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Abstract

Friedman & Tukey commented on their initial paper on projection pursuit in 1974 that "the technique used for maximising the projection index strongly influences both the statistical and the computational aspects of the procedure." While many projection pursuit indices have been proposed in the literature, few concerns the optimisation procedure. In this paper, we developed a system of diagnostics aiming to visually learn how the optimisation procedures find its way towards the optimum. This diagnostic system can be applied to more generally to help practitioner to unveil the black-box in randomised iterative (optimisation) algorithms. An R package, ferrn, has been created to implement this diagnostic system.

Keywords: optimisation, projection pursuit, guided tourr, visual, diagnostics, R

*The authors gratefully acknowledge ...

1 Introduction

In an optimization problem the goal is to find the best solution within the space of all feasible solutions which typically is represented by a set of constraints. The problem consists in optimizing an objective function $f : S \to \Re$ with $S \in \Re^n$ in a reduced space given by the problem constraints to either minimize or maximize a function.... Gradient based optimization has been typically used to solve such problems. However, there are many situations where derivatives of an objective function are unavailable or unreliable and therefore traditional methods based on derivatives are not the best option to solve an optimization problem.

Derivative free methods provide another option to optimise the objective function without evaluating any gradient or Hessian information and a particular class of methods, direct search, has gained popularity through its conceptual simplicity. However, the whole searching process in the algorithm remains a black-box. Plots are usually used to evaluate and compare the performance of different algorithms but it can easily become tedious because the code will have to be modified significantly when comparing different parameters in the algorithms. For example, a categorical variable with 5 levels can be easily mapped onto colour while mapping another categorical variable with 30 levels will not make the plot informative. Thus the plot needs to be re-designed to better suit the characteristics of the parameter (whether the parameter is a scalar or a matrix? whether the parameter is quantitative or categorical? If categorical, how many levels does the parameter have?). This motivates the design of a visual diagnostic framework for optimisation algorithms based on the idea of a *global object*.

The remainder of the paper is organised as follows. Section 2 gives a general overview of optimisation methods, specifically derivative free optimisation. Section 3 introduces the optimisation problem in a specific context: projection pursuit guided tour and existing derivative free algorithms for solving it. Section 4 and 5 together present the new construction of a visual diagnostic framework that unveils the black-box of optimisation. Section 4 focuses on motivational ideas and data structure and Section 5 gives definitions of different diagnostic plots using grammar of graphic and examples. Finally, Section 6 mentions the R package: ferrn that implements the visual diagnostics described above.

2 Derivative free optimisation

In modern optimisation problems, gradient information can be hard to evaluate or sometimes even impossible and Derivative-Free Optimisation (DFO) methods can be useful to approach these problems. A traditional and still reliable in solving complicated practical problems, is *line search method* (Fletcher 2013). In the context of a simple one-dimensional problem of finding the x that minimises $f(x)$, line search achieves the goal via an iterative algorithm in the form of Equation 1.

$$x^{(k+1)} = x^{(k)} + \alpha_k * d^{(k)} \tag{1}$$

where $d^{(k)}$ is the searching direction in iteration k, and α_k is the step-size. Strictly speaking, α_k is chosen by another minimisation of $f(x^{(k)} + \alpha * d^{(k)})$ with respect to α and theoretical results have demonstrated the global convergence of the algorithm when the exact minimisation of α_k is attained (Curry 1944). In practice, this second minimisation is rarely implemented due to its computational demanding or even the existence of such a minimisation. A more realistic approach is to impose a mandatory decrease in the objective function for each iteration: $f^{(k+1)} > f^{(k)}$ and despite we lose the guarantee on global convergence, this approach turns out to be efficient in practical problems.

[Are we using projection pursuit/guided tour to better understand the convergence of optimization algorithms visually in combination with the algorithms discussed below? Or we are focusing on the optimisation problem only within the projection pursuit context? Some of the problems listed below are also applicable to optimization problem in general too. ppp]

3 Projection pursuit guided tour

Modern development of the line search methods focuses on proposing different computation on the seraching direction: $d^{(k)}$ and various approximations on the step size: α_k catered for practical optimisation problems. The specific problem context we are interested in is called projection pursuit guided tour. Projection pursuit and guided tour are two separate methods in exporatory data analysis focusing on different aspects: coined by Friedman & Tukey (1974), projection pursuit detects interesting structures (i.e. clustering, outliers and skewness) in multivariate data via low dimensions projection; whilst guided tour is a particular variation in a broader class of data visualisation method called tour.

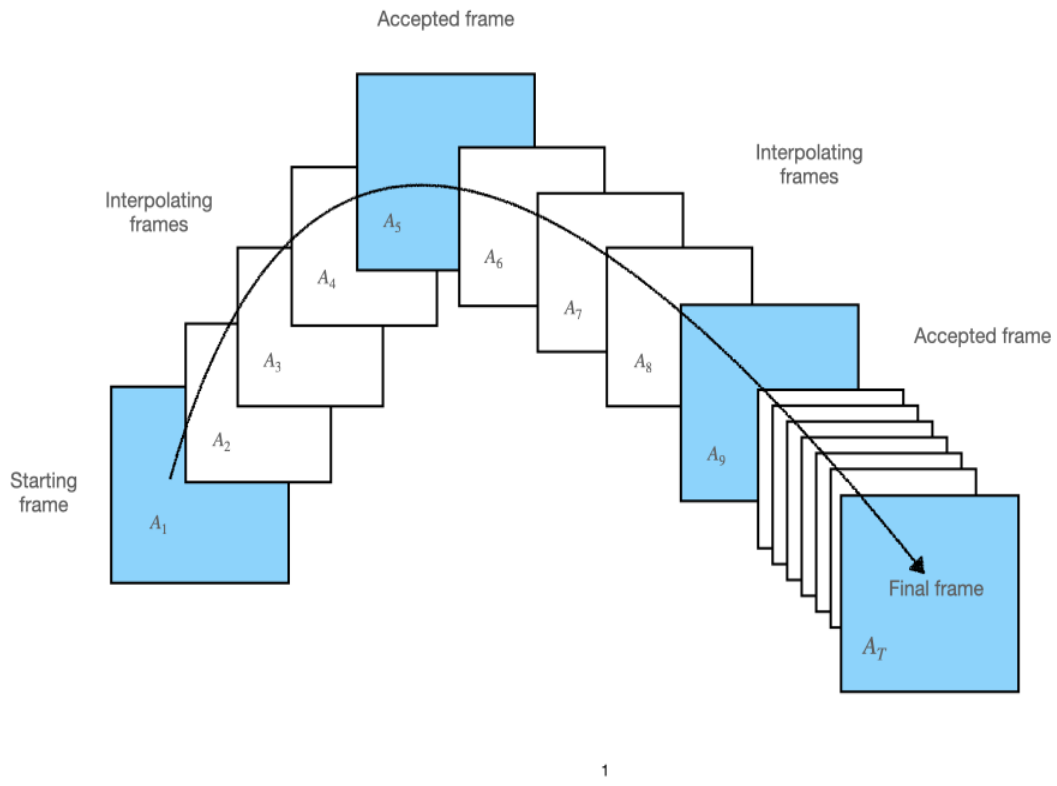
Let $\mathbf{X}_{n\times p}$ be the data matrix, an n-d projection can be seen as a linear transformation $T : \mathbb{R}^p \mapsto \mathbb{R}^d$ defined by $\mathbf{P} = \mathbf{X} \cdot \mathbf{A}$, where $\mathbf{P}_{n\times d}$ is the projected data and $\mathbf{A}_{p\times d}$ is the projection basis. Define $f : \mathbb{R}^{p\times d} \mapsto \mathbb{R}$ to be an index function that maps the projection basis $\mathbf{A}$ onto an index value I, this function is commonly known as the projection pursuit index (PPI) function, or the index function and is used to measure the "interestingness" of a projection. A number of index functions have been proposed in the literature to detect different data structures, including Legendre index (Friedman & Tukey 1974), Hermite index (Hall et al. 1989), natural Hermite index (Cook et al. 1993), chi-square index (Posse 1995), LDA index (Lee et al. 2005) and PDA index (Lee & Cook 2010).

In their initial paper, Friedman & Tukey (1974) noted that "..., the technique used for maximising the projection index strongly influences both the statistical and the computational aspects of the procedure." Hence, effective optimisation algorithms are necessary for projection pursuit to find the bases that give interesting projections. While we leave the formal construction of the optimisation problem and existing algorithms to section 3.1, we outline the general idea here. Given a random starting (current) basis, projection pursuit repeatedly searches for candidate bases nearby until it finds one with higher index value than the current basis. In the second round, that basis becomes the current basis and the repetitive sampling continues. The process ends until no better basis can be found or one of the termination criteria is reached.

