

Tetrahedron: Barycentric Measure Visualizer

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Abstract. Each machine learning task comes equipped with its own set of performance measures. For example, there is a plethora of classification measures that assess predictive performance, a myriad of clustering indices, and equally many rule interestingness measures. Choosing the right measure requires careful thought, as it can influence model selection and thus the performance of the final machine learning system. However, analyzing and understanding measure properties is a difficult task. Here, we present *Tetrahedron*, a web-based visualization tool that aids the analysis of complete ranges of performance measures based on a two-by-two contingency matrix. The tool operates in a barycentric coordinate system using a 3D tetrahedron, which can be rotated, zoomed, cut, parameterized, and animated. The application is capable of visualizing predefined measures (86 currently), as well as helping prototype new measures by visualizing user-defined formulas.

1 Introduction

Classifier selection and evaluation are difficult tasks requiring time and knowledge about the underlying data. One of the most important ingredients when assessing classifiers is the used *classification performance measure*. An analogous decision has to be made in association rule mining, where the overwhelming number of generated rules is usually trimmed by a selected *interestingness measure*. However, many researchers often carry out their experiments with respect to few selected measures, without discussing their properties and justifying their choice simply by the measure's popularity.

To aid the analysis of properties of measures based on two-by-two contingency tables, we put forward *Tetrahedron*, a web-based visualization tool for analyzing *entire ranges* of measure values. The proposed application visualizes 4D data in 3D using the barycentric coordinate system [1,2]. *Tetrahedron* produces 3D WebGL plots with zooming, rotating, animation, and detailed configuration capabilities. The presented tool can be used to compare properties of existing measures, as well as devise new metrics.

2 The Visualization Technique

A confusion matrix for binary classification (Table 1) consists of four entries: *TP*, *FP*, *FN*, *TN*. However, for a dataset of n examples these four entries are

Table 1. Confusion matrix for two-class classification

Actual \ Predicted	Positive	Negative	total
	Positive	TP	FN
Negative	FP	TN	N
total	\hat{P}	\hat{N}	n

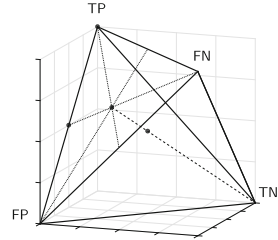


Fig. 1. Tetrahedron

sum-constrained, as $n = TP + FP + FN + TN$. Therefore, for a given constant n , any three values in the confusion matrix uniquely define the fourth value. This property allows to visualize any classification performance measure based on the two-class confusion matrix using a 4D barycentric coordinate system, tailored to sum-constrained data. The same holds for any 2×2 matrix, for example, those used to define rule interestingness measures [2].

The *barycentric coordinate system* is a coordinate system in which point locations are specified relatively to hyper-sides of a simplex. A 4D barycentric coordinate system is a tetrahedron, where each dimension is represented as one of the four vertices. Choosing vectors that represent TP, FP, FN, TN as vertices of a regular tetrahedron in a 3D space, one arrives at a barycentric coordinate system depicted in Fig. 1.

In this system, every confusion matrix $\begin{bmatrix} TP & FN \\ FP & TN \end{bmatrix}$ is represented as a point of the tetrahedron. Let us illustrate this fact with a few examples. Figure 1 shows a skeleton of a tetrahedron with four exemplary points:

- one located in vertex TP , which represents $\begin{bmatrix} n & 0 \\ 0 & 0 \end{bmatrix}$,
- one located in the middle of edge TP – FP , which represents $\begin{bmatrix} n/2 & 0 \\ n/2 & 0 \end{bmatrix}$,
- one located in the middle of face $\triangle TP$ – FP – FN , which represents $\begin{bmatrix} n/3 & n/3 \\ n/3 & 0 \end{bmatrix}$,
- one located in the middle of the tetrahedron, which represents $\begin{bmatrix} n/4 & n/4 \\ n/4 & n/4 \end{bmatrix}$.

One way of understanding this representation is to imagine a point in the tetrahedron as the center of mass of the examples in a confusion matrix. If all n examples are true positives, then the entire mass of the predictions is at TP and the point coincides with vertex TP . If all examples are false negatives, the point lies on vertex FN , etc. Generally, whenever $a > b$ ($a, b \in \{TP, FN, FP, TN\}$) then the point is closer to the vertex corresponding to a rather than b .

Using the barycentric coordinate system makes it possible to depict the originally 4D data (two-class confusion matrices) as points in 3D. Moreover, an additional variable based on the depicted four values may be rendered as color. In the presented tool, we adapt this procedure to color-code the values of classification performance and rule interestingness measures. A more in-depth description of the visualization and its possible applications can be found in [1, 2].

