

# Appendix to “New Metrics for Assessing Projection Pursuit Indexes, and Guiding Optimisation Choices”

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Let  $Y = XA$  denote the projection of a  $p$ -dimensional dataset,  $X \in \mathbb{R}^{n \times p}$ , onto  $d$ -dimensional space,  $Y \in \mathbb{R}^{n \times d}$ , where the projection is defined by an orthonormal matrix  $A \in \mathbb{R}^{p \times d}$ . Projection pursuit aims to find the matrix  $A$  that maximizes an index function  $f(\cdot)$ , which measures interesting features of the projection, such as multi-modality, linear or non-linear relationship:

$$\max_A f(XA) \quad \text{subject to} \quad A'A = I \quad (1)$$

This appendix defines all indexes  $f(\cdot)$  used in the paper, namely holes, MIC, TIC, dcor, loess, skinny, splines, and stringy). Since all the indexes are defined for 2D projections ( $d = 2$ ), the projected data can also be written as  $Y = (y_1, y_2)$ .

## The holes index

The holes index (Cook, Buja, and Cabrera 1993) defines as follows detects the presence of multi-modality in the projection:

$$I_{\text{holes}} = \frac{1 - \frac{1}{n} \sum_{i=1}^n \exp(-\frac{1}{2y_i y_i'})}{1 - \exp(-\frac{d}{2})}$$

## The dcor index

The dcor index (Grimm 2016), sometimes called dcor2D, measures the **d**istance **c**orrelation between the two projection axes  $(y_1, y_2)$ . The index uses pair-wise distance to define column sum, row sum, and overall sum and then calculates distance correlation from distance variance and covariance.

- pair-wised distance:  $a_{ij} = \|y_1^i - y_1^j\|$  and  $b_{ij} = \|y_2^i - y_2^j\|$  for  $i, j = 1, 2, \dots, n$
- column sum, row sum, and overall sum:

$$a_{i.} = \sum_{l=1}^n a_{il}, \quad a_{.j} = \sum_{k=1}^n a_{kj}, \quad a_{..} = \sum_{k,l=1}^n a_{kl}$$

$$b_{i.} = \sum_{l=1}^n b_{il}, \quad b_{.j} = \sum_{k=1}^n b_{kj}, \quad b_{..} = \sum_{k,l=1}^n b_{kl}$$

- distance covariance (and variance defined similarly):

$$\text{dCov}(a_{ij}, b_{ij}) = \frac{1}{n(n-3)} \sum_{i \neq j} a_{ij} b_{ij} - \frac{2 \sum_{i=1}^n a_{i.} b_{i.}}{n(n-2)(n-3)} + \frac{a_{..} b_{..}}{n(n-1)(n-2)(n-3)}$$

- distance correlation:

$$I_{\text{dcor}} = \text{dCor}(a_{ij}, b_{ij}) = \frac{\text{dCov}(a_{ij}, b_{ij})}{\sqrt{\text{dVar}(a_{ij}) \text{dVar}(b_{ij})}}$$

## The MIC and TIC index

Maximal Information Coefficient (MIC) and Total Information Coefficient (TIC) (Reshef et al. 2016) are information-based indexes derived from mutual information. These indexes calculate the mutual information after partitioning the space  $(y_1, y_2)$  into  $k \times l$  rectangles, with a constraint on the grid size to limit complexity:  $k \times l < B(n) = n^\alpha$ , where  $n$  is the number of observations in the data. A commonly used value for  $\alpha$  in the previous studies is 0.3 to balance flexibility and overfitting.

The MIC index finds the **maximum** mutual information over possible grids configuration that satisfy the constraint, and then normalized by the grid size:  $\log(\min(k^*, l^*))$ :

$$I_{\text{MIC}} = \frac{I(y_1, y_2 | k^*, l^*)}{\log(\min(k^*, l^*))}$$

where  $(k^*, l^*)$  is the grid configuration that maximizes the mutual information  $I(y_1, y_2 | k, l)$  under the constraint  $k \times l < B(n) = n^{0.3}$ .