Before introducing the guided tour, we shall be familiar with the general tour method (Cook et al. 2008). A tour produces animated visualisation of the high dimensional data via

rotating low dimension planes. The smoothness of the animation is ensured by computing a series of intermediate planes between two low dimension planes via geodesic interpolation and we refer readers to Buja et al. (2005) for the mathematical details. Iteratively choose different low dimension planes and interpolate between them forms a tour path. Different types of tour methods choose the low dimensional planes differently and we mention two other type of tour that are commonly used. A grand tour selects the planes randomly in the high dimensional space and hence serves as an initial exploration of the data. Manual control allows researches to fine-tuning an existing projection by gradually phase in and out one variable.

Guided tour chooses the planes produced by optimising the projection pursuit index function. Figure 1 shows a sketch of the tour path consisting of the blue frames produced by the projection pursuit optimisation algorithm iteratively and the white frames, which are the interpolations between two blue frames. The tour method has been implemented in the *tourr* package in R, available on the Comprehensive R Archive Network at `https://cran.r-project.org/web/packages/tourr/` (Wickham et al. 2011).



1

Figure 1: An illustration of the tour path

3.1 Optimisation problem

Now we begin to formulate the optimisation problem. Given a randomly generated starting basis $\mathbf{A}_1$, projection pursuit finds the final projection basis $\mathbf{A}_T = [\mathbf{a}_1, \cdots, \mathbf{a}_d]$, where $\mathbf{a}_i \in \mathbb{R}^p$, satisfies the following optimisation problem:

$$\arg\max_{\mathbf{A}\in\mathcal{A}} f(\mathbf{X}\cdot\mathbf{A}) \tag{2}$$

$$s.t. \langle \mathbf{a}_i, \mathbf{a}_j \rangle = \delta_{ij}, \forall \mathbf{a}_i, \mathbf{a}_j \in \mathbf{A} \tag{3}$$

Where δ_{ij} is the kronecker delta that takes 1 if $i = j$ and 0 otherwise.

There are several features of this optimisation that are worth noticing. First of all, it is a multivariate constraint optimisation problem. Since the decision variables are the entries of a projection basis, it is required to be orthonormal. It is also likely that the objective function is non-differentiable or the gradient information is simply not available. In this case, we will need to either use some approximation of the gradient or turn to derivative free methods. Given the goal of projection pursuit as finding the basis with the largest index value, the optimisation problem need to be able to find the global maximum. Along the way, locla maximum may also be of our interest since they could present unexpected interesting projections. There is also one computational consideration: the optimisation procedure needs to be easy to compute since the tour animation is played in real-time.

3.2 Existing algorithms

Below we introduce three possible algorithms: `search_better` and `search_better_random` are derivative free methods that sample candidate basis in the neighbourhood whilst `search_geodesic` approximates the gradient information and acts as a non-derivative version of the gradient acsent.

Posse (1995) proposed a random search algorithm that samples a candidate basis $\mathbf{A}_l$ in the neighbourhood of the current basis $\mathbf{A}_{\text{cur}}$ by $\mathbf{A}_l = \mathbf{A}_{\text{cur}} + \alpha\mathbf{A}_{rand}$, where α controls the radius of the sampling neighbourhood and $\mathbf{A}_{\text{rand}}$ is a randomly generated matrix with the same dimension as $\mathbf{A}_{\text{cur}}$. The optimiser keeps sampling bases near the current basis until it finds one with higher index value than the current basis and then outputs it for guided tour to construct the interpolation path. A new round of search continues to find a better basis after the interpolation finishes. The halving parameter c with default value of 30 is designed to adjust the searching neighbourhood α. When the search needs to sample more than c number of basis to find an accpeted basis, the neighbourhood parameter α will be reduced by half in the next iteration. If the optimiser can't find a better basis within the maximum number of tries $l_{\max}$, the algorithm stops. The algorithm is summarised in Algorithm 1 for one iteration. [mention orthonormalise to ensure the constaint is fulfilled; don't use derivative information but a random search]

Simulated annealing (Bertsimas et al. 1993, Kirkpatrick et al. (1983)) modifies `search_better` based on a non-increasing cooling scheme $T(l)$. Given an initial T_0, the temperature at iteration l is defined as $T(l) = \frac{T_0}{\log(l+1)}$. When a candidate basis fails to have an index value larger than the current basis, simulated annealing gives it a second chance to be accepted with probabiliby

$$P = \min\left\{\exp\left[-\frac{I_{cur} - I_l}{T(l)}\right], 1\right\}$$

where $I_\cdot$ denotes the index value of a given basis. This implementation allows the algorithm to jump out of a local maximum and enables a more holistic search of the whole parameter space. This feature is particularly useful when the dimension of the projected space is smaller than the number of informative variables in the dataset (i.e. a one dimenional projection of the dataset with two informative variables). The algorithm can be written as replacing line 5-11 of Algorithm 1 with Algorithm 2.

Algorithm 1: random search

input : $\mathbf{A}_{\text{cur}}$, f, α, $l_{\max}$

output: $\mathbf{A}_l$

initialisation;

Set $l = 1$ and $c = 0$;

while $l < l_{\max}$ **do**

  Generate $\mathbf{A}_l = \mathbf{A}_{\text{cur}} + \alpha \mathbf{A}_{\text{rand}}$ and orthonormalise $\mathbf{A}_l$;

  Compute $I_l = f(\mathbf{A}_l)$;

  if $I_l > I_{cur}$ **then**

    return $\mathbf{A}_l$;

  else

    $c = c + 1$;

  end

  $l = l + 1$;

end

We repeat this loop and if $c > 30$, half the α. Reset c to zero.

Algorithm 2: simulated annealing

Compute $I_l = f(\mathbf{A}_l)$ and $T(l) = \frac{T_0}{\log(l+1)}$;

if $I_l > I_{cur}$ **then**

  return $\mathbf{A}_l$;

else

  Compute $P = \min\left\{\exp\left[-\frac{I_{\text{cur}} - I_l}{T(l)}\right], 1\right\}$;

  Draw U from a uniform distribution: $U \sim \text{Unif}(0, 1)$;

  if $P > U$ **then**

    return $\mathbf{A}_l$;

  end

end

Cook et al. (1995) used a gradient ascent algorithm with pseudo-derivative. Instead of computing the actual gradient of the index function with respect to the projection basis matrix, `search_geodesic` samples $2n$ bases that are randomly generated on a uniform open ball with the radius controlled by the δ parameter and finds the most promising one to construct the geodesic direction as an approximation to the graident. The δ parameter is usually set to be tiny to ensure the geogesic direction is a good local approximation to the graident. Once the searching direction is determined, the optimiser finds the best projection $\mathbf{A}_{**}$ on the geodesic as the candidate. $\mathbf{A}_{**}$ is outputted for the current iteration if the percentage change in the index value between $\mathbf{A}_{**}$ and $\mathbf{A}_{\text{cur}}$ is greater than a threshold value or the algorithm repeats the above steps until $l_{\max}$ is reached and the searching terminates. Algorithm 3 summarise the steps in geodesic search.

Algorithm 3: search geodesic

input : $\mathbf{A}_{\text{cur}}$, f, $l_{\max}$, n, δ

output: $\mathbf{A}_{**}$

initialisation;
Set $l = 1$;
while $l < l_{\max}$ **do**
    Generate $2n$ bases in n random directions: $\mathbf{A}_l : \mathbf{A}_{l+9}$ within a small neighbourhood δ;
    Find the direction with the largest index value: $\mathbf{A}_*$ where $l < * < l + 9$;
    Construct the geodesic $\mathcal{G}$ from $\mathbf{A}_{\text{cur}}$ to $\mathbf{A}_*$;
    Find $\mathbf{A}_{**}$ on the geodesic $\mathcal{G}$ that has the largest index value ;
    Compute $I_{**} = f(\mathbf{A}_{**})$, $p_{\text{diff}} = (I_{**} - I_{\text{cur}})/I_{**}$;
    if $p_{diff} > 0.001$ **then**
        return $\mathbf{A}_{**}$;
    end
    $l = l + 1$;
end

4 Visual diagnostic system

4.1 Motivation

We can see from Figure 1 that only the data projected using the accepted and interpolated bases are animated by tour; none of the searching bases sampled by the optimsiation algorithms are presented in the tour animation. Although these algorithms have been demonstrated to find the global maximum in various literature as we cited above, they focus solely on finding the global maximum and fewer tools are available to explore how each algorithm searches the parameter space and compare the results between different algorithms.

