Putting Science First

Distinguishing Visualizations from Pretty Pictures

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In 1987, Bruce McCormick led an extensive study of the benefits of combining computer graphics and computational-science methods. This culminated in the US National Science Foundation panel report “Visualization in Scientific Computing,” in which I was (serendipitously) a participant. Many people identify this event as the birth of scientific visualization as a distinct discipline. It was soon followed, for example, by the creation of the IEEE Visualization Conference, thanks largely to Larry Rosenblum, Arie Kaufman, and Gregory Nielson. (A few of us still fondly remember the inaugural 1990 meeting in San Francisco.) The discipline achieved maturity in 1995, when Arie Kaufman became the founding editor in chief of IEEE Transactions on Visualization and Computer Graphics.

Today, the worlds of science, computing, and visualization continue to evolve at a dizzying pace. Visual analytics is competing valiantly with visualization per se, and the newcomers big data and cloud computing pose novel challenges to the integration of visualization. While the problems of extracting useful information from ever-growing datasets that dominated the panel’s original concerns continue unabated, here I will ponder the parallel issue of understanding the scientific quality of visualization content.

Art or Science?
The essence of visualization is the creation of appealing images that are based on scientific data and that facilitate the domain scientist’s understanding of the data. Datasets without visualizations are little more than lists of numbers, typically generated by computational models or extracted from measurements. When I construct images and animations for a visualization task, I often want them to aesthetically inspire the viewer, just as an artist wants a piece of art to attract attention and comment. For some tasks artistic goals might seem irrelevant, but, more often than not, an attractive presentation can make the difference between a widely used visualization and a neglected one. Creating artistic images isn’t easy, but producing meaningful visualizations isn’t easy either, and producing a good visualization that’s also artistically attractive is doubly difficult.

Interestingly, we can find cases for which an image of a legitimate scientific data domain is remarkably close to pure art, and vice versa. For example, Figure 1a shows a masterpiece by Jackson Pollock, in a style instantly recognizable to almost any patron of the arts. In this painting, Pollock brings together chaotic elements that each seem to have a place in the intuitive process of attracting the viewer’s attention and appreciation. Compare that work of art to Figure 1b, which is an instance of The Symplectic Piece, an image introduced as a work of art. Indeed, this image is attractive for the reasons that any good work of art is attractive. It captures the eye with forms and patterns in shape and color, yet it’s slightly unpredictable, inviting further examination. However, it’s not a deliberately designed piece of art, but the output of a computer program visualizing the butterfly effect. It illustrates the large-scale, unpredictable behaviors resulting from the propagation of infinitesimally small differences in numerical initial conditions for the simulated motion of 10 moons and two massive suns. The essential processes that produced the Jackson Pollock painting and The Symplectic Piece seem closely related. Figure 2a shows another Jackson Pollock painting that strongly resembles the technically correct but uninformative visualization in Figure 2b, which depicts a 4D mathematical object called a K3 surface. This leads us to consider the question, when should we label such images as science or art?
Stretching the Truth Too Far
Visualizations with artistically motivated features that are difficult to justify aren’t hard to find. The temptation to introduce and exploit artistic exaggeration can sometimes get the upper hand. A particularly irresistible domain for this seems to be planetary-surface data from spacecraft. One example, from the Mars Odyssey mission, is a widely shown animation seemingly flying through the valleys and mountains of Mars. Most presentations viewed by the general public don’t mention that the elevations are exaggerated by a factor of 2.5.

An even more striking example occurs in the images of the Gula Mons feature on the surface of Venus, reconstructed from the Magellan radar data survey. The press releases accompanying the images didn’t mention the unusual transformations applied to the surface-reconstruction process that produced the images. Figures 3a and 3b are exaggerated vertically by a factor of 22.5. In contrast, Figure 3c, available on an apparently later website

Figure 1. Art and science with common features. (a) Jackson Pollock’s *Number 1, 1950 (Lavender Mist)* is considered one of his masterpieces. (Courtesy of the National Gallery of Art. © 2013 The Pollock-Krasner Foundation/Artists Rights Society [ARS], New York.) (b) The *Symplectic Piece* is a similar image that appears artistic but is the output of a precise simulation of many-body gravitational dynamics. (Courtesy of Alec Jacobson, ETH.)

