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Abstract

1. check consistency of using PP for projection pursuit and PPI for projection pursuit index

Keywords: 3 to 6 keywords, that do not appear in the title

*The authors gratefully acknowledge ...

1 Introduction

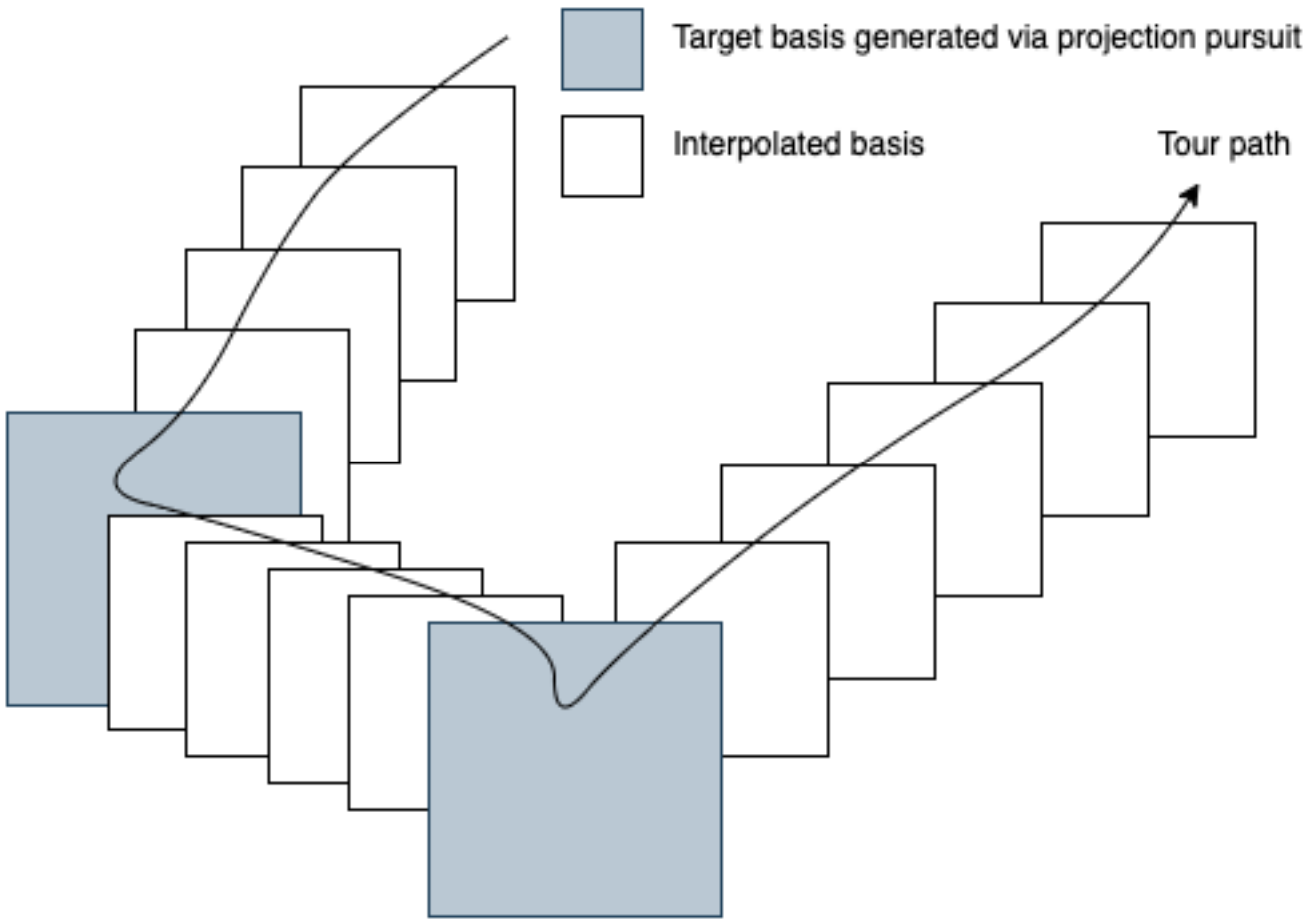
1.1 Tour

Tour provides a way to explore multivariate data interactively via an established tour path. A tour path is formed by interpolating between randomly generated plane. Different types of tours are available depends on the purpose of the exploration i.e. a grand tour is suitable for randomly exploring the data from different angles; a guided tour detects a particular structure in the data. a manual tour allows user to manually control the projection (**?**).

1.2 Guided tour

Guided tour is usually used in conjunction projection pursuit, a method coined by **?** to detect "interesting" low-diemsion projection of multivariate data. A projection pursuit requires the definition of a projection pursuit index function and an optimisation routine. The projection pursuit index measures the "interestingness" of data defined as its departure from normality. Numerous indices have been proposed in the literature, including lengendre index (**?**), hermite index (**?**), natural hermite index (**?**), chi-square index (**?**), LDA index (**?**) and PDA index (**?**). An optimisation routine is required to find the projection basis (thus projection) that maximises the projection pursuit index. The discussion of existing optimisation procedure will be discussed in the next section.

Guided tour creates visualisation for the projections found by projection pursuit by constructing a tour path. An illustration modified from (**?**) entails the geodesic interpolation bewteen the plane generated by projection pursuit.



1.3 Optimisation methods in projection pursuit literature

As **?** said "..., the technique use for maximizing the (one- and two-dimensional) projection index strongly influences both the statistical and the com- putational aspects of the procedure." The quality of the optimisation procedure largely affect the tour view and thus, the interesting projection one could possibly observe. An ideal optimisation procedure needs to have following characteristics:

- *Being able to handle non-differentiable index function*: the index function could be noisy and non-differentible
- *Being able to optimise with constraints*: the projection matrix is restricted to an orthornormal matrix.

