

# Manual for Software that Constructs Local IMSPE-optimal Simulator Designs Using Particle Swarm + Quasi-Newton Optimization

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This manual explains the Matlab software written to find simulator-only IMSPE-optimal designs. The sections below detail the inputs of the software, the outputs of the software, and give an example of how to run the software.

## 1 Inputs

The syntax to run the PSO + fmincon optimization routine to construct local IMSPE-optimal simulator designs is as follows:

```
[ PSO_ex1, fmin_ex1] = IMSPEopt_simulator(n, d, rho, Ndes, Nits, id);
```

where all inputs must be present in the order specified in the syntax. The inputs in the syntax above, plus one additional, are listed in further detail below. See Section 3 for a specific example that uses all inputs that are described below.

- $n \in \mathbb{N}$  – defines the number of rows in the simulator design matrix
- $d \in \mathbb{N}$  – defines the number of columns in the simulator design matrix
- $\rho$  – the  $1 \times d$  row vector of simulator correlation parameters. Each element must be in  $[0, 1]$ .
- $Ndes \in \mathbb{N}$  – defines the number of designs (particles) for PSO
- $Nits \in \mathbb{N}$  – defines the number of iterations for PSO
- $id$  – the character string used to identify which example is being run
- $yourpath$  – the character string containing the path where the IMSPE optimization MATLAB functions are stored

## 2 Outputs

There are two output structures for the software that constructs IMSPE-optimal designs for the simulator-only setting. The first structure is denoted PSO and contains the outputs from the PSO part of the optimization routine. The elements of the PSO structure are as follows:

- $PSO.IMSPE$  – the best IMSPE value found using PSO
- $PSO.Xbest$  – the  $n \times d$  IMSPE-optimal simulator design matrix constructed using PSO
- $PSO.Xbest\_vect$  – the  $nd \times 1$  reshaped design vector of the  $n \times d$  IMSPE-optimal simulator design matrix constructed using PSO

- PSO.PSOtime – the actual time elapsed during the PSO routine

The second structure is denoted fmin and contains the outputs from the fmincon part of the optimization routine. The elements of the fmin structure are as follows:

- fmin.IMSPE – the best IMSPE value found using fmincon.m
- fmin.Xbest – the  $n \times d$  IMSPE-optimal simulator design matrix constructed using fmincon
- fmin.exitflag – the exit flag describing why the fmincon search was terminated
- fmin.output – the fmincon.m output structure
- fmin.fmintime – the actual time elapsed during the fmincon.m routine

### 3 Example

```
%% Example: IMSPE-optimal simulator-only design

% Clean work space
clear all
close all
format compact
format shortG

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% User-Specified Section %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% Only change items in this section! %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% state design size
n = 10;      %number of simulator runs
d = 2;      %number of simulator inputs
% (resulting IMSPE-optimal design matrix will be of size (n \times d)

% state point-prior for correlation parameters in (1 \times d) row vector
rho = [0.75, 0.75];

% state number of PSO desgins (particles) and iterations to be used
Ndes = n*d*4; %number of designs (particles)
Nits = Ndes*2; %number of iterations

% state identification name to be used to save files
id = 'example';

% add path where IMSPE functions live
yourpath = '../software';
if exist(yourpath,'dir')
    addpath(yourpath)
    disp(' ')
    disp(['PATH ', yourpath, ' ADDED'])
else
    end
clear yourpath
```

```

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% construct design
[ PSO_ex1, fmin_ex1] = IMSPEopt_simulator(n, d, rho, Ndes, Nits, id);

%%% save results
save(strcat('out_',id))

%%% see results
% simulator design
sprintf('The resulting (%d x %d) IMSPE-optimal simulator design matrix is:',n,d)
fmin_ex1.Xbest

% IMSPE value
sprintf('The IMSPE value for the resulting design is %d', fmin_ex1.IMSPE)

% calculation times
sprintf(strcat('The total (PSO + fmincon) calculation time to find',...
    ' this design was %d seconds. '),PSO_ex1.PSOtime + fmin_ex1.fmintime)

```