Data-Driven Colormap Optimization for 2D Scalar Field Visualization

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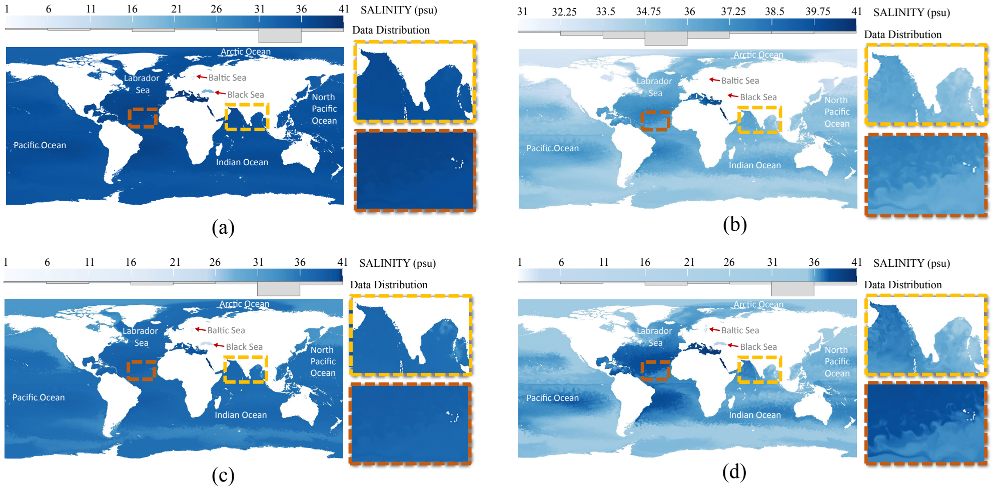

Figure 1: Visualizing ocean salinity with different colormaps. (a) A *white-blue* colormap used by domain scientists, where the boundary characteristics in the highlighted regions are not clearly revealed; (b) our domain expert limits the data range between 31 and 41 psu; (c) applying histogram equalization [20] to shift the colormap in (a); (d) the colormap generated by adapting the colormap in (a) to the data with our method.

Abstract

Colormapping is an effective and popular visual representation to analyze data patterns for 2D scalar fields. Scientists usually adopt a default colormap and adjust it to fit data in a trial-and-error process. Even though a few colormap design rules and measures are proposed, there is no automatic algorithm to directly optimize a default colormap for better revealing spatial patterns hidden in unevenly distributed data, especially the boundary characteristics. To fill this gap, we conduct a pilot study with six domain experts and summarize three requirements for automated colormap adjustment. We formulate the colormap adjustment as a nonlinear constrained optimization problem, and develop an efficient GPU-based implementation accompanying with a few interactions. We demonstrate the usefulness of our method with two case studies.

Keywords: Scientific visualization, scalar fields, color mapping, visualization optimization

Index Terms: Human-centered computing—Visualization—Visualization application domains—Scientific visualization

1 Introduction

Scientific simulations and applications produce massive 2D scalar fields: temperature in meteorology, density in physics, and diffusion in aerodynamics are all examples. 2D scalar field visualization plays an essential role for scientists to discriminate values, understand patterns and analyze trends that are hidden in data. The most effective and popular visual representation for 2D scalar fields is color mapping [3, 21, 22], which aims to map distinguishable colors in a given colormap to quantitative data values. For 2D scalar field analysis, inspecting patterns is one of the most important task for users, and during this task, users' perception for patterns is heavily affected by the colormap [22]. A good colormap makes patterns clearly visible, while a bad one might mislead readers [16].

In practice, scientists often select an existing colormap via visualization tools (e.g., SciVisColor [2], ColorMeasures [7]), and apply it to data through color mapping schemes (e.g., linear mapping). One challenge in this procedure is caused by the inconsistency between the wide range of data and the nuanced range of interesting patterns. To reveal data patterns, scientists usually interactively adjust a chosen colormap in a trial-and-error manner, which is a tedious procedure especially for unevenly distributed data.

