Simple workflow example for a population model

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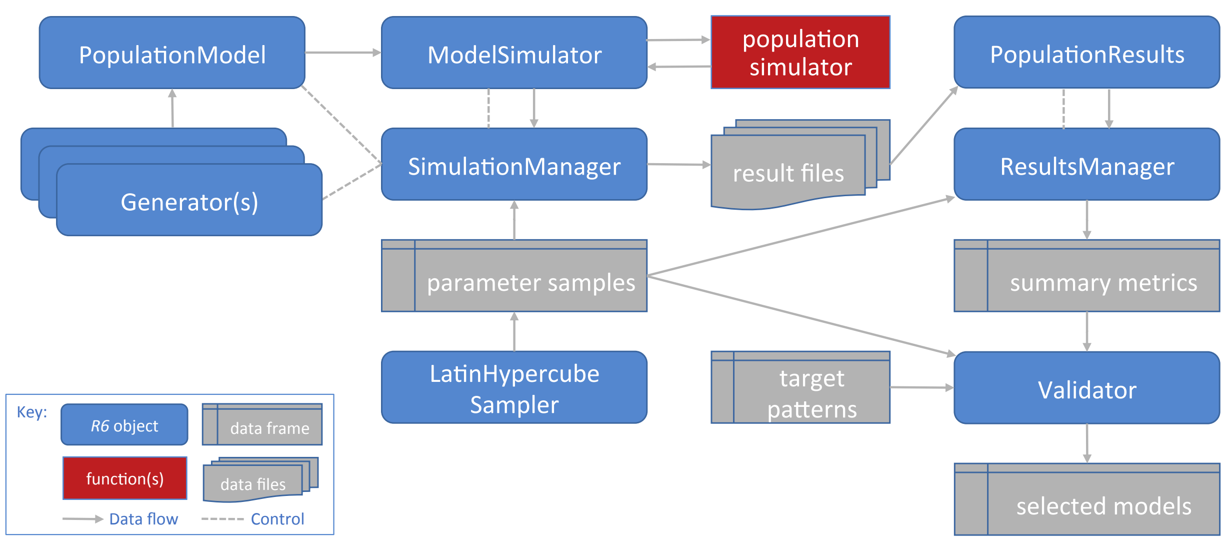
In this vignette we present a simple example of the *poems* workflow using a fictitious population model. The purpose of this example is to demonstrate how the components of the package are used to build an ensemble of viable models that best match known or desired patterns. Although the package is designed to facilitate building complex models and running multitudes of sample simulations, the scale and complexity of this demonstration model is deliberately minimal so as to easily examine the outputs at every stage of the workflow.

We begin by loading the *poems* package and setting our output directory.

```
library(poems)
OUTPUT_DIR <- tempdir()
```

Workflow

The *poems* workflow, which implements a pattern-oriented modeling (POM) approach (Grimm et al., 2005), is achieved via a framework of interoperable components:



The workflow is summarized by the following six steps:

1. Build the population model for the study region.
2. Build generators for dynamically generating model parameters.
3. Sample model and generator parameters for each simulation.
4. Build a simulation manager to run each simulation.
5. Build a results manager to generate summary results (metrics).
6. Build a validator to select a model ensemble.

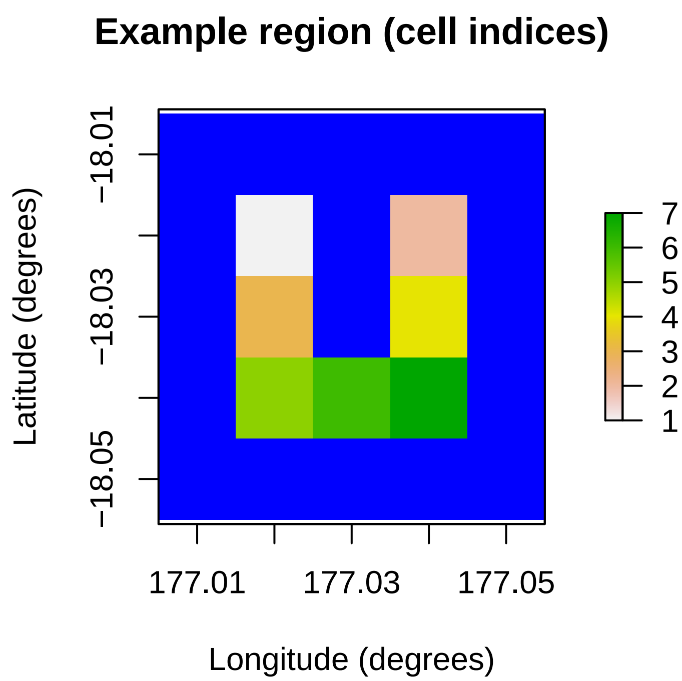
Step 1: Build the population model for the study region

