Expected Hyper Volume Improvement

Development of Expected Improvement for multi-objective problem

Łukasz Łaniewski-Wołłk

Institute of Aeronautics and Applied Mechanics
Warsaw University of Technology

Reseach for: Institute of Fluid Science
Tohoku University

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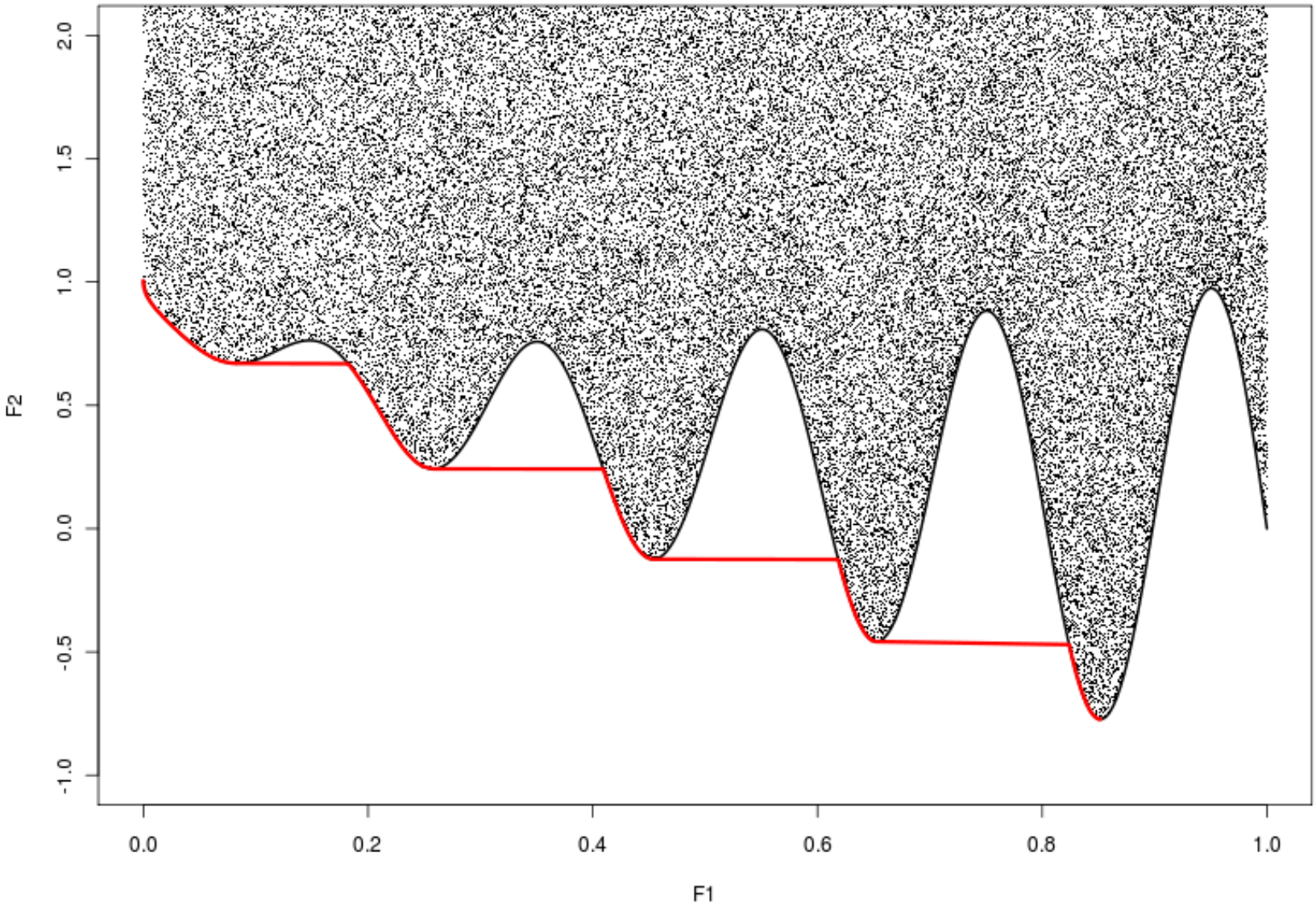
1. Problem