- *Being able to reveal both local and global maximum*: Although the primary interest is to find the global maximum, distinct local structures are also of our interest.

Below present three existing methods in tour.

? presented a random search algorithm that samples new basis in the neighbourhood of the current basis. The neighbourhood is defined via the radius of the p-dimenionsal sphere, c. The new basis is taken as the target basis if it has higher index value, or the sampling continues. If no basis is found to have higher index value after a certain humber of tries n, the radius c is halved. The algorithm stops when the maximum numbere of iteration is attained or the radius c is less than a pre-determined number. [Pursuit package uses this method and it works greate! But I don't think we implement this - although don't think it is too hard to do it].

? explained the use of a gradient ascent optimisation with the assumption that the index function is continuous and differentiable. Since some indices could be non-differentiable, the computation of derivative is replaced by a psudo-derivative of evaluating five randomly generated directions in a tiny nearby neighbourhood. Taking a step on the straight derivative direction has been modified to maximise the projection pursuit index along the geodesic direction.

Simulated annealing (**?**, **?**) is a non-derivative procedure based on a non-increasing cooling scheme $T(i)$. Given an initial T_0, the temperature at iteration i is defined as $T(i) = \frac{T_0}{log(i+1)}$. The simulated annealing algorithm works as follows. Given a neighbourhood parameter α and a randomly generated orthonormal basis B, a candidate basis is constructed as $B_j = (1-\alpha)B_i + \alpha B$ where B_i is the current basis. If the index value of the candidate basis is larger than the one of the current basis, the candidate basis becomes the target basis. If it is smaller, the candidate is accepted with probability $A = \min\left(\exp(-\frac{I(B_j)-I(B_i)}{T(i)}), 1\right)$ where $I(.)$ is the index function.

1.4 problems and difficulties in PP optimisation

Below listed several issues in projection pursuit optimisation. Some are general optimisation problems, while others are more specific for PP optimisation.

- *Finding global maximum*: Although finding local maximum is relatively easy with developed algorithms, it is generally hard to guarantee global maximum in a problem where the objective function is complex or the number of decision variables is large. Also, there are discussions on how to avoid getting trapped in a local optimal in the literature.

- *optimising non-smooth function*: When the objective function is non-differentiable, derivative information can not be obtained, which means traditional gradient- or Hessian- based methods are not feasible. Stochastic optimisation method could be an alternative to solve these problems.

- *computation speed*: The optimisation procedure needs to be fast to compute since tours produces real-time animation of the projected data.

- *consistency result in stochastic optimisation*: In stochastic algorithm, researchers usually set a seed to ensure the algorithm producing the same result for every run. This practice supports reproducibility, while less efforts has been made to guarantee different seeds will provide the same result.

- *high-dimensional decision variable*: In projection pursuit, the decision variable includes all the entries in the projection matrix, which is high-dimensional. Researcher would be better off if they can understand the relative position of different projection matrix in the high-dimensional space.

- *role of interpolation in PP optimisation*: An optimisation procedure usually involves iteratively finding projection bases that maximises the index function, while tour requires geodesic interpolation between these bases to produce a continuous view for the users. It would be interesting to see if the interpolated bases could, in reverse, help the optimisation reach faster convergence.

Think about how does your pacakge help people to understand optimisation

- diagnostic on stochastic optim
- vis the progression of multi-parameter decision variable

- understanding learning rate - neightbourhood parameter
- understand where the local & global maximum is found - trace plot - see if noisy function

2 Iterative algorithm and its diagnostics

2.1 Tour components

Guided tour, along with other types of tour, 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/` (**?**). A tour includes two major components: a *generator* that generating the projection basis according to projection pursuit and an *interpolator* that performing geodesic interpolation between the projection basis.

The psudo-code below illustrates the implementation of guided tour in the tourr package. Given an projection pursuit index function and a randomly generated projection basis (current basis), the optimisation procedure produces a target basis inside `generator()` Both the current basis and the target basis will be supplied to `tour_path()` to prepare information needed for constructing a geodesic path. This information is then used to compute a series of interpolating bases inside the `tour()` function. All the basis will be sent to create animation for visualising the tour in the `animate()` function.

```
animation <- function(){

  # compute projection basis
  tour <- function(){

    # construct bases on the tour path
    new_geodesic_path <- function(){
      tour_path <- function(){

        # GENERATOR: generate projection basis via projection pursuit
```

```
        guided_tour <- function(){
          generator <- function(){

            # define projection pursuit index
            # generate the target basis from the current basis via optimisation
          }
        }

        # prepare geodesic information needed for interpolating along the tour path
      }
    }

    # INTERPOLATOR: interpolate between the current and target basis
    function(){
      # generate interpolating bases on the geodesic path
    }
  }

  # animate according to different display methods
}
```

2.2 Diagnostics

Visualisatioin has been widely used for exploring and understanding data. Visualisation presents information in a graphicial manner and often allows people to see information they would otherwise not seen in the reporting of numerical summarisation. Visual diagnostics can be real-time or post-run. Real time diagnostic directly uses the data produced in the algorithm to produce visual representation and thus doesn't need to store the data. This section focuses on the definition and production of post-run diagnoistics and the next section discusses real-time diagnostics.

Post-run diagnostics requires the data produced during the algorithm to be stored/

saved in order to produce plot diagnostics.

The graphical system in R is established based on the conception gramma of graphic (**?**), where a graphic is defined using stacked layers in a coordination system. A layer includes 1) the dataset that powers the plot; 2) a geometric object that represents the visual shape of the plot and 3) relevant statistical transformation if needed. An important concept in the gramma of graphic is *aesthetic mapping*. Aesthetic mapping links the variable in a dataset to information needed to produce a geometric object. For example, we map one variable on the x-axis and another on the y-axis to create a scatterplot. To create a boxplot, we first map one variable on the x-axis and then map the five point summary of another variable on the y-axis. This computation of five point summary from the origin variable is statistical transformation. This definition of graphic through layers provides advantages to produce complex plots since all the plots, however complex, can be decomposed into basic geometric objects shaped by the variable supplied.