Visualisation has been widely used in exploratory data analysis. Presenting information in a graphical format often allows people to see information they would otherwise not see. This motivates us **to develop a visual framework to diagnose optimisation algorithms in projection pursuit with the aim to understand and compare different existing algorithms.** This study is meaningful because **as more complex index functions are proposed based on statistical theory, only computationally effective optimisation algorithms allow us to find the projection basis that presents interesting structure in the data**.

The idea of generalised framework for diagnostic plots is inspired by the concept of grammar of graphic (Wickham 2010), which powers the primary graphical system in R, ggplot2 (Wickham 2016). In grammar of graphic, plots are not defined by its appearance (i.e. boxplot, histogram, scatter plot etc) but by "stacked layers". Using this design, ggplot does not have to develop a gazillion of functions that each produces a different type of plot from a different data structure. Instead, it aesthetically maps variables (and its statistical transformation) in a dataset to different geometric objects (points, lines, box-and-whisker etc) and builds the plot through overlaying different layers.

There are different ways to represent the same data in rectangular form. Certain cleaning steps are needed, before using ggplot2, to bring the data into a tidy data format (Wickham et al. 2014) where 1) each observation forms a row; 2) each variable forms a column and 3) each type of observational unit forms a table. In a tidy format, data wrangling

and visualisation are greatly simplified.

Hence the study **contributes to set up a tidy data structure for collecting observations from optimisation algorithms and prescribe a set of rules for generalising diagnostic plots for optimisation algorithms, specifically those used for projection pursuit.**

4.2 Global object

Global object is a data construction with key components from optimisation algorithms and is designed for making diagnostic plots easier. In the optimisation algorithms for projection pursuit, three key elements are 1) projection bases: $\mathbf{A}$, 2) index values: I and 3) State: S, which labels the observation with detailed stage of searching or interpolation.

Multiple iterators are needed to index the data collected at different levels. t is a unique identifier that prescribes the natural ordering of each observation; j is the counter for each search-and-interpolate round, which remains the same within one round and has an increment of one once a new round starts. l is the counter for each search/interpolation allowing us to know how many basis the algorithm has searched before finding one to output.

There are other parameters that are of our interest and we denote them as V_p. In projection pursuit, this includes V_1 = method, which tags the name of the algorithm used and V_2 = alpha, the neighbourhood parameter that controls the size in sampling candidate bases. The data structure can thus be shown as in Equation 4.

$$
\left[\begin{array}{c|c|c|c|c|c|c|c}
t & \mathbf{A} & I & S & j & l & V_1 & V_2 \\
\hline
1 & \mathbf{A}_1 & I_1 & S_1 & 1 & 1 & V_{11} & V_{12} \\
\hline
2 & \mathbf{A}_2 & I_2 & S_2 & 2 & 1 & V_{21} & V_{22} \\
3 & \mathbf{A}_3 & I_3 & S_3 & 2 & 2 & V_{31} & V_{32} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & 2 & l_2 & \vdots & \vdots \\
\hline
\vdots & \vdots & \vdots & \vdots & 2 & 1 & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & 2 & 2 & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & 2 & k_2 & \vdots & \vdots \\
\hline
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\hline
\vdots & \vdots & \vdots & \vdots & J & 1 & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
T & \mathbf{A}_T & I_T & S_T & J & l_J & V_{T1} & V_{T2} \\
\hline
\vdots & \vdots & \vdots & \vdots & J & 1 & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & J & k_J & \vdots & \vdots \\
\hline
\vdots & \vdots & \vdots & \vdots & J+1 & 1 & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
T' & \mathbf{A}_{T'} & I_{T'} & S_{T'} & J+1 & l_{J+1} & V_{T'1} & V_{T'2}
\end{array}\right]
=
\left[\begin{array}{c}
\text{column name} \\
\hline
\text{search (start basis)} \\
\hline
\text{search} \\
\text{search} \\
\vdots \\
\text{search (accepted basis)} \\
\hline
\text{interpolate} \\
\text{interpolate} \\
\vdots \\
\text{interpolate} \\
\hline
\vdots \\
\hline
\text{search} \\
\vdots \\
\text{search (final basis)} \\
\hline
\text{interpolate} \\
\vdots \\
\text{interpolate} \\
\hline
\text{search (no output)} \\
\vdots \\
\text{search (no output)}
\end{array}\right]
\tag{4}
$$

where $T' = T + k_J + l_{J+1}$. Note that we deliberately denote the last round of search as $j = J + 1$ and in that round there is no output/interpolation basis and the algorithm terminates. This notation allows us to denote the last complete search-and-interpolate round as round J and hence the final basis is A_T and highest index value found is I_T.

[outside the paper: I find the notation of current/target basis is confusing because the target basis in round j becomes the current basis in round $j + 1$. Also, when we start to have polish, the target basis may not be the current basis in the next round... The place where current/target is most appropriate is probably when describing the interpolation where the first one is always the current basis and the last is always the target basis. I

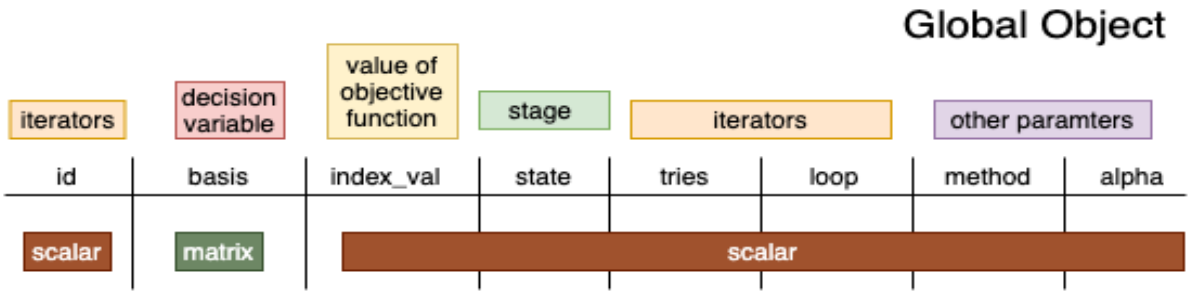


Figure 2: The global object in projection pursuit guided tour.

think it is better to leave this language in the code]

A sketch of the global object for projection pursuit guided tour is presented in Figure 2.

[I feel this sketch was initially useful but now since we have the data matrix and the printed output of the global object, it doesn't any additional information. I'm still keeping it here but we may need to remove it if it's not useful :(]

4.3 Simulated data

We simulate some random variables of size 1000 with different structures. `x1`, `x8`, `x9` and `x10` are simulated from normal distribution with zero mean and variance of one as in equation 5. When using projection pursuit to explore the data structure based on its departure from normality, the entry in the projection basis for these variables should be close to zero in theory. `x2` to `x7` are mixture of normal distributions with different weights and locations. Equation 6 to 11 outlines the distribution where each variable is simulated from and Figure 3 shows the histogram of each variable except `x3`. All the variables are then scaled to have unit variance before running the projection pursuit.