Create a model template using the *PopulationModel* class. If the model is spatially explicit, then define the study region via the *Region* class. All fixed model inputs, such as environmental correlations, as well as any user-defined functions for processes such as harvesting, should be set at this stage.

We could create these components in any order and set model parameters separately, but let's setup our study region, generate environmental correlations, and define a harvest function prior to initializing the template model with all the fixed parameters.

Study region First, we'll define our study region (denoted U Island) with some longitude-latitude coordinates.

```
# Demonstration example region (U Island)
coordinates <- data.frame(x = rep(seq(177.01, 177.05, 0.01), 5),
                          y = rep(seq(-18.01, -18.05, -0.01), each = 5))
template_raster <- Region$new(coordinates = coordinates)$region_raster # full extent
template_raster[][-c(7, 9, 12, 14, 17:19)] <- NA # make U Island
region <- Region$new(template_raster = template_raster)
raster::plot(region$region_raster, main = "Example region (cell indices)",
             xlab = "Longitude (degrees)", ylab = "Latitude (degrees)",
             colNA = "blue")
```



Enviromental correlation Next, we'll define a distance-based spatial correlation for applying environmental stochasticity within our model. The generated correlation data is compacted for computational efficiency (with large-scale models).

```
# Distance-based environmental correlation (via a compacted Cholesky decomposition)
env_corr <- SpatialCorrelation$new(region = region, amplitude = 0.4, breadth = 500)
correlation <- env_corr$get_compact_decomposition(decimals = 2)
correlation # examine
```

```
#> $matrix
#>      [,1] [,2] [,3] [,4] [,5] [,6] [,7]
#> [1,]    1 0.01 0.04 0.04 0.04 0.02 0.04
#> [2,]    0 1.00 1.00 0.01 1.00 0.02 0.01
#> [3,]    0 0.00 0.00 1.00 0.00 0.05 0.05
#> [4,]    0 0.00 0.00 0.00 0.00 1.00 1.00
#>
#> $map
#>      [,1] [,2] [,3] [,4] [,5] [,6] [,7]
#> [1,]    1    1    1    2    3    3    4
#> [2,]   NA    2    3    3    5    4    5
#> [3,]   NA   NA   NA    4   NA    5    6
#> [4,]   NA   NA   NA   NA   NA    6    7
```

Harvest function Let's now define a simple harvest function, which is optionally list-nested with a harvest rate parameter. We'll also define an alias to the harvest rate so we can sample this parameter later.

```
# User-defined harvest function (list-nested) and alias
harvest <- list(rate = NA, # sample later
                function(params) round(params$stage_abundance*(1 - params$rate)))
harvest_rate_alias <- list(harvest_rate = "harvest$rate")
```

Template model Finally, we can build our template model with these and other fixed parameters.

