


SENSITIVITY ANALYSIS, UNCERTAINTY PROPAGATION AND INTENSIVE OPTIMIZATION WITH FAST SIMULATORS

CONTEXT

- Your simulator is sufficiently fast/cheap to be called intensively for Monte-Carlo sampling
 - For intensive exploration
 - For sensitivity analysis
 - For uncertainty propagation
 - For “intensive” optimization : e.g. multi-objective optimization, robust optimization ...

Define your fast simulator as a user-defined surrogate model

- The user-defined Surrogate Models should be located in a folder in `modules/surrogatemodels`
Here : *Analytic_models/Analytic_model1.R*

> lagun > modules > surrogatemodels > Analytic_models			
Nom	Modifié le	Type	Taille
 Analytic_model1.R	10/06/2025 18:15	Fichier R	3 Ko

- Add the new folder (here *Analytic_models*) to the list of surrogates in the file «`modules/surrogatemodels/SurrogateFolders.R` »

DEFINE YOUR FAST SIMULATOR AS A USER-DEFINED SURROGATE MODEL

1. The « build » function is used only to define the model structure

```
Analytic_model1.build <- function(Xmodel, y, Ytype){  
  # Build the metamodel and return the output list  
  # Here: the model is fixed (no learning step)  
  obj <- list()  
  
  # This example is a 2d model with 2 linear outputs each defined by 3 coefficients  
  # output1 = 1 + 2*x1 + 3*x2  
  # output2 = -x1 + 2*x2  
  coef0 = c(1,0)  
  coef1 = c(2,-1)  
  coef2 = c(3,2)  
  
  # Store model coefficients in a structure to be used by predict function  
  # the model structure can contain more complex information as the name of a code to be called  
  
  obj$model <- list(coef0=coef0,coef1=coef1,coef2=coef2)  
  
  # Returns directly y as predictions and Q2=1 because the model is fixed (no learning phase)  
  obj$yloo <- y  
  
  # In case of multiple outputs of the models, it is useful to store names of the expected output in model obj for prediction  
  function  
  obj$ynome <- colnames(y)  
  obj$Q2loo <- 1  
  return(obj)  
}
```

DEFINE YOUR FAST SIMULATOR AS A USER-DEFINED SURROGATE MODEL

2. The « predict » function calls the fast simulator based on the information stored in model structure (defined in « build » function)

```
Analytic_model1.predict <- function(obj, Xmodel, computed){  
  
  #  
  npred <- nrow(Xmodel)  
  ysd <- NULL #no variance of prediction  
  
  model = obj$model  
  
  # In case of multiple outputs of the models, retrieve the expected output (colnames of obj initialized in  
  # Analytic_model1.build function)  
  if (obj$yname == "output1"){  
    ymean = model$coef0[1] + model$coef1[1]*Xmodel[,1] + model$coef2[1]*Xmodel[,2]  
  } else if (obj$yname == "output2"){  
    ymean = model$coef0[2] + model$coef1[2]*Xmodel[,1] + model$coef2[2]*Xmodel[,2]  
  }  
  
  Outputs <- list(ymean = ymean, ysd=ysd)  
  return(Outputs)  
}
```

→ Your simulator !

