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Model fitting in $(n+1)$ dimensions

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Conventionally, fitting a mathematical model to empirically derived data is achieved by varying model parameters to minimize the deviations between expected and observed values in the dependent dimension. However, when functions to be fit are multivalued (e.g., an ellipse), conventional model fitting procedures fail. A novel $(n+1)$-dimensional $[(n+1)$-D$]$ model fitting procedure is presented which can solve such problems by transforming the n-D model and data into $(n+1)$-D space and then minimizing deviations in the constructed dimension. While the $(n+1)$-D procedure provides model fits identical to those obtained with conventional methods for single-valued functions, it also extends parameter estimation to multivalued functions.

Fitting a model to empirical data is typically achieved by minimizing the deviation (i.e., error) between the model and the data in the dependent dimension for all data values in the independent dimension. One of the most simple and effective methods of estimating model error is the sum-of-squares error, which is integrally related to maximum likelihood estimation and chi-square error (Press, Teukolsky, Vetterling, & Flannery, 1992). The present report is restricted to sum-of-squares error minimization, for simplicity, though the procedure applies more broadly.

Although conventional model fitting is adequate for the large majority of cases, when there is a single dependent value for a given independent value (i.e., a single-valued function), it fails when there are multiple dependent values for a given independent value (i.e., a multivalued function). This problem can be solved with the construction of a new dimension in which error is minimized. The $(n+1)$-dimensional $[(n+1)$-D$]$ model fitting procedure will first be introduced in the context of linear modeling for simplicity and then applied in a situation where $(n+1)$-D fitting is required.

$(n+1)$-D Model Fitting Procedure

The linear model

$$y = mx + b \tag{1}$$

with slope m and y-axis intercept b specifies the dependent value y for any given value of x. For a data set consisting of at least 2 points of the form $(x_{\text{data}}, y_{\text{data}})$, unique parameter values m and b can be obtained with numerous methods (e.g., general linear least squares, simplex method, or Marquardt algorithm; see Press et al., 1992) through error minimization between all values of y_{exp} (the expected value of y from the model) and y_{data}. Although model fitting is constrained to error minimization at specific values of x_{data}, the model is valid for any value of x. In a perfectly fitting model, any value of y_{data} would be identical to the corresponding value of y_{exp}, which depends on model parameter estimates and x_{data}. In equation form, this translates to

$$y_{\text{data}} = mx_{\text{data}} + b \tag{2}$$

where $(mx_{\text{data}} + b)$ represents y_{exp}. Note that Equation 2 is a special case of Equation 1 where the values of y and x are constrained by the data.

The first step of the $(n+1)$-D fitting procedure is to algebraically set the left side of Equation 2 equal to zero, resulting in

$$0 = mx_{\text{data}} + b - y_{\text{data}}. \tag{3}$$

In Equation 3, $mx_{\text{data}} + b$ and y_{data} are data dependent values, their difference representing the quantity to be minimized in conventional model fitting procedures. As such, minimization of this difference is the aim of both conventional model fitting and $(n+1)$-D model fitting. The second step of the $(n+1)$-D fitting procedure is to square Equation 3:

$$0 = (m_{\text{data}}x + b - y_{\text{data}})^2. \tag{4}$$

This is necessary to ensure that positive and negative errors of fit are weighted equivalently. Although other operators are also viable (e.g., absolute value), squaring the equation has the advantage of ensuring that larger deviations are weighted more heavily. The third step of the $(n+1)$-D fitting procedure is to replace the left side of Equation 4 with a new dimension:

$$z = (mx_{\text{data}} + b - y_{\text{data}})^2. \tag{5}$$

The fourth step of the $(n+1)$-D fitting procedure is to minimize the sum-of-squares error in the new dimension, z in this case, for all independent values of x_{data} and y_{data}, using the model fitting algorithm of choice. Note that the