This idea of decompositing a graph to basic elements inspires me to characterise the diagnostics of iterative algorithm in a similar fashion. The optimisation in many machine learning algorithms these days is iterative in nature, while remains as a black box. Being able to diagnose it visually allows researchers to have the tool to unfold the myth and thus provides more understand to the algorithm.

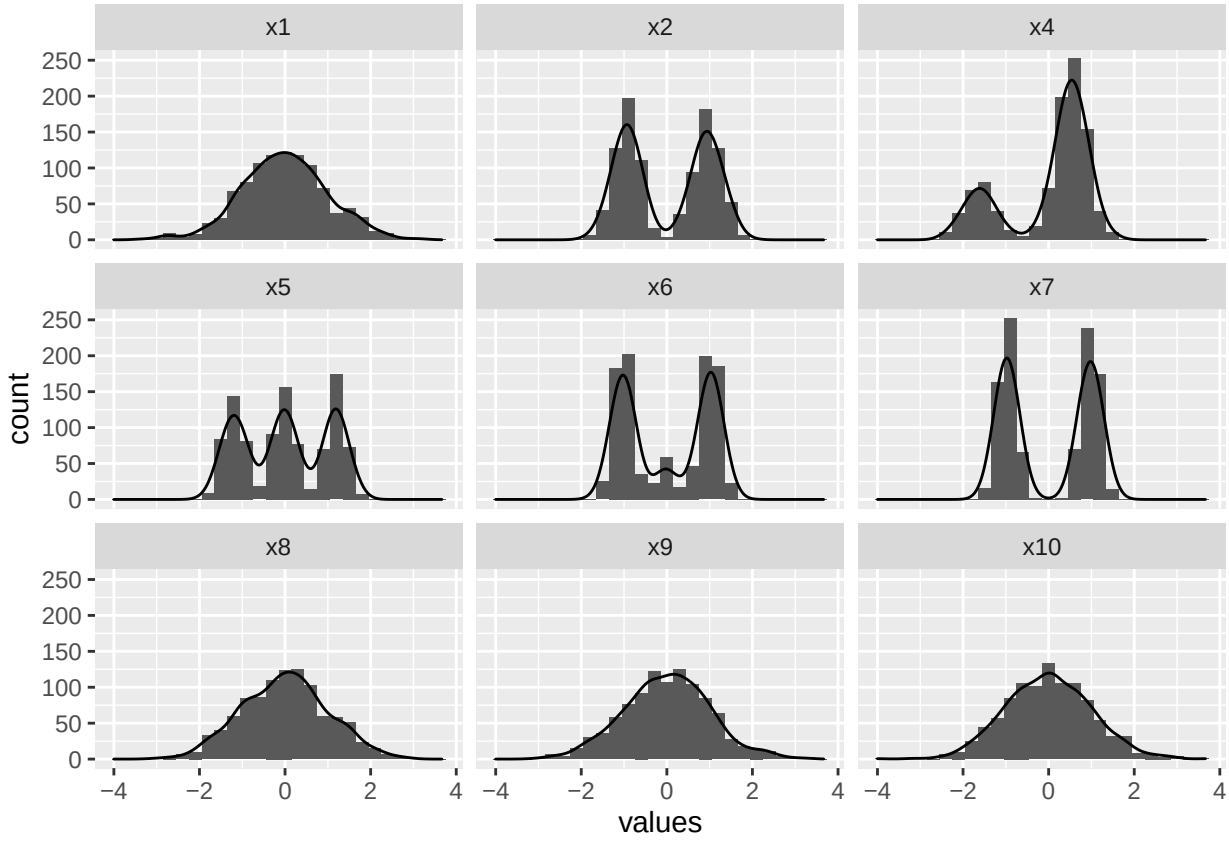
The concept of gramma of graphic requires a dataset to be supplied in making a plot, thus a global object needs to be created in the iterative algorithm. The variables will be mapped into element of a graphic to explore and thus should contain all the parameters of interest. The next section shows how a global object is created in projection pursuit guided tour.

2.3 Data Structure

In the current implementation of the `tourr` package, while the target basis generated by the projection pursuit can be accessed later via `save_history()`, interpolating bases and those randonly nearby bases generated in the optimisation are not stored. This creates difficulties for fully understand the behaviour of the optimisation and interpolation of tour in complex scenario [**needa rephrase this part**].

Two set of simulated data are used in the demonstration of the visualiation and diagnostics of the tour optimisation. A small dataset consists of 1000 randomly simulated observations of five variables (`x1`, `x2`, `x8`, `x9`, `x10`). `x2` is the informative variable simulated from two bi-modal normal distribution centered at -3 and 3 with variance being 1 and the other four are simulated from `N(0, 1)`. The data has been scaled to ensure `x2` has variance of 1.