Figure 2. More art and science with common features. (a) Jackson Pollock’s *Number 18, 1950* qualitatively resembles (b) a raw image of the 4D edges tessellating a K3 surface projected to 3D. (Figure 2a courtesy of the Guggenheim Museum. ©2013 The Pollock-Krasner Foundation/Artists Rights Society [ARS], New York.)
thread, is scaled to the actual relative left–right versus top–bottom proportions of the surface geometry of Venus. It shows roughly what you would see if you were actually standing on Venus.

I can understand the motivation to enhance these images to reveal more details. But does failing to mention such extreme exaggeration serve any purpose, say, in inspiring young students to go into science? Such artistic license will more likely induce skepticism and disbelief in the claims of scientists in general. Exaggerating science with excessive showmanship does little service to either art or science.

Some Useful Visualization Principles

We clearly must seek some well-defined principles to guide us when we want our visualizations to have artistic qualities while preserving the integrity of our science. Among many such principles that have been proposed and advocated, the following two in particular seem universally useful.

Einstein’s Razor

Einstein has been quoted as saying,

Everything should be made as simple as possible, but no simpler!

This principle sets forth the contrast between the value of simplicity and the demands of science. Applied to visual representations, it advocates whittling down our visualizations to the essential features necessary to meet a given goal of the data analyst. However, given that data must be selected, filtered, and identified with a contextual model before we can even begin, we also see that these features are fundamentally in the (possibly artistic) eye of the beholder.

(Interestingly, that wasn't what Einstein actually said. You might find it amusing to wonder about the traditional homily’s self-referential relationship to the truth. What Einstein really said was, “It can scarcely be denied that the supreme goal of all theory is to make the irreducible basic elements as simple and as few as possible without having to surrender the adequate representation of a single datum of experience.”)

Falsifiability

What’s the difference between an attractive but rigorous solution to a visualization problem and a beautiful image whose artistic appeal far outweighs its value as visualization? As someone who has spent a significant part of my career as a domain scientist, I’m inclined to believe that the ultimate tests of value come from the principles of natural science. We should be able to exploit the same methods in evaluating visualizations that we use to distinguish a valid scientific framework from an untestable one.

A key method by which we make such distinctions in science is the principle of falsifiability, championed by Karl Popper. (This term doesn’t imply any deliberate intent to falsify data or to deceive but refers to a standard of provability.) Despite being periodically challenged on philosophical grounds, this principle is still one of our most powerful tools to identify and correct erroneous and shaky claims. The process of evolving our often qualitative discipline toward an actual science...
could be enhanced by systematically applying this principle to evaluate the validity of our visualizations. If we can tell the difference between an image containing a fatal factual defect and one whose features have clearly identifiable scientific sources, we can then approach our goal of distinguishing the components of art in our work, however beautiful they might be, from our science.

**Case Study: Fermat Surfaces**

Being most familiar with the nuances of my own work, I will perhaps be forgiven for concluding with a narrative involving my experiences developing a broad set of visualizations, thus exposing the perils of trying to follow my own advice. This is the saga of a particularly amusing class of examples from my own library of visualizations, all related to Fermat’s equation, a simple equation that produces a class of surfaces called Fermat surfaces.6

The equation is

$$(z_1)^n + (z_2)^n = 1,$$

where $z_1$ and $z_2$ are complex variables and $n \geq 2$ is an integer. There are four real variables and two equations (a real and an imaginary part), leaving two degrees of freedom defining a surface. Because the surface is embedded in 4D, it must be projected to 3D to exploit standard computer graphics rendering methods.

My 25 years of continuous work in this domain provide a compelling story. The development of clear strategies to introduce falsifiability into the images of these surfaces has been counterbalanced by the amazing difficulty of convincing any given client to prefer the falsifiable forms to forms excessively manipulated (to my mind) by artistic license.

These images first appeared in the animation “Visualizing Fermat’s Last Theorem” (www.youtube.com/watch?v=xG63O03IWZI), shown at Siggraph 1990 and described in a technical article at the inaugural IEEE Visualization Conference the same year.7 Happily, interest in these images continued to grow in the next few years owing to the development of the successful proof of Fermat’s last theorem by Andrew Wiles and his associates in 1994 and 1995.