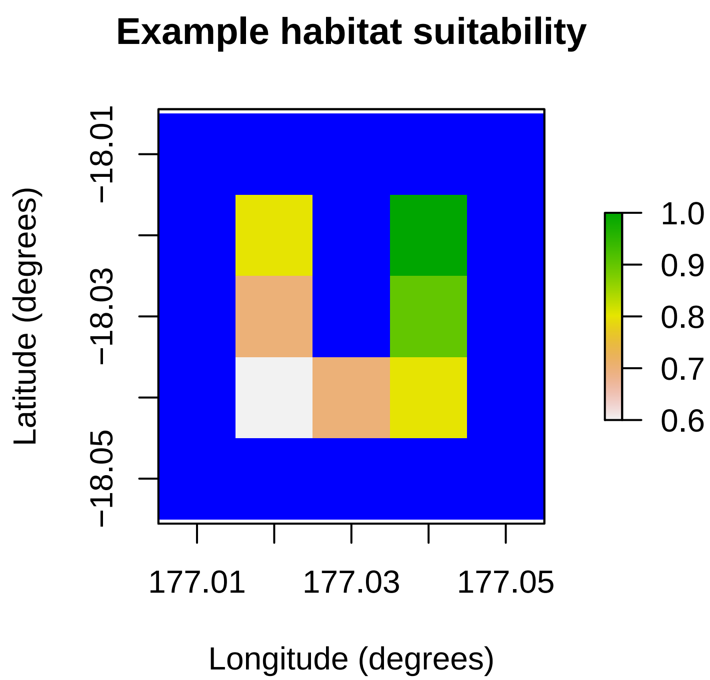
```
# Population (simulation) model template for fixed parameters
stage_matrix <- matrix(c(0,   2.5, # Leslie/Lefkovitch matrix
                         0.8, 0.5), nrow = 2, ncol = 2, byrow = TRUE,
                       dimnames = list(c("juv", "adult"), c("juv", "adult")))
stage_matrix # examine
#>       juv adult
#> juv   0.0   2.5
#> adult 0.8   0.5
model_template <- PopulationModel$new(region = region,
                                      time_steps = 10, # years
                                      populations = region$region_cells, # 7
                                      stages = 2,
                                      stage_matrix = stage_matrix,
                                      demographic_stochasticity = TRUE,
                                      standard_deviation = 0.05,
                                      correlation = correlation,
                                      density_dependence = "logistic",
                                      harvest = harvest,
                                      results_selection = c("abundance", "harvested"),
                                      attribute_aliases = harvest_rate_alias)
```

Step 2: Build generators for dynamically generating model parameters

Some model parameters are single values, whilst others are represented as arrays and other multi-value data structures. Usually, we don't wish to sample each individual value within these multi-value parameters (in step 3), but to generate them dynamically via one or more intermediate sampled parameters. Here we build generators for model initial abundance, carrying capacity, and dispersal.

Habitat suitability Firstly, our initial abundance and carrying capacity generator utilizes an example (mock) habitat suitability for our defined study region.

```
# Example habitat suitability
example_hs <- c(0.8, 1, 0.7, 0.9, 0.6, 0.7, 0.8 )
example_hs_raster <- region$region_raster
example_hs_raster[region$region_indices] <- example_hs
raster::plot(example_hs_raster, main = "Example habitat suitability",
             xlab = "Longitude (degrees)", ylab = "Latitude (degrees)",
             colNA = "blue")
```



Initial abundance and carrying capacity generator The generator utilizes generic templating functionality for user-defined custom functions. It uses sampled input parameters (initial total abundance and maximum cell density), along with habitat suitability, to generate the desired output model parameters (initial abundance and carrying capacity) via these user-defined functions. Generators can also be configured to read values from files or generate values via probabilistic distributions.

```
# Initial abundance and carrying capacity generated via example habitat suitability
capacity_gen <- Generator$new(description = "Capacity generator",
                              example_hs = example_hs, # template attached
                              inputs = c("initial_n", "density_max"),
                              outputs = c("initial_abundance", "carrying_capacity"))
capacity_gen$add_generative_requirements(list(initial_abundance = "function",
                                              carrying_capacity = "function"))
capacity_gen$add_function_template("initial_abundance",
                                   function_def = function(params) {
                                     stats::rmultinom(1, size = params$initial_n,
                                                      prob = params$example_hs)[,1]
                                   },
                                   call_params = c("initial_n", "example_hs"))
```

```r
capacity_gen$add_function_template("carrying_capacity",
                                   function_def = function(params) {
                                     round(params$density_max*params$example_hs)
                                   },
                                   call_params = c("density_max", "example_hs"))
capacity_gen$generate(input_values = list(initial_n = 500, density_max = 100)) # test
#> $initial_abundance
#> [1] 76 94 63 85 52 64 66
#>
#> $carrying_capacity
#> [1]  80 100  70  90  60  70  80
```