A larger dataset contains more informative variables (`x3` to `x7`) of different types. `x3` takes 500 positive one and 500 negative one. The distribution of all the variables except `x3` is plotted below. *[should I introduce the dist for each var?]*



Once the dataset is sent to the tourr package, all the information generated will be stored in a global structure. The global structure consists of six columnes: `basis`, `index_val`, `tries`, `info`, `loop`, `id` and captured all the basis generated during whole tour process. The example below presents the global object of a 1D projection of the small dataset with geodesic seraching method.

```
holes_1d_geo %>% head(5)
```

```
## # A tibble: 5 x 8
##   basis           index_val tries info            loop method        alpha    id
##   <list>              <dbl> <dbl> <chr>          <dbl> <chr>         <dbl> <int>
## 1 <dbl[,1] [5 x ~     0.749     1 start             NA <NA>            0.5     1
## 2 <dbl[,1] [5 x ~     0.749     1 direction_sea~     1 search_geode~  NA       2
## 3 <dbl[,1] [5 x ~     0.749     1 direction_sea~     1 search_geode~  NA       3
## 4 <dbl[,1] [5 x ~     0.749     1 direction_sea~     1 search_geode~  NA       4
## 5 <dbl[,1] [5 x ~     0.749     1 direction_sea~     1 search_geode~  NA       5
```

`tries` has an increment of one once the generator is called (equivalently a new target basis is generated); `info` records the stage the basis is in. This would include the `interpolation` stage and the detailed stage in the optimisation i.e. `direction_search`, `best_direction_search`, `line_search`and `best_line_search` for geodesic searching (`search_geodesic`); `random_search` and `new_basis` for simulating annealing (`search_better`). `loop` is the counter used for the optimisation procedure and thus will be `NA` for interpolation steps. `id` creates a sequential order of the basis. This information will be stored and printed when the optimisation ends and can be turned off via `print = FALSE`. Additional messages during the optimisation can be displayed via `verbose = TRUE`. Another examples is a 2D projection of the larger dataset with two informative variable (`x2` and `x7`) using search_better method. Notice in this example, the dimension of the bases becomes 6 by 2.

```
holes_2d_better %>% head(5)
```

```
## # A tibble: 5 x 8
##   basis             index_val tries info           loop method        alpha    id
##   <list>                <dbl> <dbl> <chr>         <dbl> <chr>         <dbl> <int>
## 1 <dbl[,2] [6 x 2]>     0.804     1 start            NA <NA>            0.5     1
## 2 <dbl[,2] [6 x 2]>     0.793     1 random_search     1 search_bett~   0.5     2
## 3 <dbl[,2] [6 x 2]>     0.784     1 random_search     2 search_bett~   0.5     3
## 4 <dbl[,2] [6 x 2]>     0.773     1 random_search     3 search_bett~   0.5     4
## 5 <dbl[,2] [6 x 2]>     0.795     1 random_search     4 search_bett~   0.5     5
```

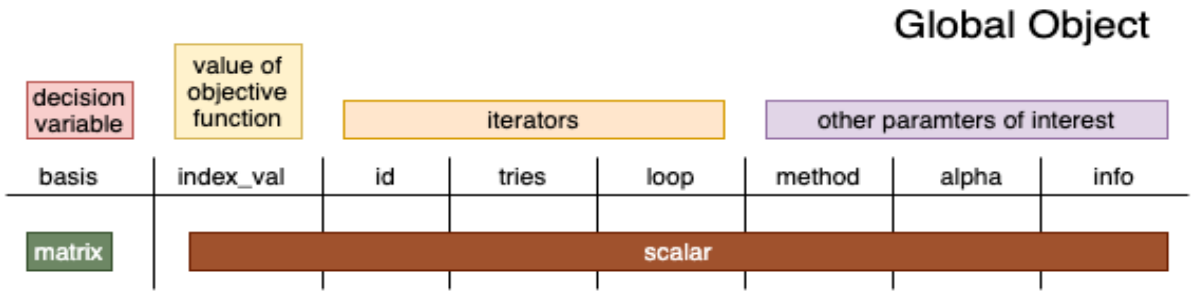


Figure 1: this is xxxx

3 Post-run static diagnostics plots

Given all the information of interest in a global object, the next thing is to design its visual representation that can diagnose our algorithm. In an iterative algorithm, one would be interested to know how one parameter changes as the algorithm iterates. The parameter could be could be the decision variable, the value of the optimisation function or other parameter that facilitate the algorithm. In projectio pursuit guided tour, apart from the decision variable projection basis, the value of index function (`index_val`), we are also interested to explore the effect the different searching methods, the neighbourhood parameter alpha, and the stage a particular observation is in (`info`). These are the variables that will be mapped into the diagnostic plot. The global object also has its time series nature since the observations are recorded as the algorithm progresses and thus can't be switch in rows. This time series structure is always hierachical and nested since each row can be labelled with the smallest unit `id` and up by the iterative structure of the algorithm. Take our example, in the global object, each row has an `id` label which is the smallest unit the observation is ordered. A larger ordering unit is `tries` since it is updated everytime a new target basis is found. A nested ordering unit is `loop`, which increases by one as searching method iterates and starts over at a new `tries`. These features explain the definition of the global object for projection pursuit guided tour in Figure **??**.

3.1 Explore scalar parameters

The most interesting parameter to explore is the value of objective function. The points recorded in the global object can be divided into two broad categories: searching points and interpolating points

- *Searching points* include the observations that are recorded in the searching algorithm in order to find the target basis. The points for target bases is also included in the searching points and there is one such point per `tries`.
- *interpolating points* exist in the guided tour to produce continuous animated view from one target basis to another and it doesn't have `loop` value.

3.1.1 Explore searching points

As mentioned previously, the largest difficulties of exploring searching points is its unknown number of observations per `tries`. Mapping `id` on the x-axis will leave the `tries` with few observations a small space in the plot, while those `tries` with large number of search points towards the end occupying the vast majority of the space in the plot.

This motivates the use of summarised statistics. At each iteration, rather than knowing the index value of *every* points, we are more interested to know a general summary of all the points and more importantly, the point with the largest `index_val` since it prescribes the geodesic interpolation and future searches.

Boxplot is a suitable candidate that provides five points summary of the data, while it has one drawback: it doesn't report the number of point in each box. We may risk losing information on how long it takes for the search to find the target basis by displaying the boxplot alone for all `tries`. Thus, the number of point for each `tries` is displayed at the bottom of each box and we provide options to switch `tries` with small number of points to a point geometry. This is achieved via the `cutoff` argument. A line geometry is also added to link the points with the largest index value for each `tries`. This helps to visualise the improvement made by each `tries`.