2. Algoritm
   - Kriging Model
   - Criterion
   - Sampling

3. Summary

Zitzler et al. (2000) test-case function no. 3

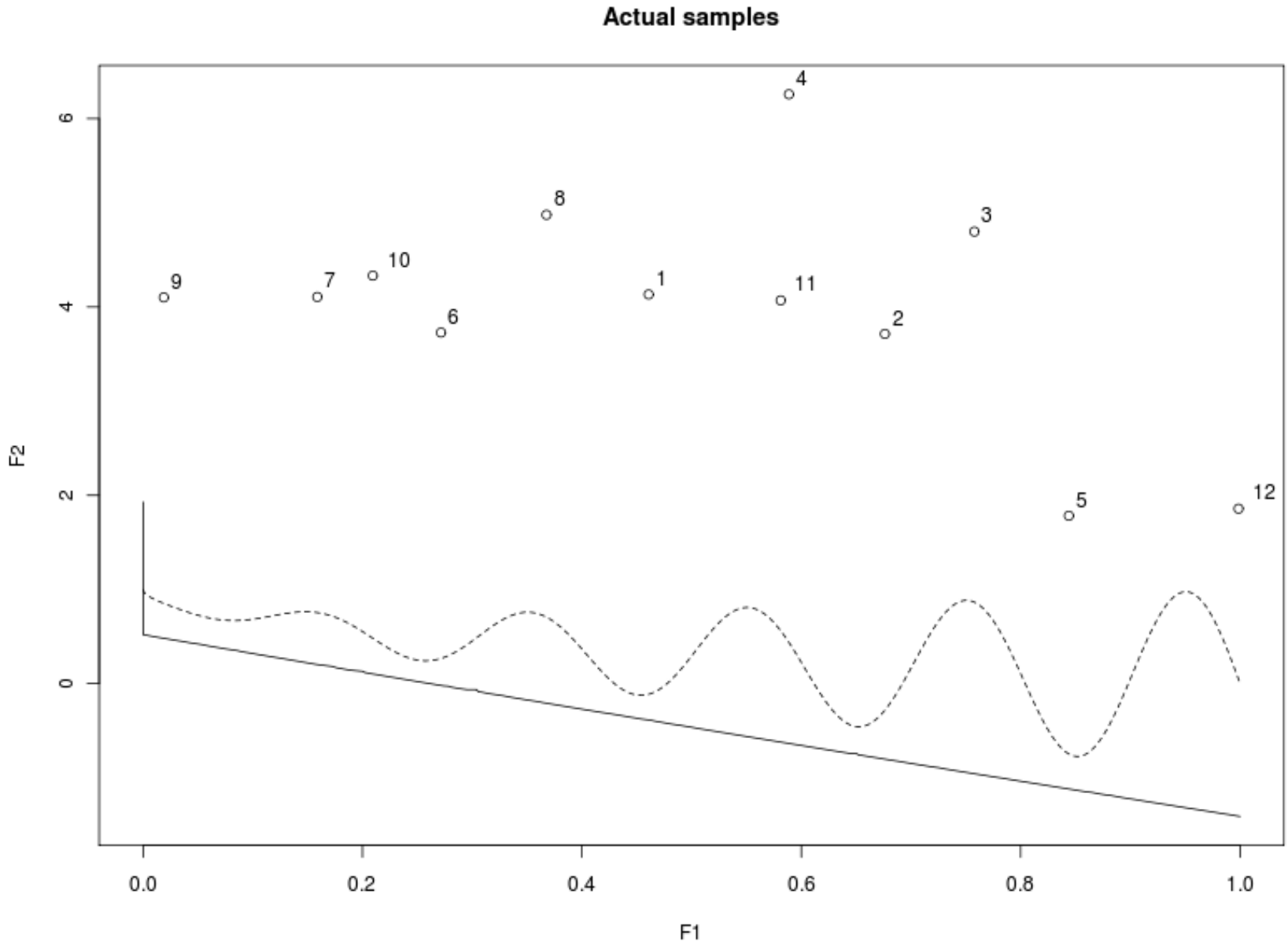


Surrogate Model based Optimization