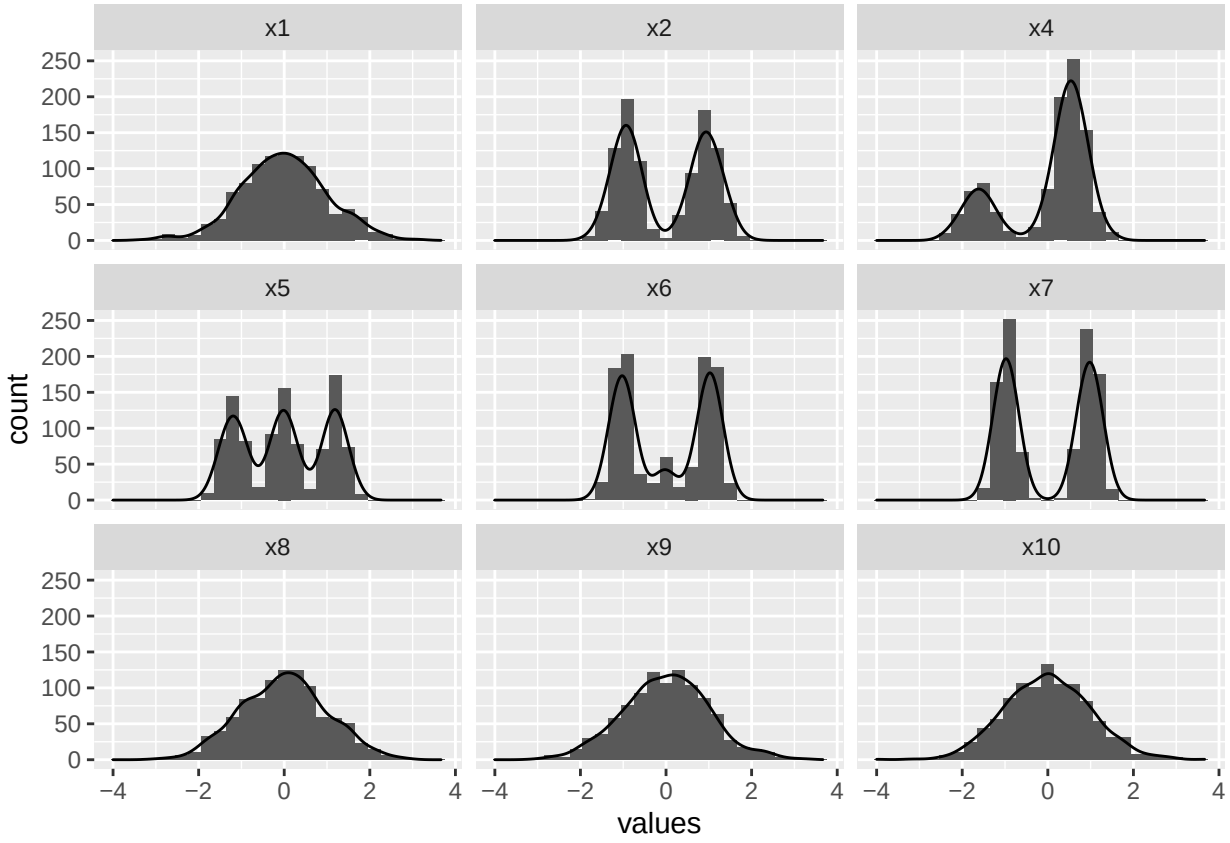


Figure 3: The distribution of simulated data except x3

$$x_1 \overset{d}{=} x_8 \overset{d}{=} x_9 \overset{d}{=} x_{10} \sim \mathcal{N}(0,1) \tag{5}$$

$$x_2 \sim 0.5\mathcal{N}(-3,1) + 0.5\mathcal{N}(3,1) \tag{6}$$

$$\Pr(x_3) = \begin{cases} 0.5 & \text{if } x_3 = -1 \text{ or } 1 \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

$$x_4 \sim 0.25\mathcal{N}(-3,1) + 0.75\mathcal{N}(3,1) \tag{8}$$

$$x_5 \sim \frac{1}{3}\mathcal{N}(-5,1) + \frac{1}{3}\mathcal{N}(0,1) + \frac{1}{3}\mathcal{N}(5,1) \tag{9}$$

$$x_6 \sim 0.45\mathcal{N}(-5,1) + 0.1\mathcal{N}(0,1) + 0.45\mathcal{N}(5,1) \tag{10}$$

$$x_7 \sim 0.5\mathcal{N}(-5,1) + 0.5\mathcal{N}(5,1) \tag{11}$$

We form our first dataset using variables `x1`, `x2`, `x8`, `x9` and `x10` and run the guided

tour with optimiser `search_better`. When the optimisation ends, the global object will be stored and printed (it can be turned off by supplying argument `print = FALSE`). Additional messages during the optimisation can be displayed by argument `verbose = TRUE`. Below shows the first ten rows of the global object. Notice that the tibble object allows the list-column `basis` to be printed out nicely with the dimension of the projection basis readily available.

[I notice that in the implementation the loop index for interpolation starts from 0 rather than 1. Need more investigation to see if it is easy to change it to 1 or we will have to change the definition of the data structure.]

```
## # A tibble: 10 x 8
##       id basis             index_val info         tries  loop method       alpha
##    <int> <list>                <dbl> <chr>        <dbl> <dbl> <chr>        <dbl>
##  1     1 <dbl[,1] [5 x 1]>     0.749 new_basis        1     1 <NA>           0.5
##  2     2 <dbl[,1] [5 x 1]>     0.730 random_sear~     2     1 search_bett~   0.5
##  3     3 <dbl[,1] [5 x 1]>     0.743 random_sear~     2     2 search_bett~   0.5
##  4     4 <dbl[,1] [5 x 1]>     0.736 random_sear~     2     3 search_bett~   0.5
##  5     5 <dbl[,1] [5 x 1]>     0.747 random_sear~     2     4 search_bett~   0.5
##  6     6 <dbl[,1] [5 x 1]>     0.725 random_sear~     2     5 search_bett~   0.5
##  7     7 <dbl[,1] [5 x 1]>     0.752 new_basis        2     6 search_bett~   0.5
##  8     8 <dbl[,1] [5 x 1]>     0.749 interpolati~     2     0 search_bett~  NA
##  9     9 <dbl[,1] [5 x 1]>     0.750 interpolati~     2     1 search_bett~  NA
## 10    10 <dbl[,1] [5 x 1]>     0.750 interpolati~     2     2 search_bett~  NA
```

5 Visual diagnostic plots

Below we will present several examples of diagnosing different aspects of the projection pursuit optimisation. We will present:

1) static plots to explore the index value,

2) animated plots to explore the projection basis and,

3) a self-contained example to optimise a complex index function.

In the first two sections, we will first provide a toy example that is easy to grasp and then more examples that can help us to understand the algorithm and parameter choice. Remember the research question we raised earlier, the purpose of visual diagnostics is to understand:

- Whether the algorithm has successfully found the maximum and how the index value changes throughout the algorithm?

- How does the searching space look like, that is, geometrically, where are the projection bases located in the space?

The first question can be answered using a static plot with x-axis showing the progression of the optimisation and y-axis showing the value of the objective function. The second question can be addressed via visualising the rotating high dimensional space or its projection on the reduced 2D space. Thus animated visualisation is needed to perceive the optimisation path in the searching space.

Since the global object is already tidy, not further tidying steps is needed, while certain data wrangling steps (Wickham & Grolemund 2016) are still needed to transform the global object into desirable format for one particular visualisation. To emphasize on this good practice of data analysis, we will describe the transformation steps needed for each diagnostic plots before stepping into visualisation.

5.1 Explore the value of objective function

5.1.1 Searching points

A primary interest of diagnosing an optimisation algorithm is to study how it finds its optimum progressively. We could plot the index value across its natural ordering, however, different iterations may have different number of points and, towards the end of the search there could easily be hundreds of bases being tested before the target basis is found. In the plot, points from those iterations towards the end will occupy the vast majority of the plot space. This motivates to use summarisation. Rather than knowing the index value of *every* basis, we are more interested to have a general summary of all the index value in that iteration and more importantly, the basis with the largest index value (since it prescribes the next geodesic interpolation and future searches).

Boxplot is a suitable candidate that provides five points summary of the data, however it has one drawback: it does not report the number of points in each box. We may risk losing information on how many points it takes to find the target basis by displaying the boxplot alone for all `tries`. Thus, the number of point in each iteration is displayed at the bottom of each box and we provide options to switch iteration with small number of

points to a point geometry, which is achieved via a `cutoff` argument. A line geometry is also added to link the points with the largest index value in each iteration. This helps to visualise the improvement made in each iteration. Using the concept of *gramma of graphics* (Wickham 2010), the plot for exploring index value can be defined in three layers as:

- Layer 1: boxplot geom
  - data: group by j and filter the observations in the group that have count greater than `cutoff = 15`.
  - x: j is mapped to the x-axis
  - y: the statistical transformed index value: $Q_{I_t'}(q)$ is mapped to the y-axis where $Q_X(q)$, $q = 0, 25, 50, 75, 100$ finds the qth-quantile of X and I_t' denotes the index value of all the searching bases defined in Matrix 4.
- Layer 2: point geom
  - data: group by j and filter the observations in the group that have count less than `cutoff = 15`.
  - x: j is mapped to the x-axis
  - y: I is mapped to the y-axis
- Layer 3: line geom
  - data: filter the points with the highest index value in group j
  - x: j is mapped to the x-axis
  - y: I is mapped to the y-axis

Toy example: exploring searching points We choose variables `x1`, `x2`, `x3`, `x8`, `x9` and `x10` to perform a 2D projection with tour. Parameter `search_f = tour::search_better` and `max.tries = 500` is used. The index value of the searching points are shown in Figure 4. The label at the bottom indicates the number of observations in each iteration and facilitates the choice of `cutoff` argument (by default `cutoff = 15`). We learn that the `search_better` quickly finds better projection basis with higher index value at first and then takes longer to find a better one later.