The story continued in fall 1999 as string theorist Brian Greene was finishing his million-selling book *The Elegant Universe*. He suggested to me that Fermat surface images could be used to represent Calabi-Yau spaces, the hidden dimensions of string theory, which were central to his narrative. This turned out to be straightforward because the Fermat equation for $n = 5$ produces a 2D cross-section of the 6D complex quintic equation, which is a Calabi-Yau space and a strong candidate for the hidden string theory geometry. The 2D slices preserve many fundamental features of the quintic, particularly the fivefold symmetry. I naively considered my constructions showing unmistakable pentagonal symmetry to be wonderfully compelling examples of a falsifiable representation of these otherwise highly abstract objects.

However, when I handed over my basic construction of the Calabi-Yau quintic to a variety of graphic artists, what befell my cherished principles of falsifiability was hard to predict. Figures 4a and 4b appear in Greene’s books. The absence of color printing and a viewpoint that completely hides the fivefold symmetry leaves Figure 4a an unintelligible mish-mash; you simply have to take for granted it might be a Calabi-Yau object. Figure 4b, based on an image from my webpage, stood a chance of meeting my criteria. It showed the fivefold symmetry and different shades of gray where fivefold pie slices were color coded in the Web version. However, the art department added meaningless random lines all over the image. Apparently, they were unaware that I would have been quite happy to spend two seconds to hit my renderer’s hot key that overlays the tessellation lines in the correct places. This would have maintained the geometric falsifiability instead of destroying it in the name of art.

Of course, Figures 4a and 4b were grayscale static images printed in books. When the NOVA team started adapting these Calabi-Yau representations for extensive animated treatment in the Elegant Universe episodes in 2003, I again had some hope that the result would be mathematically informative visual representations. Figure 4c shows the beautiful results of the Red Vision animation house’s adaptation of my algorithms for the 2D cross-section. The 2D checkerboard layout of Figure 4d is supposed to represent the higher dimensions missing from the cross-section. However, this approach includes only two of the four missing dimensions. We see that every trace of the intrinsic quintic signature that the chosen modeling approach so carefully preserved is gone, and the animation becomes a sea of writhing tulips. The result is obviously no longer a visualization but pure art (although I must admit I like it).

The original corpus of my Fermat/Calabi-Yau Mathematica code deposited in the Wolfram MathSource library in the early 1990’s has been ported, with the assistance of Jeff Bryant at Wolfram, to a Wolfram Demonstration Project.8 The project easily supports the generation of both the original
falsifiable images and more artistic versions. Figure 5a is one of the latter, produced to accompany a string theory article in *Physics Today* by Gordon Kane. Figure 5b shows the amazing glasswork rendering by Bathsheba Grossman, who took my 4D equations and chose her own parameters for the projection to 3D. Her deliberately artistic results are some of the most mathematically compelling representations I’ve seen, showing that we still have much to learn from the skills of real artists.

I conclude this story of the struggle between the priorities of falsifiability and aesthetics by presenting in Figure 6a what I consider to be the definitive static visualization of the Calabi-Yau quintic 2D cross-section. This representation was chosen for the cover of Yau’s own book on string theory. Figure 6b shows a method that can be used to represent the entire 6D space. We see that the 2D checkerboard layout used to indicate the higher dimensions of string theory in previous visualizations could be considered an unnecessary oversimplification. The representations in Figure 6 possess significant additional, although subtle, information. Each color in Figure 6a has a specific mathematical meaning, and each of the hundreds of shapes in Figure 6b is different, showing the geometric variations across all six dimensions. (For more mathematical details on the Calabi-Yau quintic images, see the sidebar.)

Over the years, my laboratory has developed fully interactive high-dimensional-geometry viewing systems enabling us to study these remarkable
mathematical objects from arbitrary 4D viewpoints. I argue that such interactive exploration can significantly enhance the visualization paradigm for such objects, greatly facilitating the verification of falsifiable properties. (See, for example, 4Dice, our free iPhone App for interactively exploring the 4D hypercube, at http://itunes.apple.com/us/app/4dice/id453083422.)