Dispersal generator Our dispersal generator uses default functionality for generating dispersal rates between cells. Its sampled inputs parameterize the distance-based dispersal function (proportion dispersing and breadth of dispersal). The generator can be configured with a dispersal friction helper class object, which calculates equivalent dispersal distances for frictional landscapes and coastlines. Here it is used to ensure dispersal is not performed directly across the "water" in our example U-shaped island. The generated dispersal data is calculated via pre-calculated distance data and compacted for computational efficiency (with large-scale models).

```r
# Distance-based dispersal generator
dispersal_gen <- DispersalGenerator$new(region = region,
                                        dispersal_max_distance = 3000, # in m
                                        dispersal_friction = DispersalFriction$new(),
                                        inputs = c("dispersal_p", "dispersal_b"),
                                        decimals = 5)
dispersal_gen$calculate_distance_data() # pre-calculate
dispersal_gen$generate(input_values = list(dispersal_p = 0.5,
                                           dispersal_b = 700))$dispersal_data # test
#> [[1]]
#>    target_pop source_pop emigrant_row immigrant_row dispersal_rate
#> 1           3          1            1             1        0.10284
#> 2           5          1            2             1        0.02115
#> 3           6          1            3             1        0.01501
#> 4           4          2            1             1        0.10284
#> 5           6          2            2             2        0.01501
#> 6           7          2            3             1        0.02115
#> 7           1          3            1             1        0.10284
#> 8           5          3            2             2        0.10284
#> 9           6          3            3             3        0.05596
#> 10          7          3            4             2        0.01643
#> 11          2          4            1             1        0.10284
#> 12          5          4            2             3        0.01643
#> 13          6          4            3             4        0.05596
#> 14          7          4            4             3        0.10284
#> 15          1          5            1             2        0.02115
#> 16          3          5            2             2        0.10284
#> 17          4          5            3             2        0.01643
#> 18          6          5            4             5        0.11014
#> 19          7          5            5             4        0.02426
#> 20          1          6            1             3        0.01501
#> 21          2          6            2             2        0.01501
#> 22          3          6            3             3        0.05596
#> 23          4          6            4             3        0.05596
#> 24          5          6            5             4        0.11014
#> 25          7          6            6             5        0.11014
```

```
#> 26          2          7           1           3          0.02115
#> 27          3          7           2           4          0.01643
#> 28          4          7           3           4          0.10284
#> 29          5          7           4           5          0.02426
#> 30          6          7           5           6          0.11014
```

Note that there is no dispersal rate between cells 1 and 2 as there is "water" between those cells, and consequently dispersal between those cells must travel around the U-shaped island, which can't be achieved in one simulation time-step since the "round" distance between those cells is greater than 3000 m.

Step 3: Sample model and generator parameters for each simulation

In order to explore the model parameter space to find the best models, we generate Latin hypercube samples of model and generator parameters to be simulated, using the *LatinHypercubeSampler* class. This class has functionality for generating sample parameters via Uniform, Normal, Lognormal, Beta, and Triangular distributions. For our example we only generate 12 samples. We encourage the user to generate hundreds, or thousands, of samples.

```
# Generate sampled values for variable model parameters via LHS
lhs_gen <- LatinHypercubeSampler$new()
lhs_gen$set_uniform_parameter("growth_rate_max", lower = 0.4, upper = 0.6, decimals = 2)
lhs_gen$set_uniform_parameter("harvest_rate", lower = 0.05, upper = 0.15, decimals = 2)
lhs_gen$set_uniform_parameter("initial_n", lower = 400, upper = 600, decimals = 0)
lhs_gen$set_uniform_parameter("density_max", lower = 80, upper = 120, decimals = 0)
lhs_gen$set_uniform_parameter("dispersal_p", lower = 0.2, upper = 0.5, decimals = 2)
lhs_gen$set_uniform_parameter("dispersal_b", lower = 400, upper = 1000, decimals = 0)
sample_data <- lhs_gen$generate_samples(number = 12, random_seed = 123)
sample_data # examine
#>    growth_rate_max harvest_rate initial_n density_max dispersal_p dispersal_b
#> 1             0.50         0.09       575         111        0.26         481
#> 2             0.41         0.07       487          96        0.34         589
#> 3             0.44         0.09       483         110        0.42         509
#> 4             0.59         0.11       589          86        0.38         859
#> 5             0.56         0.06       441          92        0.21         667
#> 6             0.51         0.14       458         116        0.50         980
#> 7             0.54         0.05       416          88        0.28         447
#> 8             0.43         0.13       542         107        0.36         920
#> 9             0.46         0.12       422         101        0.43         849
#> 10            0.52         0.08       552          99        0.32         745
#> 11            0.48         0.11       525         119        0.25         789
#> 12            0.58         0.15       505          81        0.45         609
```