In the visualization community, plenty of guidance rules have been proposed for colormap design [7]. Several previous works address the importance of data distribution [17] for colormap design. For example, Schulze-Wollgast et al. [18] and Tominski et al. [20] propose to modulate control points of a colormap based on statistical metadata or histogram distribution. However, such data distribution based methods might not be able to clearly visualize the spatial

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patterns of interest, see an example in Fig. 1. So far, there is no automatic colormap design algorithm that explicitly takes the spatial patterns into account for refining a given colormap.

To fill this gap, we propose a data-driven colormap adjustment method to reveal spatial patterns in 2D scalar field visualization, based on our requirement analysis with domain experts. We formulate colormap adjustment as a nonlinear constrained optimization problem, by iteratively modulating parametric positions of control points in the colormap based on the boundary characteristics [8]. We further incorporate user interactions into our optimization framework, including ROI exploration and control point customization.

The main contributions of our approach are as follows:

- We summarize three requirements for automatic colormap adjustment through discussions with domain experts.
- We propose a novel method to automatically optimize colormap for revealing discernible data patterns.
- We demonstrate the effectiveness of our method via two cases.

2 Related Work

In this section, we investigate on data-aware colormap design measures. We refer readers to prior literature [19], [4] and [23] for a complete review of colormap design in visualization.

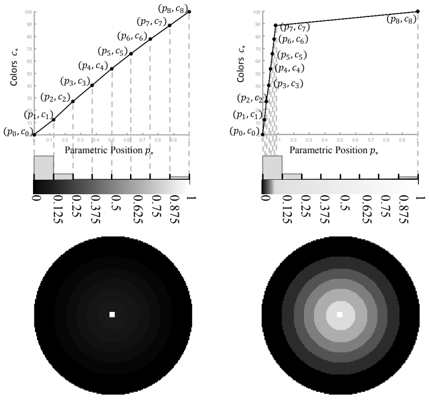
The importance of data and tasks has been addressed by previous works [9,14,22]. The most pioneering work is the system, PRAVDAColor, proposed by Bergman et al. [3], which builds a taxonomy for colormap design with consideration of spatial data frequencies and representative tasks. Similar ideas can be found in ColorBrewer [6] and ColorCAT [10]. These methods usually apply similar colormap design rules for data that are categorized in the same group. However, data with noticeably different patterns may be assigned with the same colormap, because of the limited number of categories. In our work, we aim to refine a given colormap automatically so as to better reveal continuous data patterns.

We propose to automatically adjust control points in a given colormap for a richer visualization of continuous data patterns. The methods proposed by Schulze-Wollgast et al. [18] and Tominski et al. [20] have the similar goal, which both leverage data distribution to modulate parametric positions of control points. Specifically, Schulze-Wollgast et al. [18] extract statistical metadata (e.g. median, mean or a user defined value) and adjust the colormap by shifting a control point to the corresponding position of the inferred metadata. Followed by their work, Tominski et al. [20] propose histogram equalization to improve color encoding for highlighting and segmentation tasks, aiming to shift more colors to high density data ranges. Instead of adjusting the colormap to highlight a specific value or to homogenize perceptual data distribution, our method optimizes the colormap to represent continuous data patterns by taking into account the boundary characteristics [8].

3 Requirement Analysis

To achieve our goal of optimizing colormap automatically, we firstly conduct a requirement analysis through interviews with six domain experts (E1-E6) from both visualization and scientific community. During the study, each domain expert is required to answer two 5-point Likert-scale questions based on a few prototype results, and give 1-5 sentences feedback to each question.

- Would you find it beneficial for the visualization users (e.g., designers, scientists) to have an "Auto Adjust" button next to a colormap, so that it automatically tries to match the data and provide a richer visualization?
  (1) *strongly not beneficial* (2) *not beneficial* (3) *neutral* (4) *beneficial* (5) *strongly beneficial*
- Would you expect desired results of such "Auto Adjust" to be similar to the prototype results provided by our technique?
  (1) *strongly dissimilar results expected* (2) *dissimilar results expected* (3) *neutral* (4) *similar results expected* (5) *strongly similar results expected*



(a) (b)

Figure 2: An illustration of colormap definition. (a) An unevenly distributed data is encoded with a gray colormap. (b) By shifting parametric position of control points in the gray colormap, we can produce a new colormap by linear interpolations.