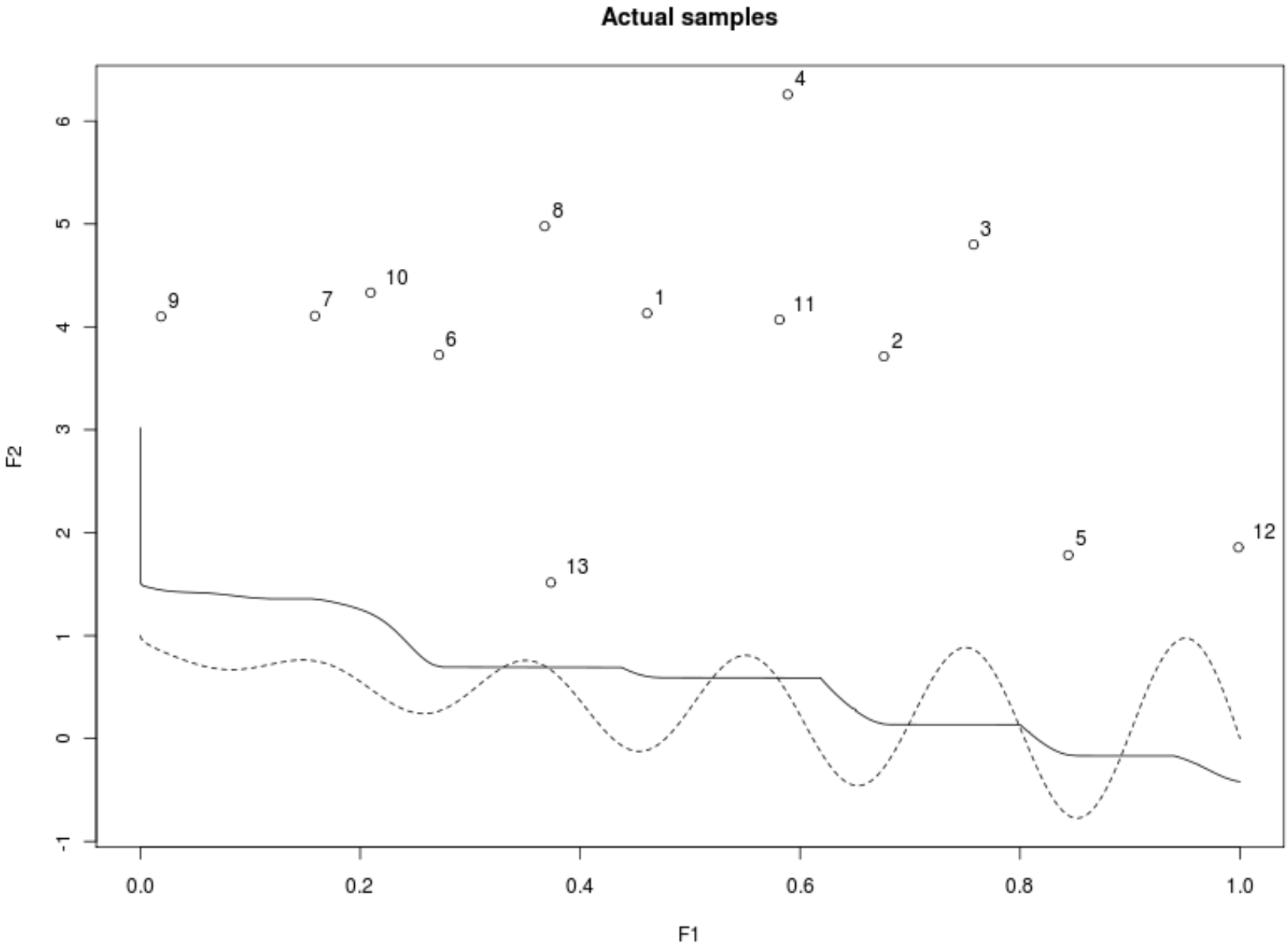
Algorithm

1. Design of Experiments
2. Objective function evaluation for sample points
3. Surrogate model fit
4. Selection of new sampling points
5. Back to 2