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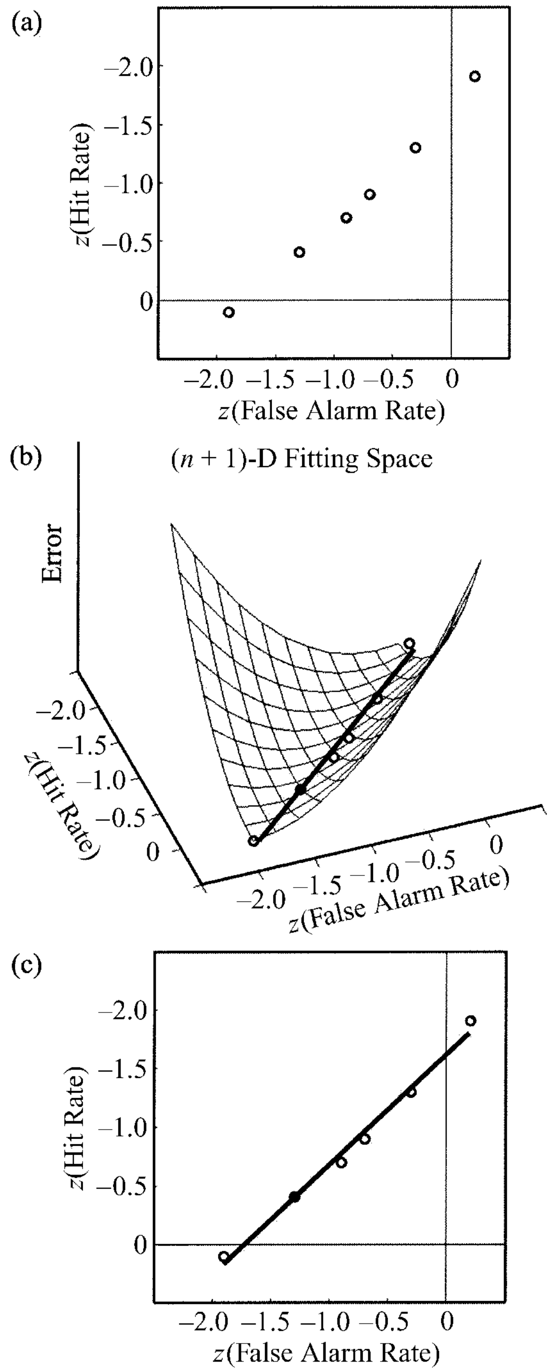

Figure 1. (a) 2-D source memory zROC data. (b) 3-D fitting space where error for all x and y is shown as a grid. The error minimum, demarcated by a line, represents the best 2-D model fit. (c) Source memory zROC with best-fit model obtained from $(n+1)$-D fit.

$(n+1)$-D fitting procedure offers a method of representing the deviation between model and data but still relies on traditional methods for parameter estimation. Finally, the fifth step of the $(n+1)$-D fitting procedure is to translate the minimum of the $(n+1)$-D model into n-D space; this is the best-fit model in n-D space.

In fitting the linear model, as with fitting other single-valued functions, the $(n+1)$-D procedure minimizes the