Example: exploring searching points The data is sourced from a 2D projection of the larger dataset and `search_better` is used with `max.tries = 500`. In Figure ?? and ??, a

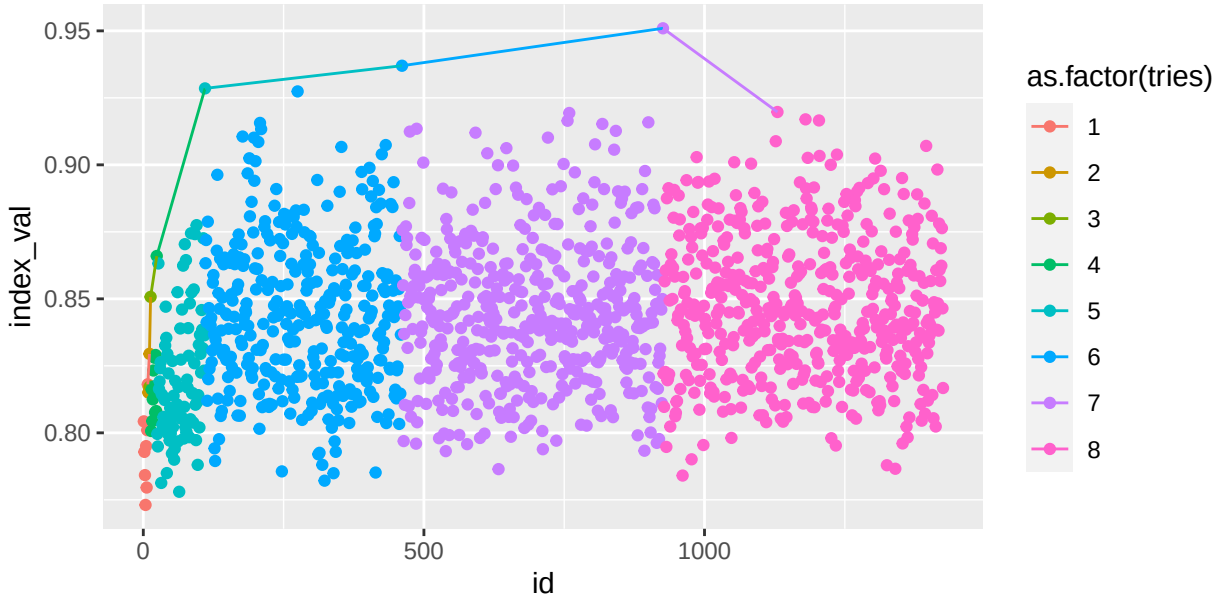


Figure 2: this is a xxx

comparison has been made on visualising the searching points with `id` and `tries` on the x-axis, colored by `tries`. In Figure **??**, the searching points of the first few `tries` are squeezed in a small width leaving the large uninteresting searching points in the last three `tries` taking a vast majority of the plotting space. While in Figure **??** the data is spaced by `tries` evenly in the plot. Label at the bottom indicates the number of observations in each tries and facilitates the choice of cutoff to switch from point geometry to boxplot geometry (`cutoff = 15`). The line geometry suggest the largest improvement happens at `tries = 5`.

3.1.2 Explore interpolating points

Plotting the interpolating points as time series data allows us to diagnose characterstics of different configurations and index functions. Here we present two examples of using plots to diagnose the tour algorithm and different index functions.

Example: Interruption This examples uses `search_better` for a 2D projection on the larger dataset using the `holes` index. As mentioned previously, the interpolation starts from the current basis to the target basis, which has been found by the projection pursuit algorithm to ahve a higher index value. After the interpolation, the target basis will become

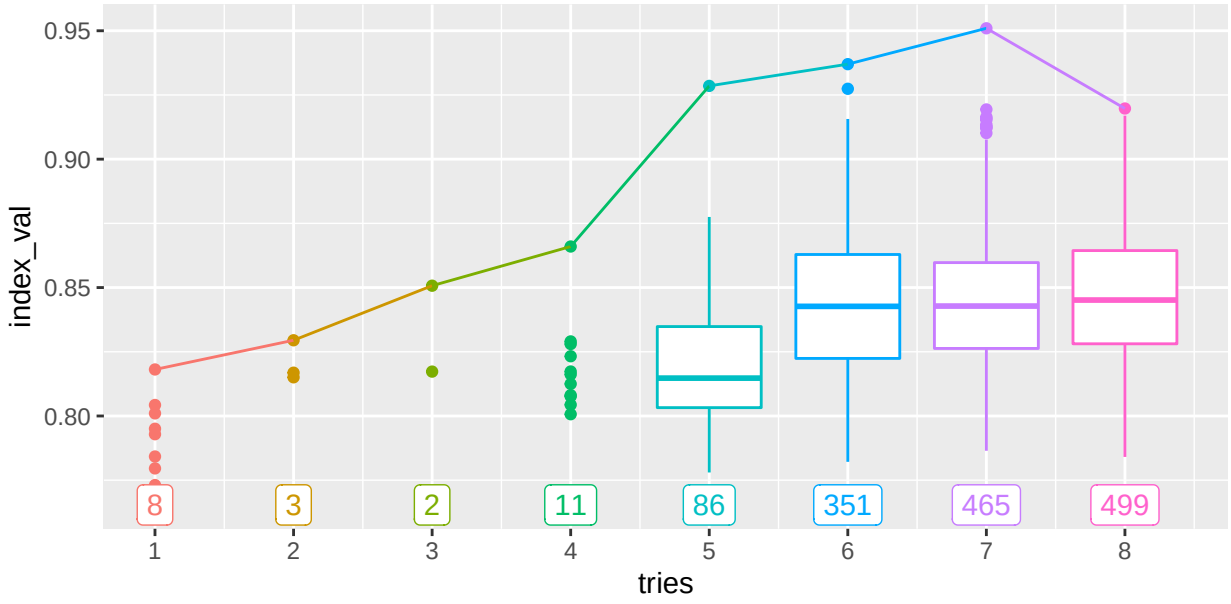


Figure 3: A comparison of plotting the same search points with different plot designs. The left plot doesn't efficiently use the plot space to convey information from the plot while the right plot provides good summarisation of data and number of points in each tries.

the current basis and send back to the projection pursuit algorithm to find the next target basis. From figure **??**, it is possible that there are bases with index value higher than the target basis on the interpolation path and these bases could be used to search for new basis in the next iteration.