Step 4: Build a simulation manager to run each simulation

We now wish to run a simulation for each set (or row) of sampled parameters. The *SimulationManager* class manages the generation of parameters (via the generators), the running the model simulations, and writing simulation results to disk. It also maintains a log of each simulation's success and any errors or warnings encountered.

```
# Create a simulation manager and run the sampled model simulations
sim_manager <- SimulationManager$new(sample_data = sample_data,
                                     model_template = model_template,
                                     generators = list(capacity_gen, dispersal_gen),
                                     parallel_cores = 2,
                                     results_dir = OUTPUT_DIR)
run_output <- sim_manager$run()
```

```r
run_output$summary
#> [1] "12 of 12 sample models ran and saved results successfully"
dir(OUTPUT_DIR, "*.RData") # includes 12 result files
#>  [1] "sample_1_results.RData"  "sample_10_results.RData"
#>  [3] "sample_11_results.RData" "sample_12_results.RData"
#>  [5] "sample_2_results.RData"  "sample_3_results.RData"
#>  [7] "sample_4_results.RData"  "sample_5_results.RData"
#>  [9] "sample_6_results.RData"  "sample_7_results.RData"
#> [11] "sample_8_results.RData"  "sample_9_results.RData"
dir(OUTPUT_DIR, "*.txt") # plus simulation log
#> [1] "simulation_log.txt"
```

Note that the output directory contains a R-data result files for each sample simulation and a simulation log file.

Step 5: Build a results manager to generate summary results (metrics)

We now wish to collate summary results for each of our simulations via the *ResultsManager* class. This manager loads the results from each sample simulation into an intermediate *PopulationResults* class object, which dynamically generates further results. We need to define functions for calculating summary metrics, as well as any matrices (one row of values per simulation) that we may be interested in examining. Each metric (or matrix) is associated with a user-defined function that utilizes results object attributes, or alternatively direct access to an attribure may be defined via a string. Once generated, the result metrics (a data frame) and/or matrices (a list) can be accessed via the manager. We may utilize the collated results in a variety of ways. However, with the objective of selecting the best models, we wish to compare (or validate) these result metrics to (with) known or desired target patterns (in step 6).

```r
results_manager <- ResultsManager$new(simulation_manager = sim_manager,
                                      simulation_results = PopulationResults$new(),
                                      summary_metrics = c("trend_n", "total_h"),
                                      summary_matrices = c("n", "h"),
                                      summary_functions = list(
                                        trend_n = function(results) {
                                          round(results$all$abundance_trend, 2)
                                        },
                                        total_h = function(results) {
                                          sum(results$harvested)
                                        },
                                        n = "all$abundance", # string
                                        h = "all$harvested"),
                                      parallel_cores = 2)
gen_output <- results_manager$generate()
gen_output$summary
#> [1] "12 of 12 summary metrics/matrices generated from sample results successfully"
dir(OUTPUT_DIR, "*.txt") # plus generation log
#> [1] "generation_log.txt" "simulation_log.txt"
results_manager$summary_metric_data
#>    index trend_n total_h
#> 1      1   -4.00     474
#> 2      2   -5.00     352
#> 3      3    3.00     475
#> 4      4  -10.60     475
#> 5      5    0.67     276
#> 6      6    4.33     751
#> 7      7   -0.67     220
#> 8      8   -5.88     620
```

```
#> 9      9    0.50     555
#> 10    10   -8.00     408
#> 11    11   -2.71     606
#> 12    12   -5.50     563
results_manager$summary_matrix_list
#> $n
#>       [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
#>  [1,]  502  478  494  481  481  478  477  446  450   501
#>  [2,]  480  468  491  487  487  448  465  462  438   442
#>  [3,]  491  466  445  452  477  540  500  512  490   460
#>  [4,]  447  419  419  389  372  365  357  366  375   337
#>  [5,]  463  430  437  465  436  486  417  469  436   449
#>  [6,]  454  446  453  448  447  483  480  476  510   463
#>  [7,]  414  395  419  414  438  427  403  436  382   401
#>  [8,]  498  442  436  398  384  390  402  401  403   395
#>  [9,]  412  399  389  405  403  424  407  420  396   403
#> [10,]  516  511  509  495  471  428  420  447  458   458
#> [11,]  537  496  487  492  452  483  475  490  477   484
#> [12,]  378  358  296  317  312  302  316  296  317   285
#>
#> $h
#>       [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
#>  [1,]   50   48   49   49   47   48   45   43   44    51
#>  [2,]   37   35   37   38   36   35   34   33   34    33
#>  [3,]   49   44   44   44   49   52   50   50   49    44
#>  [4,]   55   52   52   48   46   44   43   46   47    42
#>  [5,]   27   26   26   29   26   30   26   31   28    27
#>  [6,]   75   72   73   73   73   81   76   75   80    73
#>  [7,]   23   21   23   22   22   23   20   22   20    24
#>  [8,]   74   66   65   59   59   58   59   60   60    60
#>  [9,]   55   55   54   55   54   58   58   56   54    56
#> [10,]   43   43   43   43   42   39   36   40   40    39
#> [11,]   67   60   64   59   56   57   59   64   59    61
#> [12,]   66   64   52   57   56   55   55   51   58    49
```