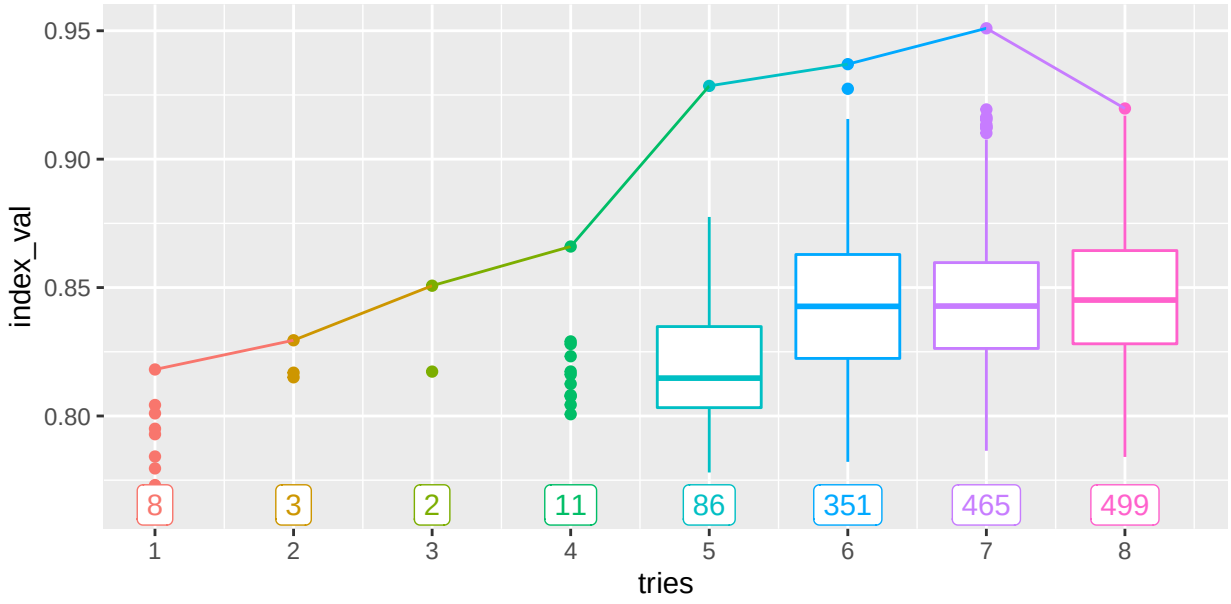


Figure 4: A comparison of plotting the same search points with different plot designs. The left plot does not use the plot space efficiently to convey information from the plot while the right plot provides good summarisation of data and number of points in each tries.

5.1.2 Interpolating points

Sometimes, rather than exploring the searching points, we may be interested in exploring the points on the interpolation path (target and interpolating points) since these points will be played by the tour animation. Since interpolation paths are geodesically the shortest, a summarisation using boxplot geometry is no longer needed. The slightly modified plot definition is shown below:

- Layer 1: point geom
  - data: filter the observations with $S =$ interpolation and mutate t to be the row number of the subsetted tibble
  - x: t is mapped to the x-axis
  - y: I is mapped to the y-axis
- Layer 2: line geom
  - using line geometry for the same data and aesthetics

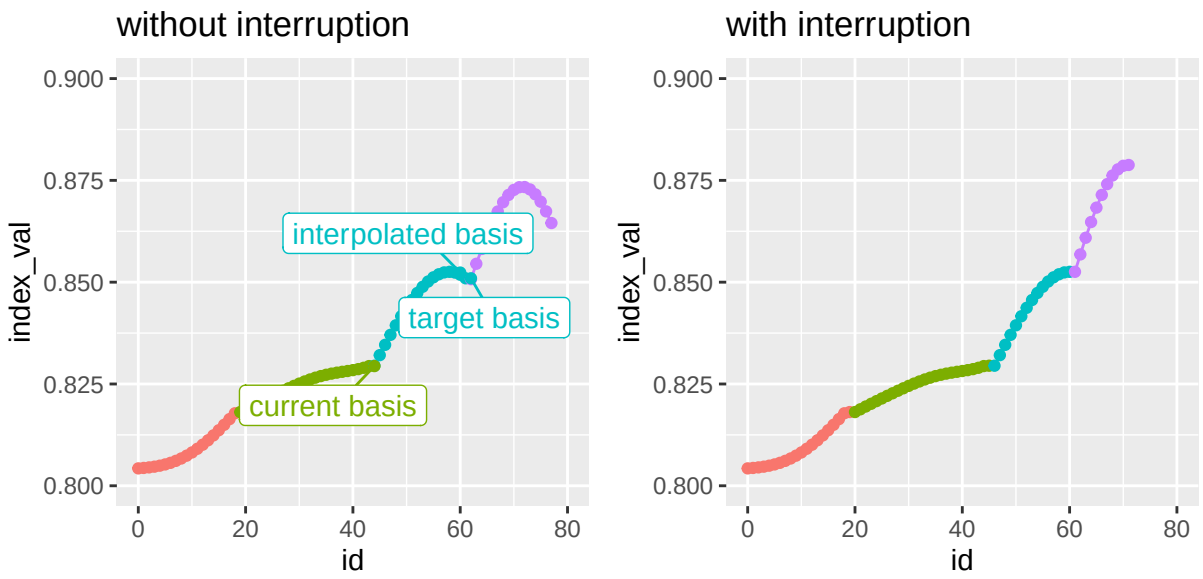


Figure 5: Trace plots of the interpolated basis with and without interruption. The interruption stops the interpolation when the index value starts to decrease at id = 60. The implementation of the interuption finds an ending basis with higher index value using fewer steps.

A more complex example: Interruption We use the same dataset as the toy example above to explore the search function `search_better` and we want to learn how the index value changes on the interpolation path for the `holes` index. From the left panel of Figure 5, we observe that when interpolating from the current basis to the target basis, the index value may not be monotone: we could reach a basis with a higher index value than the target basis on the interpolation path. In this sense, we would be better off using the basis with the highest index value on the interpolation path as the current basis for the next iteration (rather than using the target basis). Hence, an interruption is constructed to accept the interpolating bases only up to the one with the largest index value. After implementing this interruption, the search finds higher final index value with fewer steps as shown in the right panel of Figure 5.

5.1.3 Polishing points

In principle, all the optimisation routines should result in the same output for the same problem while this may not be the case in real application. This motivates the creation of a polishing search that polishes the final basis found and achieves unity across different methods.

`search_polish` takes the final basis of a given search as a start and uses a brutal-force approach to sample a large number of basis (`n_sample`) in the neighbourhood. Among those sampled basis, the one with the largest index value is chosen to be compared with the current basis. If its index value is larger than that of the current basis, it becomes the current basis in the next iteration. If no basis is found to have larger index value, the searching neighbourhood will shrink and the search continues. The polishing search ends when one of the four stopping criteria is satisfied:

1) the chosen basis can't be too close to the current basis
2) the percentage improvement of the index value can't be too small
3) the searching neighbourhood can't be too small
4) the number of iteration can't exceed `max.tries`

The usage of search_polish is as follows. After the first search, the final basis from the interpolation is extracted and supplied to the second search as the `start` argument. `search_polish` is used as the search function. All the other arguments should remain the same.

```
set.seed(123456)
holes_2d_geo <- animate_xy(data_mult[,c(1,2, 7:10)],tour_path =
                             guided_tour(holes(), d = 2,
                                         search_f = tourr:::search_geodesic),
                           rescale = FALSE, verbose = TRUE)

last_basis <- holes_2d_geo %>% filter(info == "interpolation") %>%
  tail(1) %>% pull(basis) %>% .[[1]]
```

```
set.seed(123456)
holes_2d_geo_polish <- animate_xy(data_mult[,c(1,2, 7:10)], tour_path =
                                    guided_tour(holes(), d = 2,
                                                search_f = tourr:::search_polish),
                                  rescale = FALSE, verbose = TRUE,
                                  start = last_basis)
```

A slight variation of the plot definition due to the addition of polishing points is as follows:

- Layer 1: point geom
  - data: filter the observations with S = interpolation; bind the global object from optimisation and interpolation and form polishing; mutate t to be the row number of the binded tibble.
  - x: t is mapped to the x-axis
  - y: I is mapped to the y-axis
  - colour: V is mapped to the colour aesthetic
- Layer 2: line geom

Another example: Polish Again using the same data, we are interested to compare the effect of different `max.tries` in the 2D projection setting. `max.tries` is a hyperparameter that controls the maximum number of try before the search ends. The default value of 25 is suitable for 1D projection while we suspect it may not be a good option for the 2D case and hence want to compare it with an alternative, 500. As shown in Figure 6, both trials attain the same index value after polishing while the small `max.tries` of 25 is not sufficient for `search_better` to find its global maximum and we will need to adjust the `max.tries` argument for the search to sufficiently explore the parameter space.