TIC calculates the **sum** of the normalized mutual information for all grid configurations under the size constraint:

$$I_{TIC} = \sum_{k \times l < n^{0.3}} \frac{I(y_1, y_2 | k, l)}{\log(\min(k, l))}$$

## The loess and splines index

The loess and splines indexes detect non-linear structure in the projection by capturing the variance explained by the loess/ spline model. To account for the orientation of the projection, the model is run for both  $y_1 \sim y_2$  and  $y_2 \sim y_1$  and the larger of the two is used as the index value. Let  $e_{y_1 \sim y_2}^{\text{model}}$  and  $e_{y_2 \sim y_1}^{\text{model}}$  denote the residual from the loess/splines model  $y_1 \sim y_2$ , and  $y_2 \sim y_1$ . The two indexes are calculated as:

$$I_{\text{loess}} = \max \left( 1 - \frac{\text{var}(e_{y_1 \sim y_2}^{\text{loess}})}{\text{var}(y_1)}, 1 - \frac{\text{var}(e_{y_2 \sim y_1}^{\text{loess}})}{\text{var}(y_2)} \right)$$

$$I_{\text{spline}} = \max \left( 1 - \frac{\text{var}(e_{y_1 \sim y_2}^{\text{spline}})}{\text{var}(y_1)}, 1 - \frac{\text{var}(e_{y_2 \sim y_1}^{\text{spline}})}{\text{var}(y_2)} \right)$$

## The skinny and stringy index

Both skinny and stringy indexes are non-smooth indexes based on scagnostics (Wilkinson and Wills 2008; Wilkinson, Anand, and Grossman 2005). Scagnostics are defined based on graph concepts, specifically, the alpha hull for the skinny index and the minimum spanning tree for the stringy index. The skinny index is defined based on the alpha hull (AH) as:

$$I_{\text{skinny}} = 1 - \frac{\sqrt{4\pi \text{area}(\text{AH})}}{\text{perimeter}(\text{AH})}$$

The stringy index is defined based on the minimal spanning tree ( $T$ ). We adopt the definition in Wilkinson, Anand, and Grossman (2005) based on the diameter and length of the tree. The diameter refers to the longest shortest path through  $T$ , and the length refers to the total number of edges in  $T$ .

$$I_{\text{stringy}} = \frac{\text{diameter}(T)}{\text{length}(T)}$$

An alternative definition of the stringy index is based on number of vertices, given by  $\frac{|V^{(2)}|}{|V| - |V^{(1)}|}$ , where  $|V^{(2)}|$  represents the number of degree-2 vertices and  $|V| - |V^{(1)}|$  is the overall number of vertices minus the number of degree-1 vertices. However, we prefer the original definition based on the diameter and length of the minimal spanning tree, as it is more robust to noise, especially as the number of observations increases. In Figure 1, the stringy index defined based on the number of vertices (row 1) fails differentiate the non-linear sine wave from the non-pattern (left to right), while the diameter/length-based definition (row 2) does.