Figure 5. Two artistic Calabi-Yau images. (a) An image accompanying a Physics Today article on string theory by Gordon Kane, rendered using the most artistic options in the Wolfram Demonstrations Project Calabi-Yau tool. (Reprinted with permission from Physics Today, Nov. 2010, © 2010, American Institute of Physics.) (b) The Calabi-Yau quintic as treated by a professional artist, Bathsheba Grossman. Her clever choice of parameters reveals the intrinsic symmetries in this view of her laser-etched glass sculptures. This object, intended mainly as an art piece, is superior to many visualization-oriented treatments. (Courtesy of Bathsheba Grossman, http://bathsheba.com.)

Figure 6. Visualizations of the quintic Calabi-Yau 6D manifold. (a) The color-enhanced 2D cross-section emphasizing the fivefold symmetry. (b) A representation of the full 6D manifold, showing 2D cross-sections at sampled values of the remaining four dimensions.
The full Calabi-Yau quintic is a 6D manifold described in a local coordinate system by the equation $(z_1)^5 + (z_2)^5 = \Phi(z_3, z_4, z_5)$, where $\Phi = 1 - (z_3)^5 - (z_4)^5$, and each $z$ is a complex variable represented by two real variables, $z = x + iy$. I ignore for the moment the submanifold at infinity that can’t be seen in the finite local coordinates.

Figure 6a in the main article shows a 3D projection of the 2D surface embedded in 4D defined by the solutions with $\Phi(0, 0) = 1$. The surface’s coordinates are thus $x_1, y_1, x_2, y_2$. The fivefold pie slices throughout Figure 6 are checkable evidence that this is indeed a quintic equation. The 25 colors in Figure 6a uniquely identify particular phase transformations applied to the mostly hidden blue fundamental shape on the back side.

The four variables in the Figure 6b lattice are $x_3, y_3, x_4$, and $y_4$, where one coordinate axis necessarily goes off in a diagonal direction in this 3D projection. For each fixed sampled point in these variables, $\Phi(z_3, z_4)$ is a complex constant, and the solutions to $(z_1)^5 + (z_2)^5 = \Phi(z_3, z_4)$ change slightly in shape and size. Figure 6b contains $5 \times 5 \times 5 \times 5 = 625$ snapshots of the 2D surface at discretely sampled positions $(-2, -1, 0, 1, 2)$ in the four additional directions.

The resulting distinct 2D surfaces are plotted at each 4D sample point in the figure. If the samplings were made continuous, the result would be the 6D manifold required by string theory. Hidden in the sampled lattice is a “ghost surface” of zero-radius 2D objects that form a new embedded 2D surface having exactly the same shape as Figure 6a. The outer objects increase in size relative to inner objects that are near the surface of zeroes.

Full disclosure obligates me to point out that the visualizations in Figure 6 are vastly misleading. The full 6D manifold is actually closed and compact, with Euler characteristic $-200$. Among other subtle details, the 2D cross-section in Figure 6a should have its five circular outer edges that extend to infinity closed up to make a surface of genus 6. Nevertheless, the open-edged version of the quintic in Figure 6 contains enough information to check that it’s a consistent local depiction of the complete manifold and so is still a sufficient (although not ideal) representation.

Many years have passed since the 1987 appearance of Visualization in Scientific Computing, and we continue to learn about and evolve our craft. Our highest challenges reach beyond the accuracy and completeness of the data in a visualization image, beyond elegance in the sense of Einstein, and beyond appropriateness for the viewer’s chosen goals. Our work must also take into account the evaluatability of our representations in an essential way.

Einstein’s principle in sciences such as chemistry, physics, and biology is in effect supplemented by cross-checking against experimental data for validation. Visualization’s needs extend uniquely into the cognitive sciences for evaluation. The question that confronts us is this: how do we tell whether a student or colleague has produced a valid pictorial representation of the truth or just an appealing image that could have been derived inadvertently from a completely invalid process? Art and science can work brilliantly together in visualization science, but we must know when, and how, to distinguish them.

References

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