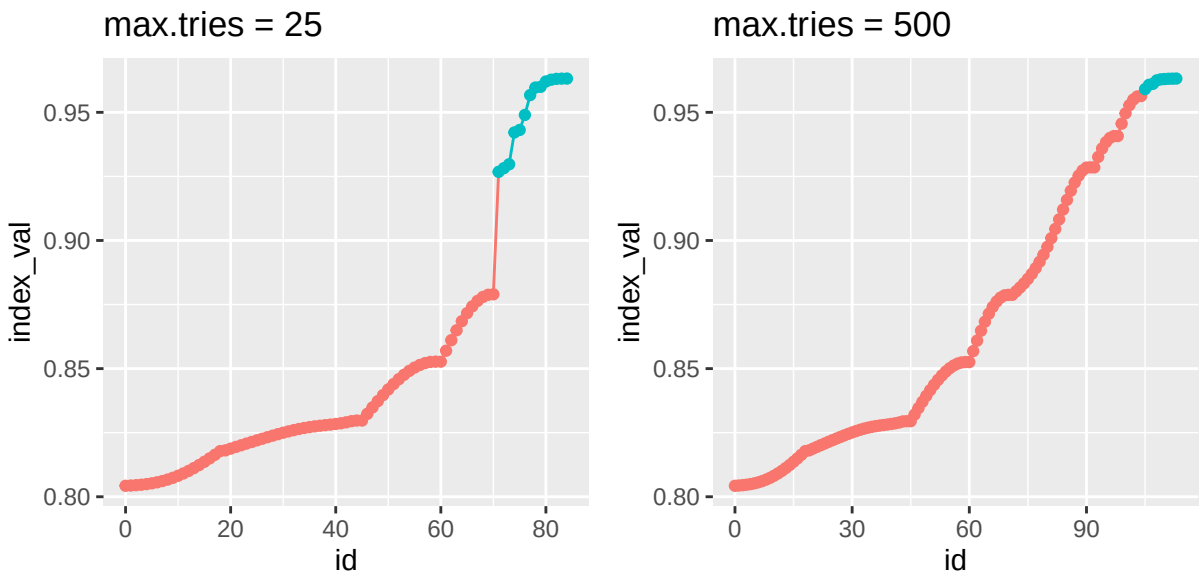


Figure 6: Breakdown of index value when using different max.tries in search better in conjunction with search polish. Both attain the same final index value after the polishing while using a `max.tries` of 25 is not sufficient to find the true maximum.

5.2 Explore searching space

In projection pursuit, the projection bases $\mathbf{A}_{p\times d}$ are usually of dimension $p \times d$ and hence can't be visualised in a 2D plot. An option to explore the searching space of these bases is to explore a reduced space via principal component analysis (PCA). The visualisation can thus be defined as

- Layer 1: point geom
  - data: subset the basis of interest and arrange into a matrix format; perform PCA on the basis matrix and compute the projected basis on the first two principal components; bind the variables from the original global object and form a tibble
  - x: the projected basis on the first principal component
  - y: the projected basis on the second principal component
  - colour: V is mapped to the colour aesthetic

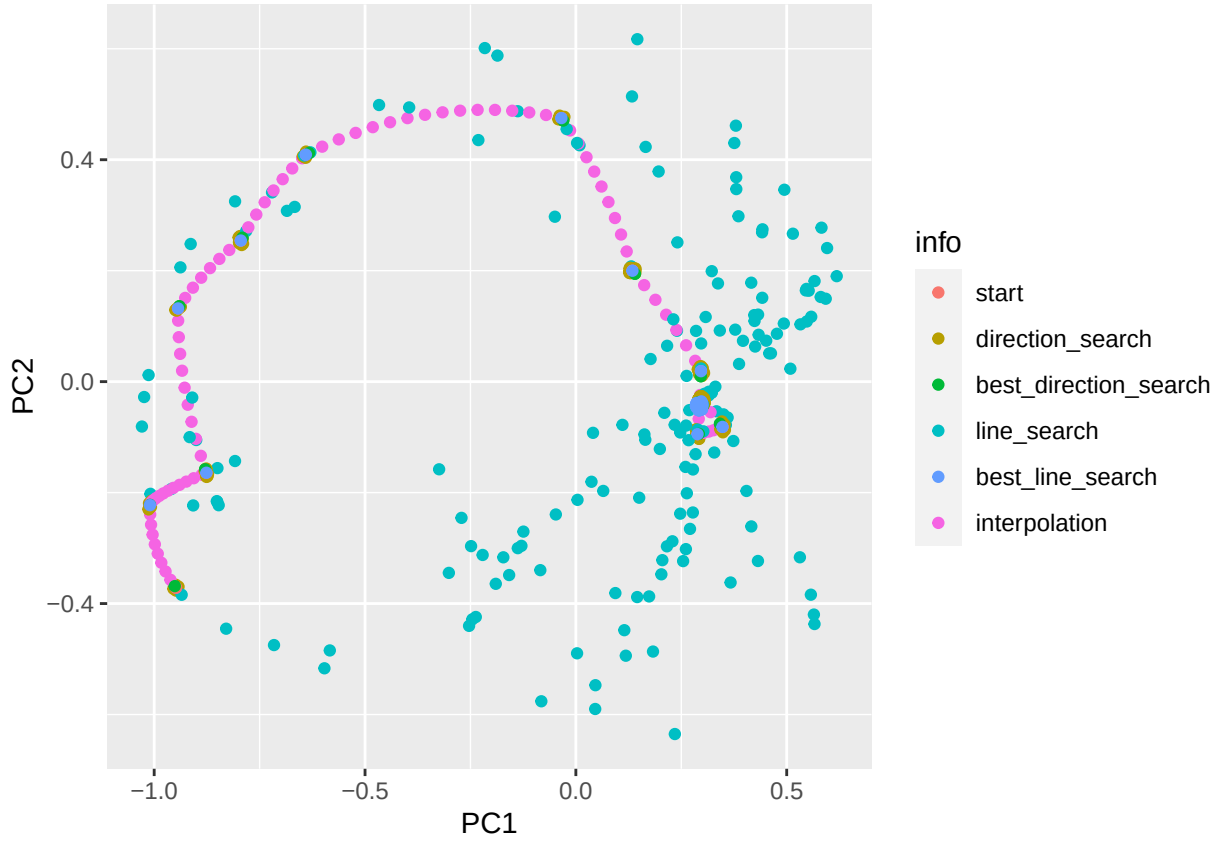


Figure 7: PCA plot of search geodesic colouring by info allows for better understanding of each stage in the geodesic search

5.2.1 A toy example: understand different stage of search_geodesic

Example: understand search_geodesic [feel like this example is merely explaining search geodesic algorithm, so maybe introduce the animated plot here? xxx] `search_geodesic` is a two-stage ascending algorithm with four different stages in the search and a PCA plot useful to understand how the algorithm progresses and the relative position of each basis in the PCA projected 2D space. Starting from the start basis, a directional search is conducted in a narrow neighbourhood on five random directions. The best one is picked and a line search is then run on the geodesic direction to find the target basis. The starting and target bases are then interpolated. In the next iteration, the target basis becomes the current basis and then the procedures continues.

5.2.2 A more complex example: Choosing the initial value for polishing parameter

Example: initial value for polishing alpha `search_polish` is a brute-force algorithm that evaluate 1000 points in the neighbourhood at each loop. Setting an appropriate initial value for polish_alpha would avoid wasting search on large vector space that are not likely to produce higher index value. The default initial value for polishing step is 0.5 and we are interested in whether this is an appropriate initial value to use after `search_geodesic`. The problem is a 1D projection of the small dataset using `search_geodesic` and followed by `search_polish`. The top-left panel of Figure 8 displays all the projection bases on the first two principal components, coloured by the `polish_alpha`. We can observe that rather than concentrating on the ending basis from `search_geodesic` as what polishing step is designed, `search_polish` searches a much larger vector space, which is unnecessary. Thus a customised smaller initial value for `polish_alpha` would be ideal. One way to do this is to initialised `polish_alpha` as the projection distance between the last two target bases. The top-right panel of Figure 8 shows a more desirable concentrated searching space near the ending basis. Both specifications of initial value allow the searches to reach the same ending index values.