Step 6: Build a validator to select a model ensemble

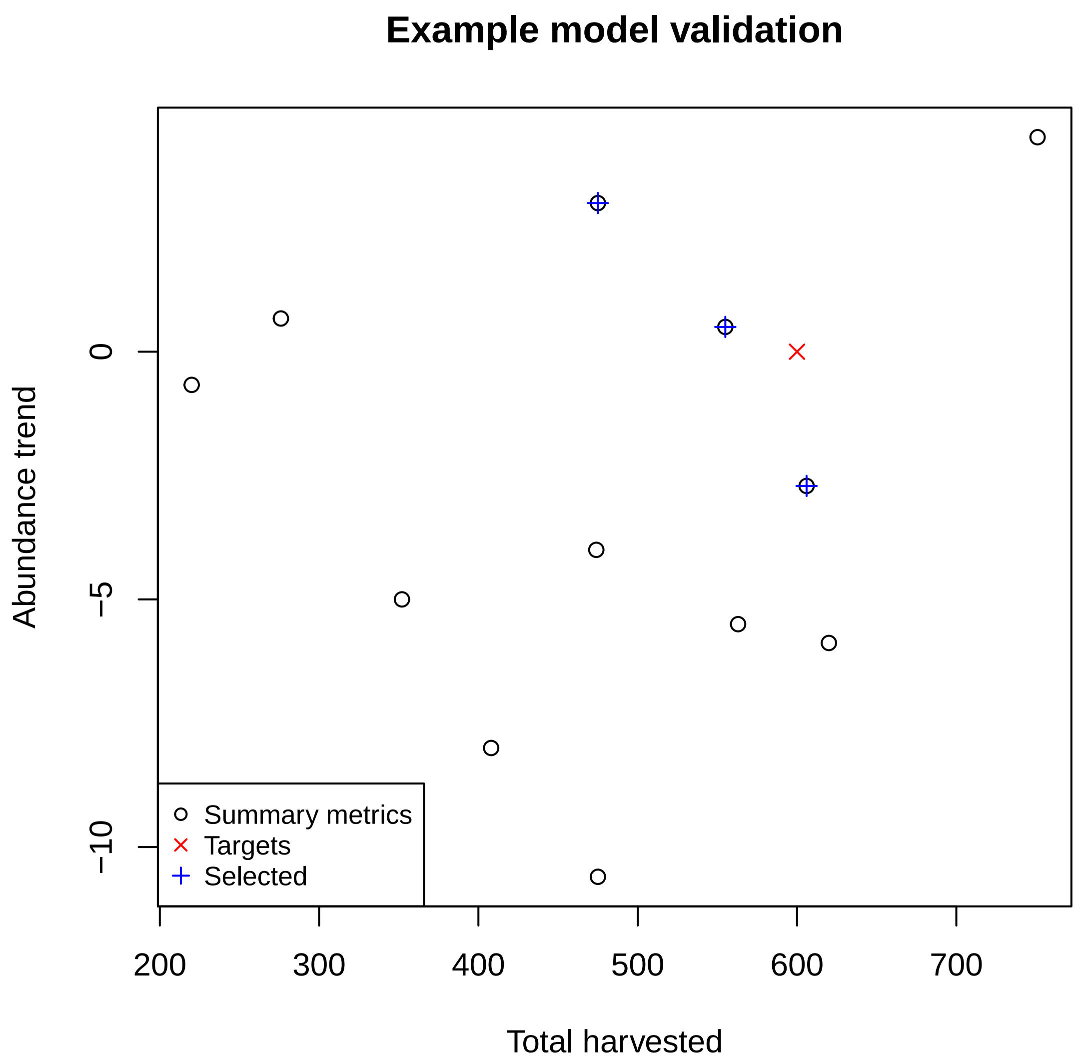
We now select and analyse our 'best' models via a *Validator* class object, which by default utilizes an approximate Bayesian computation (ABC) approach (Beaumont, Zhang, & Balding, 2002) provided by the *abc* library (Csillery et al., 2015). The validator can be configured appropriately for a problem domain (see the *abc* documentation). Here we use the default configuration to select the best 3 models, along with a weight value, which is indicative of the congruence between each model's summary metrics and the corresponding target patterns. Also provided (with the default settings) is a diagnostic output (PDF) file, containing statistical information for analysing the contribution of model parameters in the selection/validation process (see the *abc* documentation). For our simple demonstration the metrics and corresponding targets are relatively trivial, having the aim of producing stable population abundances with high harvest. However, the package facilitates the use more complex spatiotemporal metrics and targets (demonstrated in more advanced vignettes).

```
# Create a validator for selecting the 'best' example models
validator <- Validator$new(simulation_parameters = sample_data,
                           simulation_summary_metrics =
                             results_manager$summary_metric_data[-1],
                           observed_metric_targets = c(trend_n = 0, total_h = 600),
                           output_dir = OUTPUT_DIR)
suppressWarnings(validator$run(tolerance = 0.25, output_diagnostics = TRUE))
```

```
#> 12345678910
#> 12345678910
dir(OUTPUT_DIR, "*.pdf") # plus validation diagnostics (see abc library documentation)
#> [1] "validation_diagnostics.pdf"
validator$selected_simulations # top 3 models (stable abundance and high harvest)
#>   index    weight
#> 1     3 0.0000000
#> 2     9 0.9085658
#> 3    11 0.6926961
```