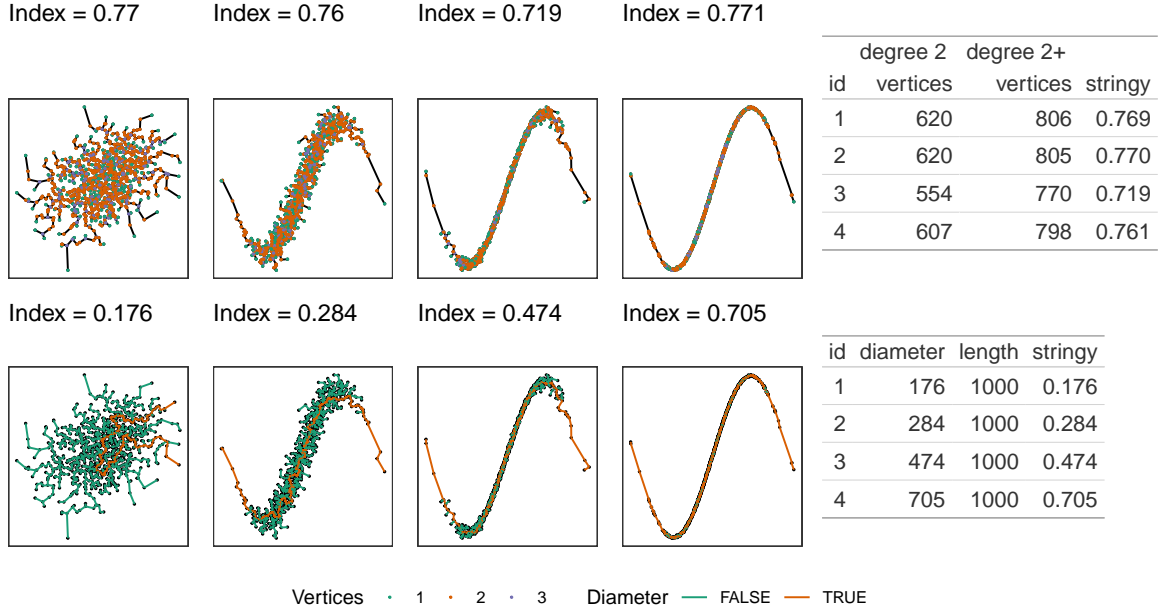


Figure 1: Projections and the stringy index values calculated based on the number of vertices definition (row 1) and the diameter/length definition (row 2) for a sine wave pattern with 1000 observations. The color represents the number of vertices in row 1 and highlights the longest minimal path (the points forming the diameter) in row 2. The noise around the sine wave creates local structures in the minimal spanning tree, resulting in a high number of degree-2 and higher vertices when calculated based on the number of vertices. This causes stringy index based on the number of vertices fails to differentiate the non-linear sine wave from the non-pattern, while the diameter/length definition, which captures the dominant main structure, is able to differentiate the sine wave form the non-pattern.

## The sine and pipe structures in the example data

Figure 2 gives an example of the sine and pipe structures data, along with index values for these projections. The syntax to generate these figures are provided below.

```
data("sine1000")
sine1000 <- as_tibble(sine1000)
dp1 <- ggplot(sine1000, aes(x=V5, y=V6)) + geom_point()
data("pipe1000")
pipe1000 <- as_tibble(pipe1000)
dp2 <- ggplot(pipe1000, aes(x=V5, y=V6)) + geom_point()
dp1 + dp2 + plot_layout(ncol=2)
```

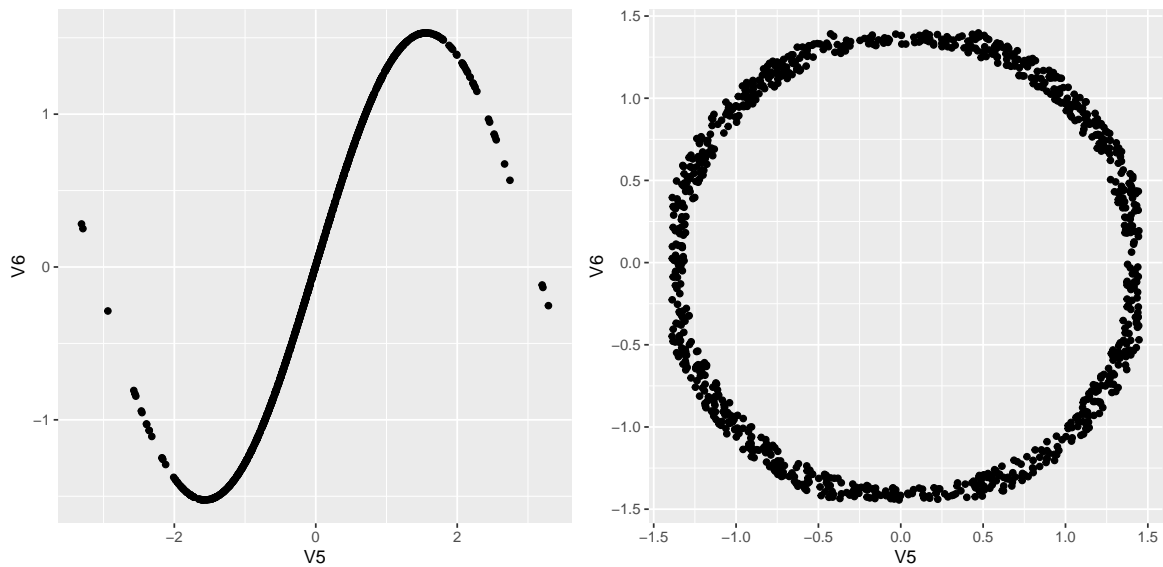


Figure 2: The sine and pipe structures in the example data, along with index values for these projections.