While explore the reduced space is an initial attempt to understand the searching space, there are existing technology for rotating a higher dimensional space for visualisation. Geozoo is an option. It generates random points on the high dimensional space and we can overlay it with the points on the optimisation path to visualise the spread of it on the high-D sphere.

[add example from geozoo]

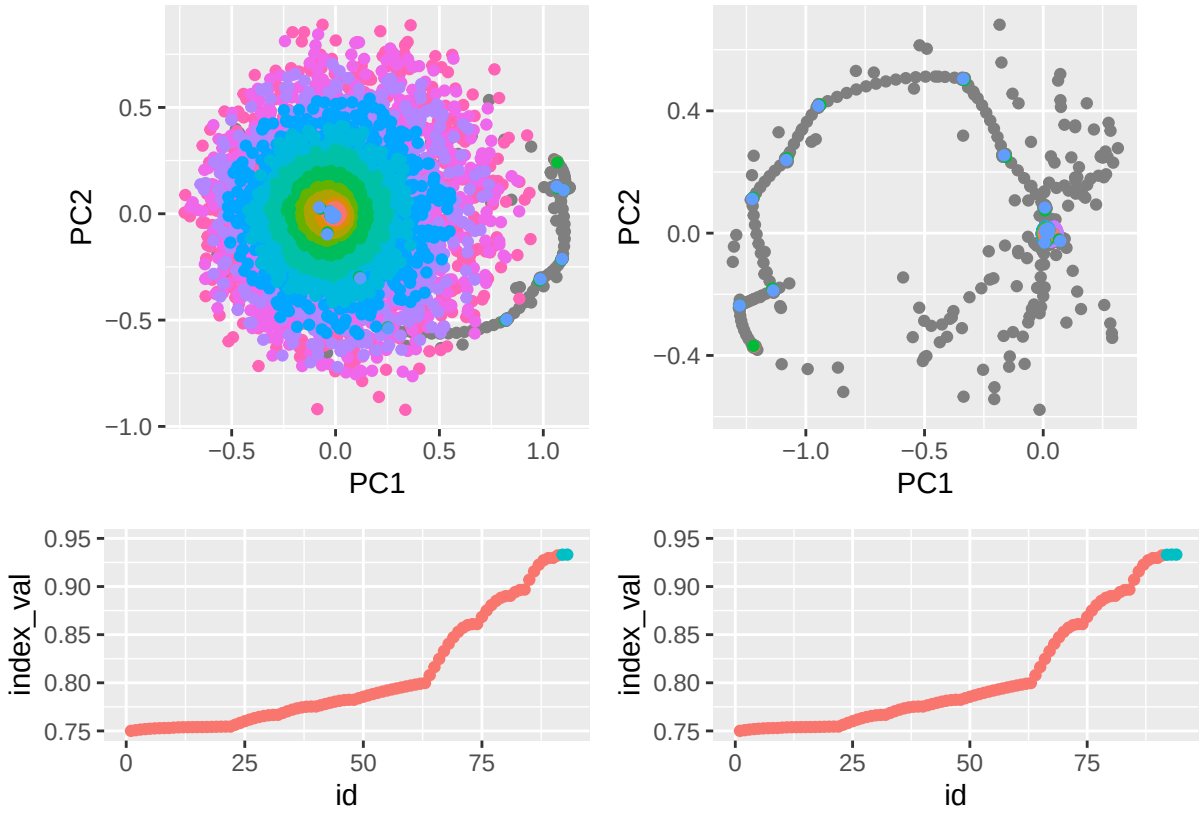


Figure 8: PCA plot of two different polish alpha initialisations. A default polish alpha = 0.5 searches a larger space that is unncessary while a small customised initial value of polish alpha will search near the ending basis. Both intialisations reach the same ending index values.

5.3 A comprehensive example of diagnosing a noisy index function

The interpolation path of holes index, as seen in Figure 5, is smooth, while this may not be the case for more complicated index functions. `kol_cdf` index, an 1D projection index function based on Kolmogorov test, compares the difference between the 1D projected data, $\mathbf{P}_{n\times 1}$ and a randomly generated normal distribution, y_n based on the empirical cumulated distribution function (ECDF). Denotes the ECDF function as $F(u)$ with subscript indicating the variable, the Kolmogorov statistics defined by

$$\max\left[F_{\mathbf{P}}(u) - F_y(u)\right]$$

can be seen as a function of the projection matrix $\mathbf{A}_{p\times 1}$ and hence a valid index function.

5.3.1 Explore index value

Figure 9 compares the tracing plot of the interpolating points when using different optimisation algorithms: `search_geodesic` and `search_better`. One can observe that

- The index value of `kol_cdf` index is much smaller than that of holes index
- The link of index values from interpolation bases are no longer smooth
- Both algorithms reach a similar final index value after polishing

Polishing step has done much more work to find the final index value in `search_geodesic` than `search_better` and this indicates `kol_cdf` function favours of a random search method than ascent method.

Now we enlarge the dataset to include two informative variables: `x2` and `x3` and remain 1D projection. In this case, two local maxima appear with projection matrix being $[0, 1, 0, 0, 0, 0]$ and $[0, 0, 1, 0, 0, 0]$.

Using different seeds in `search_better` allows us to find both local maxima d as in Figure 10. Comparing the maximum of both, we can see that the global maximum happens when `x2` is found. It is natural to ask then if there is an algorithm that can find the global maximum without trying on different seeds? `search_better_random` manages to do it via

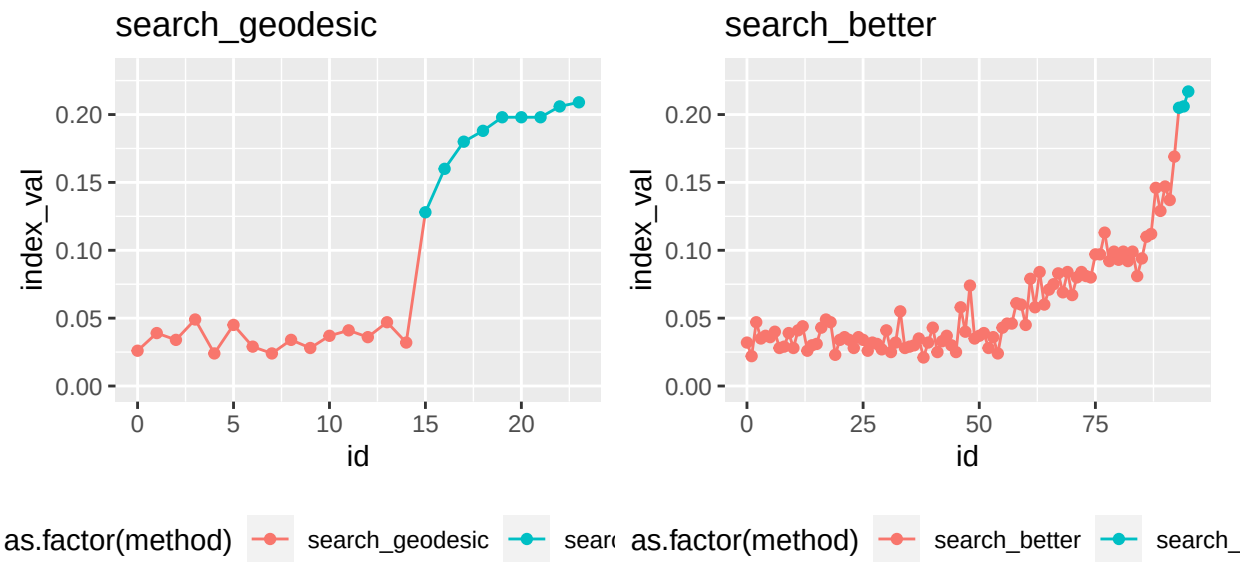


Figure 9: Comparison of two different searching methods: search_geodesic and search_better on 1D projection problem for a noisier index: kol_cdf. The geodesic search rely heavily on the polishing step to find the final index value while search better works well.

a Metropolis-hasting random search as shown in Figure 11, although at a higher cost of number of points to evaluate.

5.3.2 Explore searching space

We can also plot the searching points of all three algorithms in the searching space and explore their relative position against each other using principal components. As shown in Figure 12, the bases from better1 and better2 only search a proportion of the searching space while better_random produces a more exhaustive search. The large overlapping of better1 and better_random is explained by the fact that both algorithms find x2 in the end.