Based on the answers and feedback, we summarize three requirements for an automatic colormap optimization approach. The original answers and feedback from domain experts can be found in our supplementary materials.

R1: Adjust colormap to exhibit patterns even for the full data range. Our domain experts (E1 and E3) pointed out that scientists often set the minimum and maximum data range manually, to exhibit features not visible for the full data range under a standard linear color mapping. A good manual adjustment requires not only domain knowledge, but also comprehensive understandings on the analysis task. Otherwise, the process will be tedious and time-consuming.

R2: Preserve primary colors in the colormap. E6 mentioned that she prefers to use a familiar colormap, because her experiences working with it can improve the efficiency of data analysis, even it might produce poor visualization and misleading artifacts [11,15]. Therefore, it is necessary to preserve primary colors in the process of colormap optimization.

R3: Support interactive user-control for data exploration. E4 pointed out that users would like to keep control over a visualization system, and E5 mentioned that oceanologists often care more about specific regions of interest. In addition, E2 mentioned that the benefit of the colormap adjustment in medical visualization is highly depended on applications and user preferences. Therefore, our optimization framework also can support user interactions for a better data exploration.

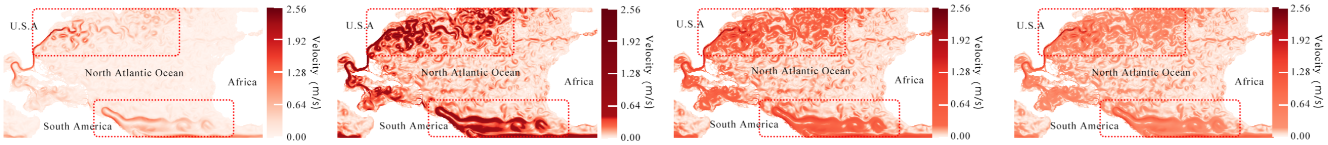
4 Technique

Based on the three requirements, we formulate an algorithm to enhance boundary characteristics for 2D scalar field visualization, improving their accessibility to domain experts for visual analysis.

Preliminaries. A colormap in our method is defined as a list of 3D colors $C = \{C_1, C_2, ..., C_n\}$ in CIELAB colorspace. Mapping colors to data requires an association between colors C and parametric data values $T = \{t_1, t_2, ..., t_n\} (0 \leq t_* \leq 1)$, denoted as $\xi : T \rightarrow C$.

To build such an association for continuous 2D scalar field, we define the discrete colormap as a set of *control points* and a *mapping function* (see Fig. 2). *Control points* refer to w constant colors $c = \{c_1, c_2, ..., c_w\}$ and corresponding parametric positions $p = \{p_1, p_2, ..., p_w\} (0 \leq p_* \leq 1)$ on the colormap. A *mapping function* describes transitions between every two control points, correlating continuous parametric positions to discrete colors. We utilize a piecewise linear mapping function to interpolate colors [13] between two neighboring control points, shown as below:

$$\hat{c} = \frac{c_w - c_{w-1}}{p_w - p_{w-1}} \times (\hat{p} - p_{w-1}) + c_{w-1}, \qquad p_{w-1} < \hat{p} < p_w \quad (1)$$



(a) Input (b) $\beta = 0$ (c) $\beta = 0.4$ (d) $\beta = 1$

Figure 3: Different settings of parameter β. (a) The input is ocean velocity at the North Atlantic Ocean, visually encoded with a *white-red* colormap. (b)-(d) Our optimized results with $\beta = 0, 0.4, 1$ respectively.

By iteratively applying the function to neighboring control points, we can recover a new colormap, denoted as $\xi = f(T; p, c)$.