## Calculated smoothness and squintability metrics for all PP indexes and data sets

Smoothness and squintability are metrics used to characterize the index function for PP tasks and are invariant to the optimizer and its hyper-parameters. Table 1 presents the Gaussian process parameters (outputscale  $\eta$ , lengthscale  $\ell$ , smoothness  $\nu$ , and nugget  $\sigma$ ) and scaled

Table 1: Parameters estimated from the Gaussian process (outputscale  $\eta$ , lengthscale  $\ell$ , smoothness  $\nu$ , and nugget  $\sigma$ ) and scaled logistic function ( $\theta_1$  to  $\theta_4$  and  $\varsigma$ ) for the pipe-finding and sine-wave finding problems. The columns  $\nu$  and  $\varsigma$  represent the smoothness and squintability measures respectively.

shape	index	d	$\eta$	$\ell$	$\nu$	$\sigma$	$\theta_1$	$\theta_2$	$\theta_3$	$\theta_4$	$\varsigma$
pipe	holes	4	0.03	0.36	2.99	0.00	1.00	0.78	4.50	0.03	0.31
pipe	holes	6	0.03	0.38	3.09	0.00	1.02	0.86	3.37	0.02	0.41
pipe	holes	8	0.02	0.33	2.90	0.00	1.01	0.87	3.26	0.03	0.41
pipe	holes	10	0.02	0.34	2.88	0.00	1.02	0.88	3.15	0.02	0.43
pipe	holes	12	0.02	0.43	2.72	0.00	1.01	0.88	3.34	0.00	0.41
sine	MIC	4	0.14	0.27	3.56	0.00	0.94	0.15	1.14	-0.04	0.39
sine	MIC	6	0.06	0.31	3.08	0.00	0.89	0.57	1.62	-0.03	0.39
sine	MIC	8	0.03	0.32	2.75	0.00	0.93	0.33	1.31	-0.04	0.38
sine	TIC	4	0.40	0.27	3.49	0.00	0.97	0.46	1.55	-0.04	0.38
sine	TIC	6	0.16	0.31	3.08	0.00	0.95	0.54	1.72	-0.03	0.37
sine	TIC	8	0.07	0.30	2.72	0.00	0.95	0.56	1.72	-0.03	0.38
sine	dcor	4	0.22	0.30	3.63	0.00	0.96	1.07	2.67	-0.03	0.56
sine	dcor	6	0.08	0.29	3.13	0.00	0.95	1.04	2.74	-0.03	0.53
sine	loess	4	0.34	0.50	2.90	0.00	1.02	1.10	2.50	0.05	0.57
sine	loess	6	0.24	0.46	3.56	0.00	1.02	1.04	2.65	0.07	0.53
sine	loess	8	0.19	0.46	3.36	0.00	1.02	1.04	2.62	0.08	0.53
sine	splines	4	0.24	0.32	3.55	0.00	1.01	1.09	2.65	-0.03	0.57
sine	splines	6	0.10	0.32	3.11	0.00	1.01	1.05	2.73	-0.02	0.54
sine	splines	8	0.05	0.29	2.74	0.00	1.02	1.06	2.68	-0.02	0.54
sine	skinny	4	0.07	0.28	2.52	0.21	0.87	0.00	3.24	0.38	0.08
sine	skinny	6	0.05	0.19	2.24	0.01	0.83	0.00	2.98	0.05	0.10
sine	stringy2	4	0.02	0.30	2.76	1.01	0.64	0.05	7.89	0.05	0.00
sine	stringy2	6	0.02	0.07	1.51	0.05	0.65	0.05	7.78	0.06	0.00

logistic function parameters ( $\theta_1$  to  $\theta_4$  and  $\varsigma$ ) for all 23 PP problems investigated in our work. The columns  $\nu$  and  $\varsigma$  represent the smoothness and squintability measures respectively.

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