3 Tool Overview

The described visualization technique has been implemented as an interactive web-based application. An online version, compatible with all modern web browsers across different client platforms, is publicly available¹. The application can visualize 86 predefined 4D measures, including 21 classification measures, 16 rule interestingness measures, and 49 general-purpose formulas based on a two-by-two matrix. The user can also visualize custom measures by providing their formula. The main functionalities of the application are:

- **Interactive 3D tetrahedron visualization.** The visualization (Fig. 2a) supports: 86 predefined measures, rotating, zooming, four rendering precisions, saving as an html with WebGL, and exporting images. The user may choose to visualize external views, inner layers, and control point-padding.
- **Cross-sections.** A useful way of visualizing measure values can also be achieved by cutting the tetrahedron with a plane and analyzing the obtained slice. In this application the user can visualize cross-sections (Fig. 2b) which correspond to different class distributions. Interestingly, this particular kind of cross-sections produces a 2D space analogous to that used in ROC charts.
- **Parameter animations.** Several of the application options can be animated. These options can change the visualization parameters automatically in constant intervals creating an animation (Fig. 2c). Such animations can be useful when attempting to analyze: consecutive layers of the tetrahedron, the

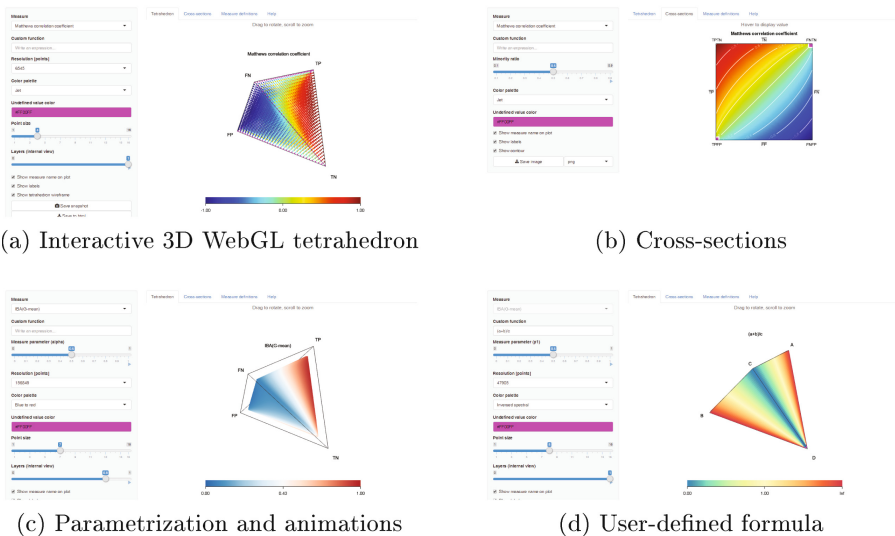


Fig. 2. Application overview

¹ <https://dabrze.shinyapps.io/Tetrahedron/>. Source codes at: <https://github.com/dabrze/tetrahedron> (MIT License).

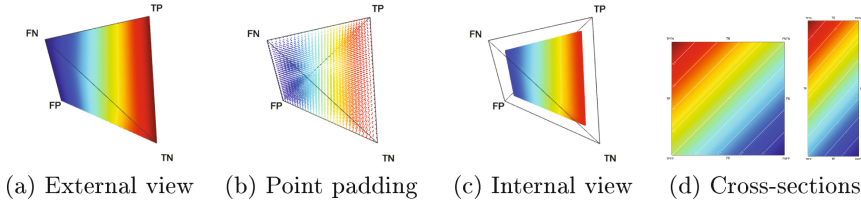


Fig. 3. Visualizations of classification accuracy (Color figure online)

impact of measure parameters (e.g. the impact of β in F_β -score), or the effect of changing class distributions on cross-sections.

- **Custom measure definition.** It is possible to define a custom measure to be visualized by providing its formula (Fig. 2d).

Since classification accuracy is one of the most intuitive performance measures, let us use it to exemplify visualizations produced by our tool with the default (blue: 0, red: 1) color map. One can notice that confusion matrices with a high number of FP and FN result in low accuracy (blue), whereas high TP and TN yield high accuracy (red). Cross-sections for two different class ratios show that on imbalanced data high accuracy can be achieved by trivial majority classifiers. More examples of visual-based analyses can be found in [1, 2] (Fig. 3).

4 Conclusions

We propose *Tetrahedron*, a web-based visualization tool for analyzing and prototyping measures based on a two-by-two matrix. Its main features include: interactive 3D WebGL barycentric plots, zooming, parameter animation, performing cross-sections, providing custom measure formulas, and saving plots with a single click. Such functionality facilitates visual inspection of various measure properties, such as determining measure monotonicity, symmetries, maximas, or undefined values. Thus, the presented tool can be used to gain further understanding of existing machine learning measures, as well as devise new ones.

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References

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