6 Implementation: Ferrn package

Everything is coded up in a package. Package structure

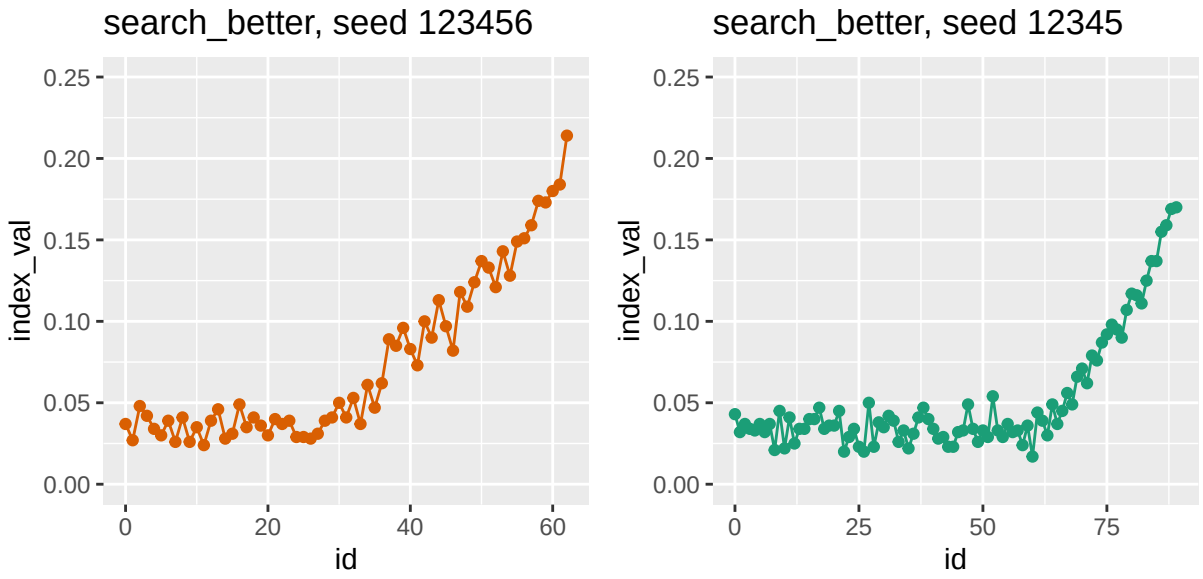


Figure 10: The trace plot search better in a 1D projection problem with two informative variables using different seeds (without polishing). Since there are two informative variables, setting different value for seed will lead search better to find either of the local maximum.

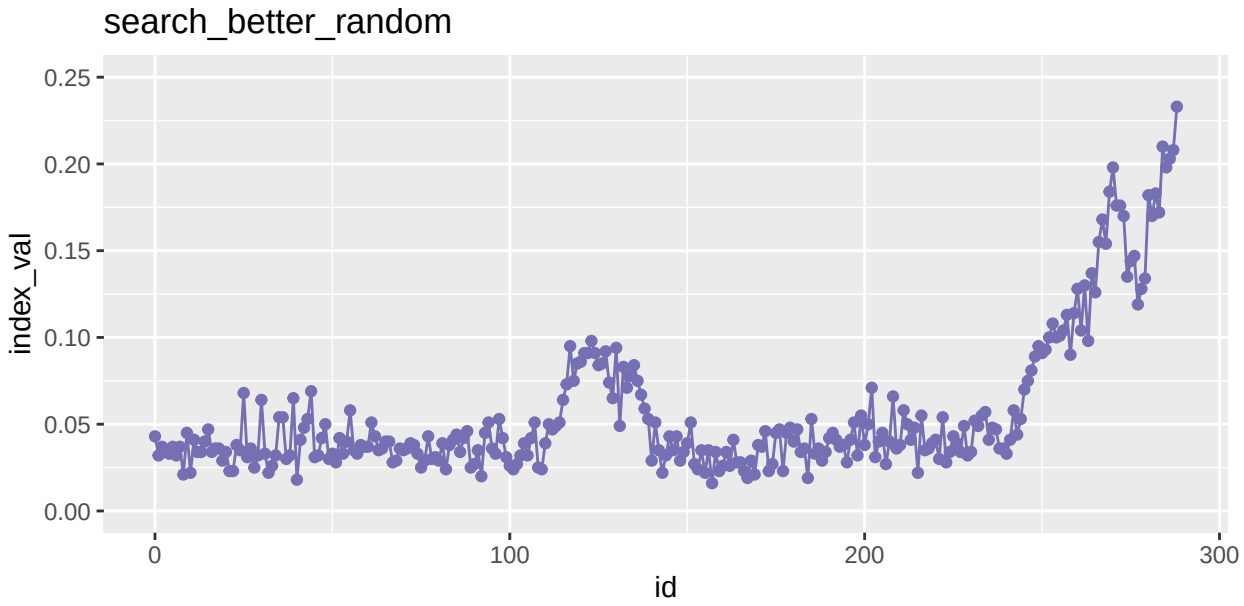


Figure 11: Using search better random for the problem above will result in finding the global maximum but much larger number of iteration is needed.

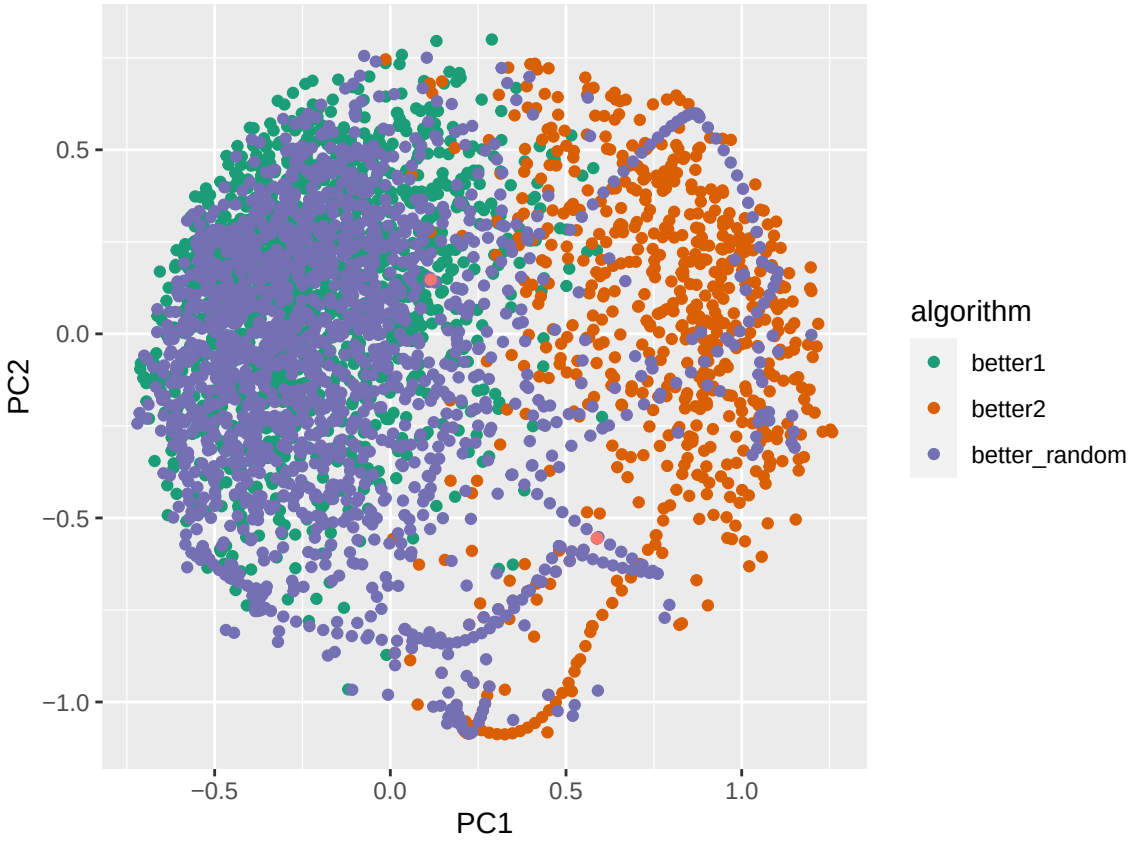


Figure 12: The projected projection basis using principal components. The bases from better1 and better2 only search a proportion of the searching space while better_random produces a more exhausive search. The large overlapping of better1 and better_random is explained by the fact that both algorithms finds x2 in the end.

7 Conclusion

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