DEFINE YOUR FAST SIMULATOR AS A USER-DEFINED SURROGATE MODEL

3. The « update » function is useless but mandatory

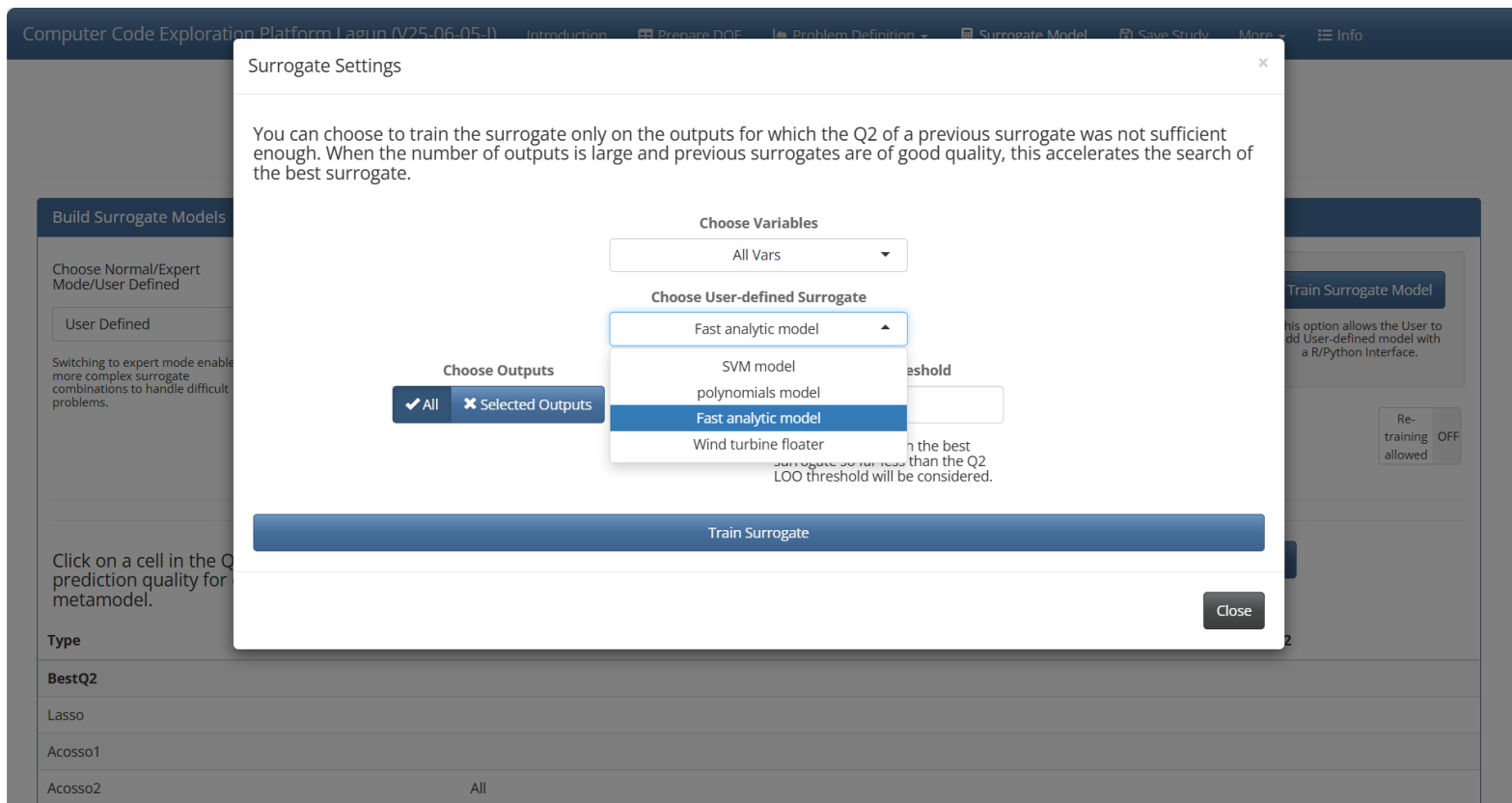
```
Analytic_model1.update <- function(obj, Xmodel, y){  
  
  obj$yloo <- y  
  obj$Q2loo <- 1  
  
  return(obj)  
}
```

4. Define the name of your model to be displayed in Lagun and its characteristics

```
Analytic_model1.description <- function(){  
  # Returns the characteristics and parameters of the surrogate model  
  #  
  # Display Name: SURROGATE  
  #  
  # OptimTags=list( "regression", "classification", "predict.sd", "CategoricalInputs")  
  #  
  # Warnings=list()  
  #  
  DisplayName="Fast analytic model"  
  
  Description="To illustrate how to plug in a fast simulator to perform SA, UQ ..."  
  
  SurrogateTags=list(classification=F, regression=T, predict.sd = F, CategoricalInputs = F)  
  Warnings=list()  
  
  return(list(dispname=DisplayName, descr=Description, tags=SurrogateTags, warn=Warnings))  
}
```

USE YOUR FAST SIMULATOR IN LAGUN

- Import a DOE with at least two different points to define the inputs and outputs of your simulator
- Surrogate model panel: select “user-defined”
- Select your fast simulator (here “Fast analytic model”)



REMARK

- You can use different types of simulators:
 - Python script : via reticulate package (See scipy example for python)
 - Executable (.exe)
 - ???
- For optimization (without uncertainties) based on your fast simulator:
rather use the simulation-based optimization functionality (Tutorial 12), there is a longer list of available optimizers and functionalities 😊