4.1 Data-Driven Colormap Optimization

To meet R1-R2, the algorithm should be able to exhibit invisible features and preserve original colors.

Problem Definition. Given a 2D scalar field x with m data samples, and w control points (p, c), our goal is to obtain w parametric positions $\bar{p} = \{\bar{p}_1, \bar{p}_3, ..., \bar{p}_w\}$ for the control points (with two endpoints constant by default), such that the new color-encoded data can reveal hidden data patterns. To map the new colormap to data, we first parameterize data values into the range between 0 and 1, denoted as $x = \{x_1, x_2, ...x_m\} (0 \leq x_* \leq 1)$. Colors on each parametric data value can be inferred from $\xi = f(x; \bar{p}, c)$, abbreviated as $f(x; \bar{p})$.

We formulate the colormap adjustment process as a nonlinear constrained optimization problem by solving an energy function using sequential quadratic programming [12]. Specifically, we seek $\bar{p}$ that minimizes the energy function $E(x; \bar{p})$:

$$\arg\min_{\bar{p}} E(x; \bar{p}) = B(x; \bar{p}) + \beta F(\bar{p}) \tag{2}$$

The function consists of a boundary term B and a fidelity term F, balanced by a parameter β. A larger β results in a colormap closer to the input one, see Fig. 3. In our implementation, we set $\beta = 0.1$ by default.

Boundary Term According to R1, an automatic algorithm is necessary for pursuing a richer visualization. We refer to a richer visualization as revealing more continuous boundary structures that indicate different data patterns. The boundary model proposed by Kindlmann and Durkin [8] is adopted to infer data patterns, for its good performance in discerning boundaries in volume rendering.

Our basic idea is to emphasize original boundary structures in the color encoded data. We first estimate the likelihood $q(x)$ of how likely a data value x belongs to boundaries, and multiply it by corresponding local differences in the visualization:

$$B(x; \bar{p}) = -\sum_{i=1}^{m} q(x_i) * \sum_{j \in \Omega} \left\| f(x_i; \bar{p}) - f(x_j; \bar{p}) \right\|^2 \tag{3}$$

where Ω denotes the neighbors of a data value x_i.

The essential feature in calculating boundary likelihood q is to associate data value to boundary regions. Kindlmann and Durkin [8] have proposed a mathematical model for mapping data value x_* to an approximate position t along an ideal boundary [1]:

$$\frac{-\sigma^2 h(x_*)}{g(x_*)} \approx t \tag{4}$$

where $g(x_*)$ is the average of the first directional derivatives over all the positions with value x_*; likewise, $h(x_*)$ is the average of the second directional derivatives at positions with value x_*. σ is a parameter to control the amount of boundary blurring in ideal boundary, defined as $\sigma\sqrt{e} = \frac{f'(0)}{f''(-\sigma)}$, where $f'(0)$ and $f''(-\sigma)$ are the maximum values of first and second derivatives in the ideal boundary model. In our situation, we estimate it according to the maximum first and second derivatives of the entire data.

Eq. 4 builds a correlation between data values and its distances to the boundary. Data value with higher first derivatives and lower second derivatives is considered as closer distance to the boundary. Thus, we provide a boundary emphasizing function $b(t) = e^{-\eta|t|}$ to set higher likelihood for data value with closer distance to the boundary. Our boundary likelihood component is defined as below:

$$q(x_*) = e^{-\eta\left|\frac{-\sigma^2 h(x_*)}{g(x_*)}\right|} \tag{5}$$

where η is an empirical boundary emphasizing factor and it is set to 0.01 by default in our implementation.

