled with evaluation based on visual inference.

To keep the statement of the position simple, we will use the term "picture" to mean *any* visual representation of data, including photographs, video, and any existing visualization outputs like bar charts, radar plots, and dynamic interactive immersive displays. We will argue that a picture results from a series of transformations, through a layer of connected vocabularies, where each layer emerges from the previous by some kind of machine learning data compression. Each compression step is responsible for finding appropriate aggregations of data, in order to support the recognition of data trends (e.g., averages of numeric data, size of measure data, etc.), which eventually get mapped to a picture vocabulary.

The result is a picture, and the interpretation of the picture by humans leads to inferences about the original or base data which has travelled through a series of compression transforms. The quality of the picture is measured in two ways: 1) how many accurate inferences are exposed for the viewer, and 2) what new relationships amongst the data are revealed by the picture.

2 INFORMAL OBSERVATIONS ABOUT "GOOD" VISUALIZATIONS

From a reprinting in Tufte's first graphical design book (Tufte, 1983), Jacques Minard's drawing of Napoleon's march on Moscow is given in Fig 1. It is immediately obvious that the declining width of the dark line represents the declining number of soldiers at the campaign proceeded.

In fact the most important aspect of an picture evaluation is really about this idea of what is immediately obvious. And since there are so many alternative ways to render a picture, it is natural to believe that some will make some inferences more obvious than others.

In this regard, we can already get a pretty good idea about how to assess alternative pictures of the same data: some will make it easier to make obvious inferences. Like the relative size of Napoleon's army in Fig 1, a relation table of a time series of numbers



Figure 1: Jacques Minard's "Napoleon's March on Moscow".

would still support the inference of how the size of the army changed over that time series. But the picture makes it easier to see.

Similarly, but perhaps less obvious, some alternative pictures of the same data will expose hypothetical relationships in the data that were simply not previously considered; for example, the Napoleon diagram includes a chart near the bottom that shows the change in temperature during the campaign, but it is not so easy to create hypotheses about the weather's impact on the size of the army as it travelled. Can the weather be considered as a factor independent of the geographical location of the army, for example? It is easy to imagine alternative pictures, e.g., that show topographical relief, and then consider factors like climbing over mountains as a potential impact on the army's progress.

The summary point is first, that evaluation of the quality of a picture produced from data is an integral component of any theory of visualization, and second, that one should distinguish between pictures which not only aid in the perspicuity of drawing inferences on the data, but also provide support for exposing plausible hypotheses on the data.

3 ABSTRACTION LAYERS IN DATA AND PICTURE DOMAINS

In contrast to traditional logical chains of inference, those within a multi-layer theory of visualization can transcend abstraction boundaries, as illustrated in Fig 2. In (Goebel et al., 2013), the use of machine learning to actually build these multi-layer models is described; here we merely note the following properties of the simple three layer model of protein structure.



Figure 2: An abstraction of three levels of protein representation.

First, at the lowest level of detail, the base data is the confirmed sequence of amino acids that comprise the protein in question. Note that conventional systems biology is able to accurately create these sequences from proteins with perfect accuracy. But the visualization in Fig 2 is not about the base data itself, but about an abstraction of that data, labelled as the protein's secondary structure. This more abstract vocabulary is of random coils (C), beta sheets (B), and helices (H). So the transformation from the amino acid level to the secondary structure is an aggregation or compression step: it compresses the simpler amino acid sequences into the secondary structure vocabulary.

Note that this transformation is not currently welldefined. The secondary structure rendered in the vocabulary of C, B, and H is a hypothesis about the protein structure, and as explained in the Wiki entry for protein secondary structure, the "C" is really a catch all for undetermined structure. But this illustrates the inductive nature of these multi-layer transformations, ending in a picture: the transformation from amino acid sequence, to secondary structure (vocabulary C, B, H), then to the tertiary structure represented by three dimensional "cartoon" models is an inductive multi-step transformation from base data to picture.

In practise, such transformation as valuable as hypothesis management systems (e.g., (Bertschi et al., 2011)), because there are relatively well defined constraints that identify the elements of each layer as hypotheses about protein structure.

Similarly, in a more general theory of visualization, the picture produced at the end of the data to picture transformation chain should at least present a picture that constrains the viewer to plausible inferences about the data in question.

4 VISUALIZATION EVALUATION

More attention is here required regarding earlier comments about the manner in which pictures support the drawing of inferences by humans. Within this sketch of a theory of visualization, a central hypothesis is that the goal of a picture is to assist humans in drawing inferences about data that would otherwise be difficult or even impossible from the base data itself. One only has to consider a practical example of how large a spreadsheet can get before one fails to see relationships intended within the cells.

So if the base data are too voluminous or complex to provide the basis for drawing inferences as humans, then one would expect a variety of different visualization methods would encourage inference, one way or another. A simple illustration of alternative methods to visualize community clusters is given below in Fig 3. The four different community clusters are layed out with the Fruchterman-Rheingold (FR), Kameda-Kawai (KK), and the COMB and COMA layout methods of Fagnan et al. (Fagnan et al., 2012). While the four different pictures are abstracted from the same base data, a viewer will have a preference for which picture is preferred when asked to infer the number of distinct communities.



Figure 3: Four alternative graphical layouts of the same data.

A more impactful illustration of the need to consider the kinds of inferences a human could draw from alternative pictures of the same data is give in Fig 4. In this case, the figure demonstrates how human perception can be fooled into incorrect inferences ((Adelson, 1995)). It is clear that it is not just that visualization evaluation must consider those inferences better enabled by alternative pictures, but that great care must be taken to not introduce artifacts that lead to incorrect inference (unless that is intended).

The summary point is that evaluation is not just necessary, but requires a formulation based on how alternative pictures support either efficient inference about confirmable data relationships, evidence for likely hypotheses consistent with but not contained within the base data, while ensuring no artifact sug-



Figure 4: Demonstration of the checkerboard illusion.

gests wrong or implausible inferences. As a component of a theory of visualization, an evaluation method will ensure all these issues are in some way addressed.

5 SUMMARY

There is still much to say about how a multi-layer theory of visualization should be structured, and how the properties at one level are selected and preserved when mapped to the subsequent layer. Indeed, dynamic visual analytics is about how direct manipulation of a picture can be constrained by the next lower level so that users exploring the properties of a picture are constrained to make only plausible adjustments to that picture (cf. (Cooper et al., 2010)).

But the primary value of such a theory is to articulate principles, which are typically domaindependent, for the multi-layer mappings from base data to picture. This ensures that anomalies are not created in the mappings, and that the resulting pictures can be evaluated with respect to their inferential value. In that regard, evaluation must focus on how alternative mappings to pictures make accurate constrained inference easy or difficult.

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