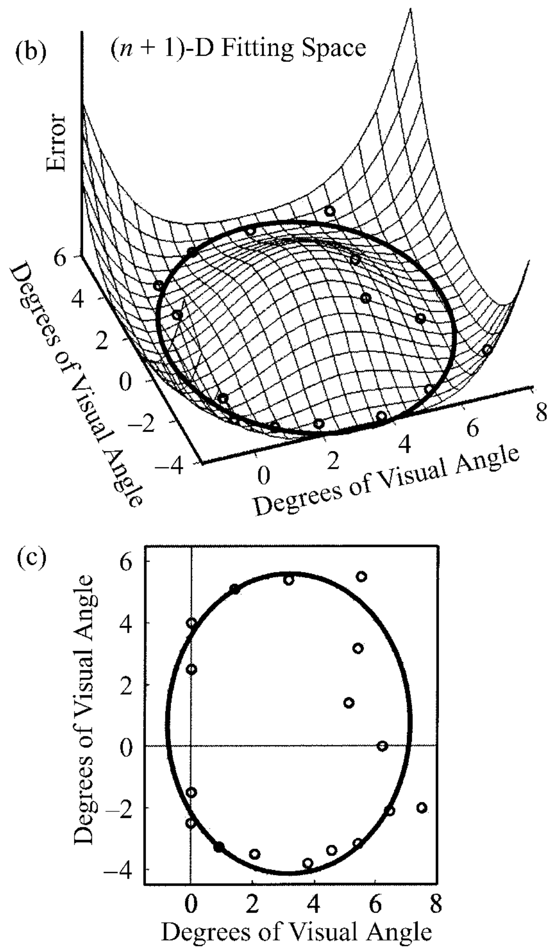

Figure 2. (a) 2-D spatial extent of attentionally mediated inhibition. (b) 3-D fitting space where error is shown as grid. The error minimum, demarcated by an ellipse, represents the best 2-D model fit. (c) Extent of attentionally mediated inhibition with best-fit elliptical model.

sum-of-squares error between expected and observed values. The conventional procedure results in the identical endpoint explaining why both methods result in the same parameter estimates under these conditions. An empirical example of linear $(n+1)$-D model fitting immediately follows.

Fitting Empirical Data

Figure 1 illustrates the $(n+1)$-D fitting procedure using actual z receiver operating characteristic (zROC) data collected in a source memory experiment (Slotnick, Klein, Dodson, & Shimamura, 2000). The Marquardt least-squares algorithm was used to minimize z in Equation 5 for all x_{data} and y_{data}, resulting in the best-fit model parameters m and b. An identical fit was produced using the conventional fitting procedure in 2-D.

In the next example, the $(n+1)$-D procedure was used to fit a multivalued function, where the conventional fitting procedure could not provide a solution. Figure 2a illustrates the spatial extent of attentionally mediated inhibition in a spatial attention experiment (Slotnick, Hopfinger, Klein, & Sutter, 2002). The aim was to model the inhibitory window with an ellipse of the form

$$1 = \frac{\left(x-\mu_x\right)^2}{a^2} + \frac{\left(y-\mu_y\right)^2}{b^2}, \tag{6}$$

where the ellipse center is located at (μ_x, μ_y), length in the x-direction is a, and length in the y-direction is b. When one applies the $(n+1)$-D fitting procedure, the final to-be-minimized equation is

$$z = \left(\frac{\left(x_{\text{data}}-\mu_x\right)^2}{a^2} + \frac{\left(y_{\text{data}}-\mu_y\right)^2}{b^2} - 1 \right)^2. \tag{7}$$

Figure 2 shows the $(n+1)$-D fitting procedure could provide the best-fit elliptical model to the data. Although other methods have previously been described to fit circular or elliptical models (Gander, Golub, & Strebel, 1994; Sutherland, 2002), the solutions are specific to those particular models. The $(n+1)$-D procedure, in comparison, applies to model fitting in general.

Conclusion

The $(n+1)$-D model fitting procedure is an alternative to conventional model estimation. It provides results identical to those of conventional model fitting, yet it can operate in cases that are conventionally insoluble. In this way, $(n+1)$-D model fitting extends the limits of conventional modeling.

REFERENCES

Gander, W., Golub, G. H., & Strebel, R. (1994). Least squares fitting of circles and ellipses. *BIT*, **34**, 556-577.

Press, W. H., Teukolsky, S. A., Vetterling, W. T., & Flannery, B. P. (1992). *Numerical recipes in C* (2nd ed.). New York: Cambridge University Press.

Slotnick, S. D., Hopfinger, J. B., Klein, S. A., & Sutter, E. E. (2002). Darkness beyond the light: Attentional inhibition surrounding the classic spotlight. *NeuroReport*, **13**, 773-778.

Slotnick, S. D., Klein, S. A., Dodson, C. S., & Shimamura, A. P. (2000). An analysis of signal detection and threshold models of source memory. *Journal of Experimental Psychology: Learning, Memory, & Cognition*, **26**, 1499-1517.

Sutherland, S. (2002). *Fitting a circle*. Retrieved September 7, 2002, from State University of New York at Stony Brook Web site: http://www.math.sunysb.edu/~scott/Book331/Fitting_circle.html.

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