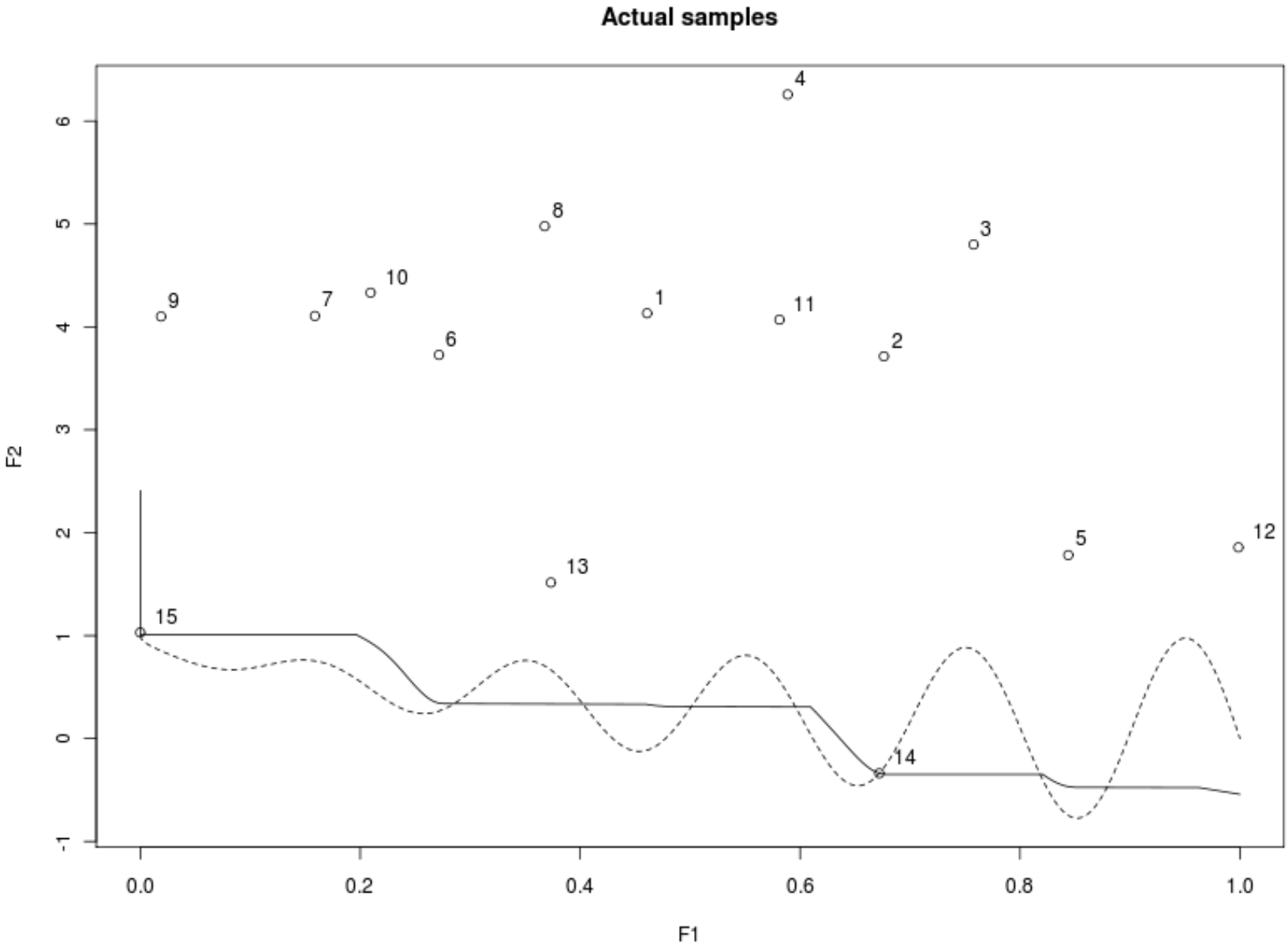
Design of experiment