We encourage the user to examine the generated diagnostics (PDF) output file, and to become acquainted with the analysis that this information facilitates (see the *abc* documentation). As our simple example only uses two metrics/targets, we can visualize the congruence of the selected models with the targets via a simple plot.

```
# Plot the simulation, targets, and selected metrics
graphics::plot(x = results_manager$summary_metric_data$total_h,
               y = results_manager$summary_metric_data$trend_n,
               main = "Example model validation",
               xlab = "Total harvested", ylab = "Abundance trend")
graphics::points(x = 600, y = 0, col = "red", pch = 4)
selected_indices <- validator$selected_simulations$index
graphics::points(x = results_manager$summary_metric_data$total_h[selected_indices],
                 y = results_manager$summary_metric_data$trend_n[selected_indices],
                 col = "blue", pch = 3)
graphics::legend("bottomleft", legend = c("Summary metrics", "Targets", "Selected"),
                 col = c(1, "red", "blue"), pch = c(1, 4, 3), cex = 0.8)
```



Summary

This demonstration has provided an overview of the *poems* workflow and modules via a simple population model example. We hope it has given you the foundation to progress to our more advanced vignettes, and towards utilizing the package for your own modeling projects.

Thank you :-)

References

Beaumont, M. A., Zhang, W., & Balding, D. J. (2002). 'Approximate Bayesian computation in population genetics'. *Genetics*, vol. 162, no. 4, pp, 2025–2035.

Csillery, K., Lemaire L., Francois O., & Blum M. (2015). 'abc: Tools for Approximate Bayesian Computation (ABC)'. *R package version 2.1.* Retrieved from https://CRAN.R-project.org/package=abc

Grimm, V., Revilla, E., Berger, U., Jeltsch, F., Mooij, W. M., Railsback, S. F., Thulke, H. H., Weiner, J., Wiegand, T., DeAngelis, D. L., (2005). 'Pattern-Oriented Modeling of Agent-Based Complex Systems: Lessons from Ecology'. *Science* vol. 310, no. 5750, pp. 987–991.