Fidelity Term According to R2, we propose a fidelity term to preserve the order of primary colors and avoid significant colormap changes during optimization. The fidelity term aims to examine the consistency of the original parametric positions p of control points and the adjusted parametric positions $\bar{p}$. Instead of simply calculating the Euclidean distance between the original and adjusted parametric positions, we take advantages of an accumulative arc length function ζ (monotonically increasing) to narrow down the optimization space. We formulate the idea as below:

$$F(x; \bar{p}) = \sum_{i=1}^{w} \|\zeta(\bar{p}_i) - \zeta(p_i)\|^2, \qquad s.t. \quad \bar{\zeta}'(\bar{p}_i) > 0 \tag{6}$$

where ζ is the accumulated arc length function of the input colormap in CIELAB colorspace. $\bar{\zeta}$ is a piecewise linear function built from $\{\zeta(\bar{p}_i), 1 \leq i \leq w\}$. $\bar{\zeta}'(\bar{p}_i)$ is the first derivative of $\bar{\zeta}$ at position $\bar{p}_i$.

4.2 User-defined Interactions

According to R3, we provide two interactive operators: ROI exploration and control point customization.

ROI Exploration. To support interactive exploration for data patterns in specific region of interest, we provide a simple "outside" lasso tool (see the white dotted region in Fig. 4). The boundary likelihood component inside the lasso region is multiplied by a weight to strengthen corresponding features.

Fig. 4(a) shows the ROI exploration on a radiotherapy dose data, encoded with the popular *rainbow* colormap in scientific visualization [5]. As shown in Fig. 4(b), more variations along the boundary of the tumor dose region are revealed. Dose variations inside the tumor region are clearly shown with our ROI exploration tool (Fig. 4(c)). We will describe domain experts' feedback in Sec. 5.

Control Point Customization. The essential idea of our optimization method is to modify parametric positions of control points, with two constant endpoints by default. To support customization of arbitrary constant control point, we provide a selection tool for adding or deleting constant control points in colormap.

Fig. 5 illustrates the results of before and after control point customization, based on an ocean salinity data around the Southwest Europe. Both optimized results (with two or three constant control points) reveal global patterns on the top of Mediterranean Sea.

5 Case Study

We have implemented our method in C++ and tested with an Intel Core i7-6700K (4GHz CPU) with 16GB memory. We also develop

[1] The ideal boundary is an integration of a step function and a Gaussian. Please refer to [8] for more details.

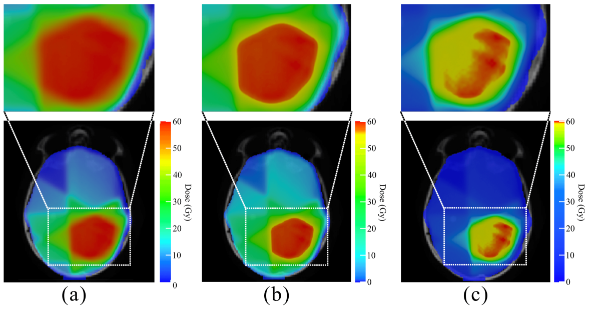


Figure 4: We show the radiotherapy dose data encoded by a *rainbow* colormap in (a). Our optimized results before and after applying ROI exploration tool are shown in (b) and (c) respectively.

a GPU implementation in CUDA that runs on an NVIDIA GTX 980 graphics card with 8GB display memory. We adopt a commercial sequential quadratic programming solver provided by Artelys Knitro [1] to optimize our energy function.

To evaluate the effectiveness and usefulness of our algorithm, we invited four domain experts (E1-E2 and E5-E6) to answer a 5-point Likert scale questionnaire. There are two categories of questions:

- **Comparison with alternatives:** does the left visualization reveal more reasonable data variations than the right one?
- **ROI exploration:** do you think our tool has provided an appropriate control for the colormap optimization?

Besides answers to the questionnaire, domain experts are requested to label exemplar regions and explain their reasons with 1-5 sentences. Please refer to our supplementary material for more details.

Case I: The first case study focuses on an ocean salinity data provided by our domain expert E1. As shown in Fig. 1(a), the salinity dissolved in ocean water is inhomogeneously distributed, with high values in the Mediterranean Sea and relatively low values in the Baltic Sea. Fig. 1(b) illustrates the visualization tuned by E1, by limiting data range to 31 and 41 psu. In (c) and (d), we show visualizations of histogram equalization [20] and our method.

