

Reproducible examples with VNDesign

VNDesign authors

1 Overview

VNDesign implements the Virtual Noise algorithm for computing D-optimal experimental designs under correlated observations. This vignette introduces the basic workflow and points to the reproducible examples included with the package.

The main steps are:

1. Define a candidate set `chi`.
2. Build the regressor or gradient matrix `Xchi`.
3. Build the covariance matrix `Sigma_chi`.
4. Run the Virtual Noise algorithm.
5. Optionally convert the approximate design measure into an exact design.

2 A minimal one-dimensional example

The following example uses a linear model with candidate points in $[-1, 1]$.

```
library(VNDesign)

chi <- seq(-1, 1, length.out = 15)
theta <- c(0, 1)
kappa <- 0.99 / length(chi)

grad_fun <- function(x, theta) {
  c(1, x)
}

res <- vndesign_Dopt(
  chi = chi,
  theta = theta,
  grad_fun = grad_fun,
  kappa = kappa,
  max_iter = 10,
  verbose = FALSE,
  cov_type = "exp",
  range = 0.4,
  vn_alt = 3,
  vn_lambda = 2,
  return_components = TRUE
)

head(res$xi)

#> [1] 0.1 0.0 0.1 0.0 0.1 0.0
```

For the classical VN algorithm implemented in `VNDesign`, `kappa` is used as a virtual-noise threshold and is typically chosen slightly below the initial uniform design weight. In the reproducible examples we use `kappa = 0.99/N`, where `N` is the number of candidate points.

An exact design can be constructed from the approximate design measure:

```
exact <- exact_design(
  res = res,
  Xchi = res$Xchi,
  Sigma_chi = res$Sigma_chi,
  chi = chi,
  n = 3,
  method = "quantile"
)

exact$points

#> [1] -0.4285714  0.1428571  0.7142857
```

3 Full reproducible examples

The package includes three full scripts in `inst/examples/`. These scripts are intended to show complete workflows for the examples discussed in the accompanying article and for a self-contained two-dimensional case.

- `example_pazman2003_ex1.R`: one-dimensional linear model with compactly supported covariance from Pázman et al. 2003.
- `example_pazman2022_ex1.R`: a classical one-parameter one-dimensional model from Pázman et al. 2022.
- `example_2D.R`: self-contained two-dimensional example on a regular grid.

The script `example_2D.R` is intentionally a toy example. It uses a regular grid and a simple planar trend only to illustrate how `VNDesign` handles a two-dimensional candidate set without requiring external spatial data. For real spatial applications, users should prepare their own candidate coordinates outside `VNDesign`; for example, a shapefile can be read, projected, and converted into an $N \times 2$ matrix or data frame of coordinates using specialised spatial packages such as `sf`. The resulting coordinate object can then be supplied directly as the argument `chi`.

After installing the package, their location can be found with:

```
system.file("examples", package = "VNDesign")
```

Run an individual example with:

```
source(system.file("examples", "example_pazman2003_ex1.R", package = "VNDesign"))
source(system.file("examples", "example_pazman2022_ex1.R", package = "VNDesign"))
source(system.file("examples", "example_2D.R", package = "VNDesign"))
```

When working from the source directory, the same scripts can be run with:

```
source("inst/examples/example_pazman2003_ex1.R")
source("inst/examples/example_pazman2022_ex1.R")
source("inst/examples/example_2D.R")
```

4 Quick Checks

For a quick check of the example scripts, set:

```
Sys.setenv(VNDESIGN_EXAMPLE_MAX_ITER = "40")  
Sys.setenv(VNDESIGN_EXAMPLE_PLOTS = "false")
```

Then source the desired script.