Thus an interruption is constructed to accpet the interpolating bases up to the one with the larget index value on the interpolation path, and that basis is taken as the current basis for the next iteration. After implementing this interruption, the tracing plot with the same configuration is shown on the lower panel. We can observe that rather than interpolating to the target basis at `id = 62`, the interpolation stops before the index value starts to decrease at `id = 60`. This implementation results in a higher index value in the end with fewer steps.

Example: Noisy index function Add an example on noisy function

xxx

Currently, I have three things to put for the noisy index function.

1) interpolating plot finds that search_geodesic is not doing a good job on optimising

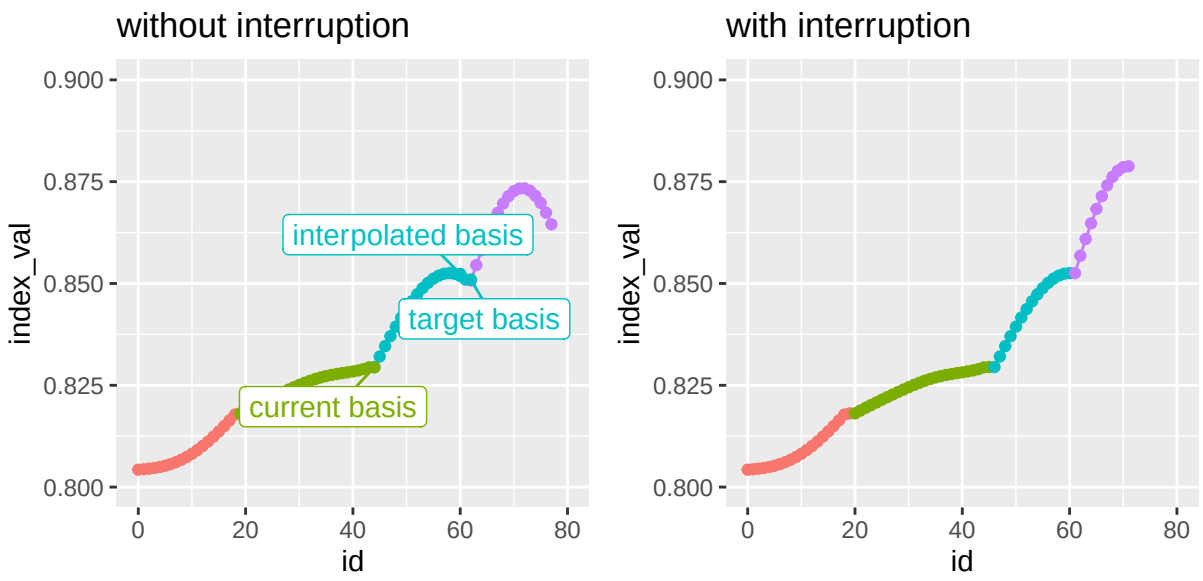


Figure 4: Trace plots of the interpolated basis with and without the interruption. The interruption stops the interpolation when the index value starts to decrease at id = 60. The implementation of the interuption finds an ending basis with higher index value using fewer steps.

the noisy index; while search_better is.

2) The interpolating plot for noisy index function is not smooth but the target basis is always increasing.

3) search_better_random sees to find both local and global maximum.

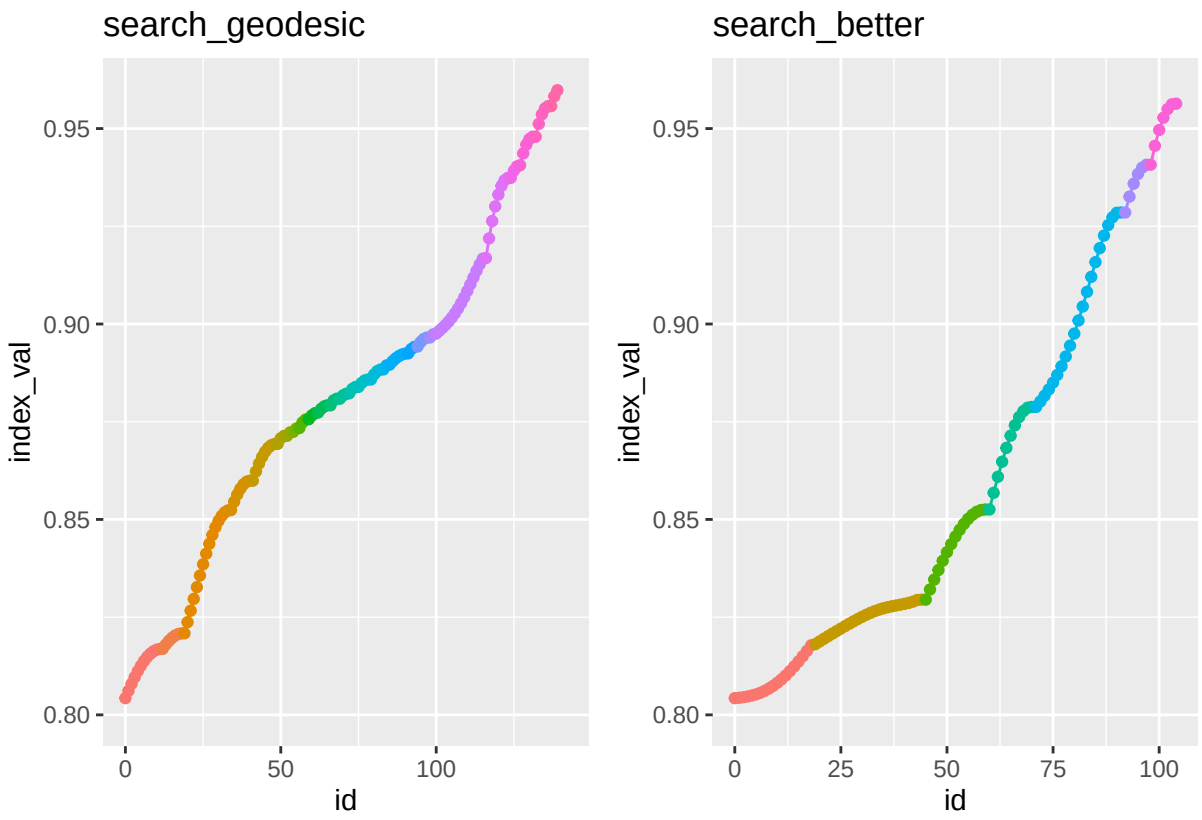
Need to decise where to put this example. Do we wan to intoduce noisy function at this stage or we put it here because they are insights draw from the interpolating plots.