We invited E1 and E5 to evaluate the four visualizations in Fig. 1. Six *comparison with alternative* questions are posed to the domain experts. According to E1 and E5's feedback, both (a) and (c) are not suitable to show the global salinity distribution. Compared with (a) and (c), our visualization in (d) reveals clearly the prominent high salinity patterns on the North and South of the Equator in the Atlantic Ocean. Regarding comparisons between our result and E1's manual adjustment in (b), E1 agreed that our result was comparable with his adjustment. Our visualization reveals the information of fresher (less salty) regions (in Baltic & Black Sea), but does not depict variations of higher salinity values on the East of the Mediterranean Sea. On the contrary, E1's visualization ignores information at fresher regions, but resolves variations in high salinity regions. This analysis was also supported by E5, "both figures lay out details structure in different areas". Though our method enables a better visualization in the global data range, we cannot always ensure a good representation in the local data range. For example, variations between 31 to 34 psu at the North of Pacific Ocean are not clearly revealed in our result. An interactive tool could be further developed to narrow down this gap.

Case II: For the second case study, we investigate on the radiotherapy dose data from a head cancer patient, which is superimposed on an anatomical CT head with 75% opacity. We invited E2 and E6 to assess the effectiveness and usefulness of our ROI exploration tool. Two *comparison with alternative* questions are posed to them, for the comparison of our visualization effect with that of the original colormap. And one *ROI exploration* question is posed to assess the usefulness of the interactive operator.

The radiotherapy dose data is visually encoded with a widely used *rainbow* colormap in the scientific community. As shown in Fig. 4(a), the tumor region is positioned on the right face with high dose on it. In this visualization, it is hard to discern intra-tumor characteristics. For our optimized colormap shown in Fig. 4(b), both E2 and E6 agreed that more data variations can be observed compared with that in Fig. 4(a). E1 mentioned that "real" high values within the tumor region can be observed in our visualization, as well as significant radiations around the right eye of the patient. And E6 pointed out that in our visualization, the boundary of the tumor region was more discernible. For our visualization in Fig. 4(c) with an interactive ROI tool, E2 expressed that "*It is really nice what you can do within a ROI*" and "*looking only at the high values area is great*", since "true" high values within the specified area can be observed. E6 mentioned that the ROI tool helped her focus on data variations inside the tumor region. Furthermore, E2 commented that a doctor would not like the useless homogeneity up to 38*Gy*. A background masking tool for hiding areas outside the ROI region could be developed in the future.

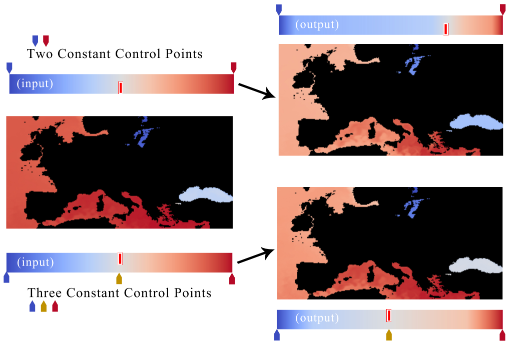


Figure 5: Here we show our optimized colormap before and after selecting a constant middle control point.

6 Conclusion

We present a data-driven colormap optimization method for 2D scalar field visualization. We conduct a pilot study under the guidance of six domain experts, and summarize three requirements for automated colormap adjustment. Following these requirements, we formulate colormap adjustment as a nonlinear constrained optimization problem, in order to reveal more data patterns with minimal shifting the control points of the input colormap. We develop an effective GPU-based implementation and interactive tool to support intuitive exploration. We demonstrate the effectiveness of our approach with two case studies.

While our case study only investigates comparisons with alternatives and ROI exploration results, in the future, we will design a task driven case study and conduct an evaluation for the interactive tool. Furthermore, we leave it as future work to develop automated colormaps for more complex data, such as sequential 2D and 3D scalar fields.

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