xxx

3.1.3 Adding more variables to the mapping

At previous two sections, only the iterator and the index value are mapped onto the x and y aesthetics of the plot; while more aesthetics i.e. color, could be added to compare other parameters in the global object. Two examples are shown below to explore and compare different searching methods and neighbourhood parameter alpha.

Example: Polish In principle, all the optimisation routines should result in the same output on the same problem. Figure **??** shows the interpolating plots for two different searching methods: search_geodesic and serach_better on a 2D projection problem for the larger dataset using the holes index. The two methods reaches different ending value in the red dots, which is not ideal. This motivates the creation of a polishing search that polishes the ending basis and achieves unity on different methods.



`search_polish` takes the ending basis of a given search as the current basis and uses a brutal-force approach to sample a larg number of basis (`n_sample`) in the neightbourhood, whose radius is controlled by `polish_alpha`. Among the `n_sample` basis, the one with the largest index value becomes the candidate. If its index value of the candidate basis 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 than the current basis, the searching neighbourhood will be shrunk and the search continues. The polishing search ends when one of the four stopping criteria is satisfied:

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

The usage of search_polish is as follows. After the first tour, the final basis from the interpolation is extracted and supplied into a new tour with the `start` argument and

`search_polish` as the searching function in the guided_tour. 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)
```

The following example conducted a 2D projection on the larger dataset using search better with different configurations. `max.tries` is a hyperparameter that controls the maximum number of try without improvement and its default value is 25. As shown in Figure **??**, after polishing, both trials attain the same index value. However, a small `max.tries` of 25 is not sufficient for the algorithm to find the true maximum. This is because 25 tries is not sufficient for the 2D searching space.

```
# nrow(holes_2d_better_max_tries)
# nrow(holes_2d_pos)
```

3.2 Explore matrix parameter

Matrix parameter could also be interested to explore, for example, in the tour, we are interested to explore the relative position of the projection basis in the vector space. A

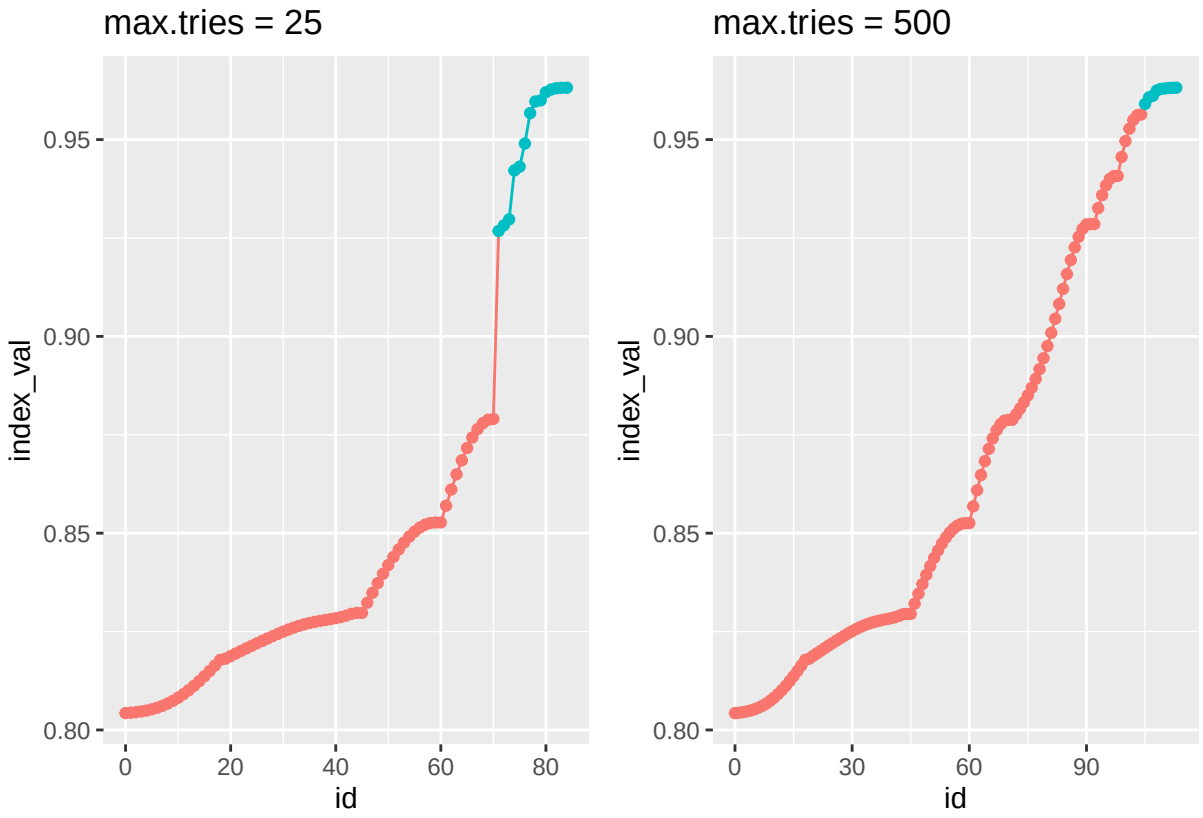


Figure 5: Breakdown of index value when using different max.tries in search better in conjunction with search polish. Both attain the same final index value after the polishing while using a max.tries 25 is not sufficient to find the ture maximum.

projection basis is a vector/matrix whose row number is the number of variable in the given dataset. This imposes difficulties in visualisation since we are bounded to preceive at most three dimensions. Thus, principal component analysis is used to reduce the dimension of the projection basi and the first two principal component are mapped to the x and y axis of the plot. Another variable of interest could be mapped to the color aesthetics to see how it changes as the projection basis changes in the projected 2D space. [have a second read here]

Example: understand search_geodesic via mapping ***info*** *to color* `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 works. 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 basis are then interpolated. In the next iteration, the target basis becomes the current basis and then procedures continues. [should probably reword this part with info levels xxx]

Example: understand the polishing alpha via mapping alpha to color `search_polish` is a brutal-force algorithm that evaluate 1000 points in the neighbourhod at each loop and an appropriate inital value in neighbourhood parameter alpha would avoid search on large vector space and concentrate on the ending basis. In Figure, two different initial alpha value is used in the polishing step. [some more illustration of the comparison of the two polish alpha here]

4 Real-time animated diagnostic plots

```
holes_1d_geo %>% explore_proj_pca(animate = TRUE, col = info)
```

5 Vis package

Everything is coded up in a package.

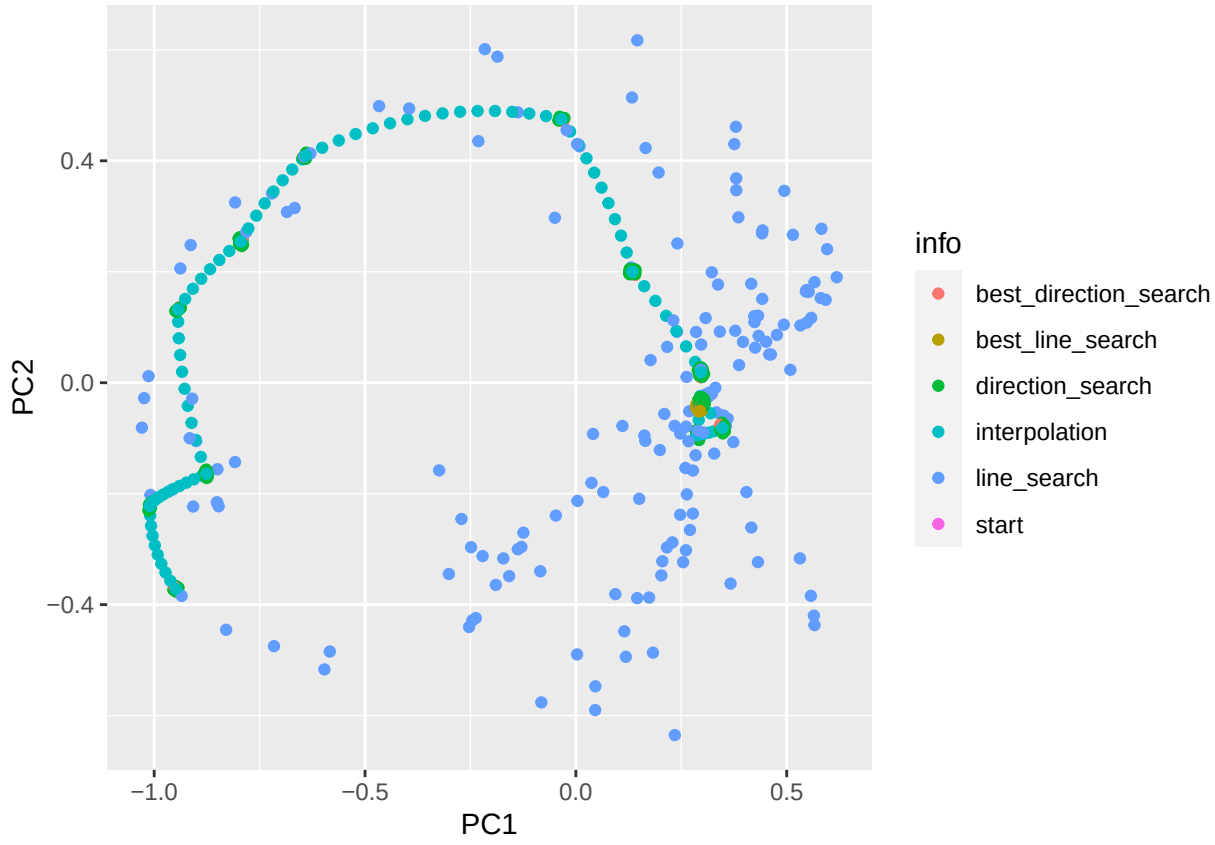


Figure 6: this is xxx