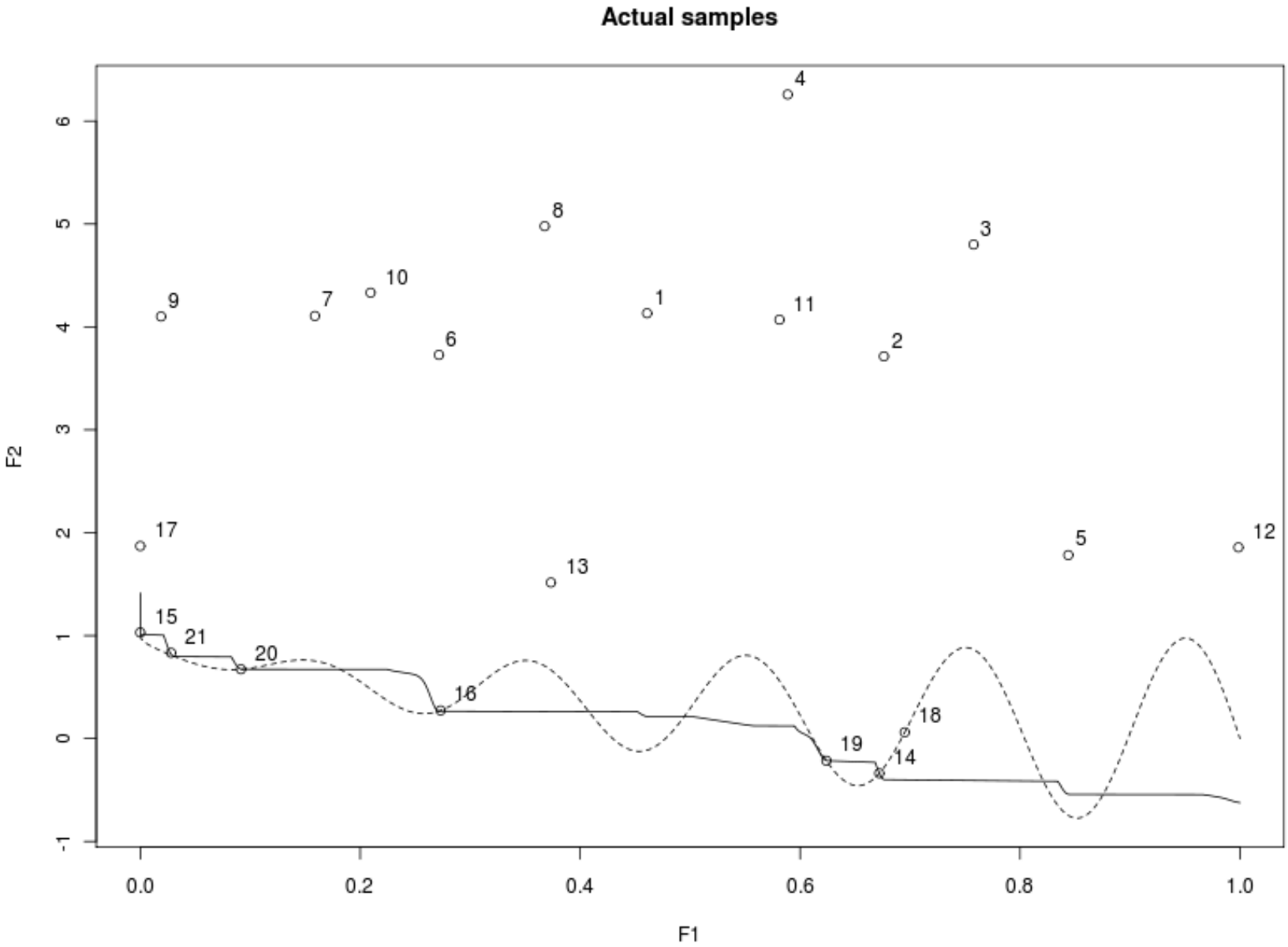
1st iteration



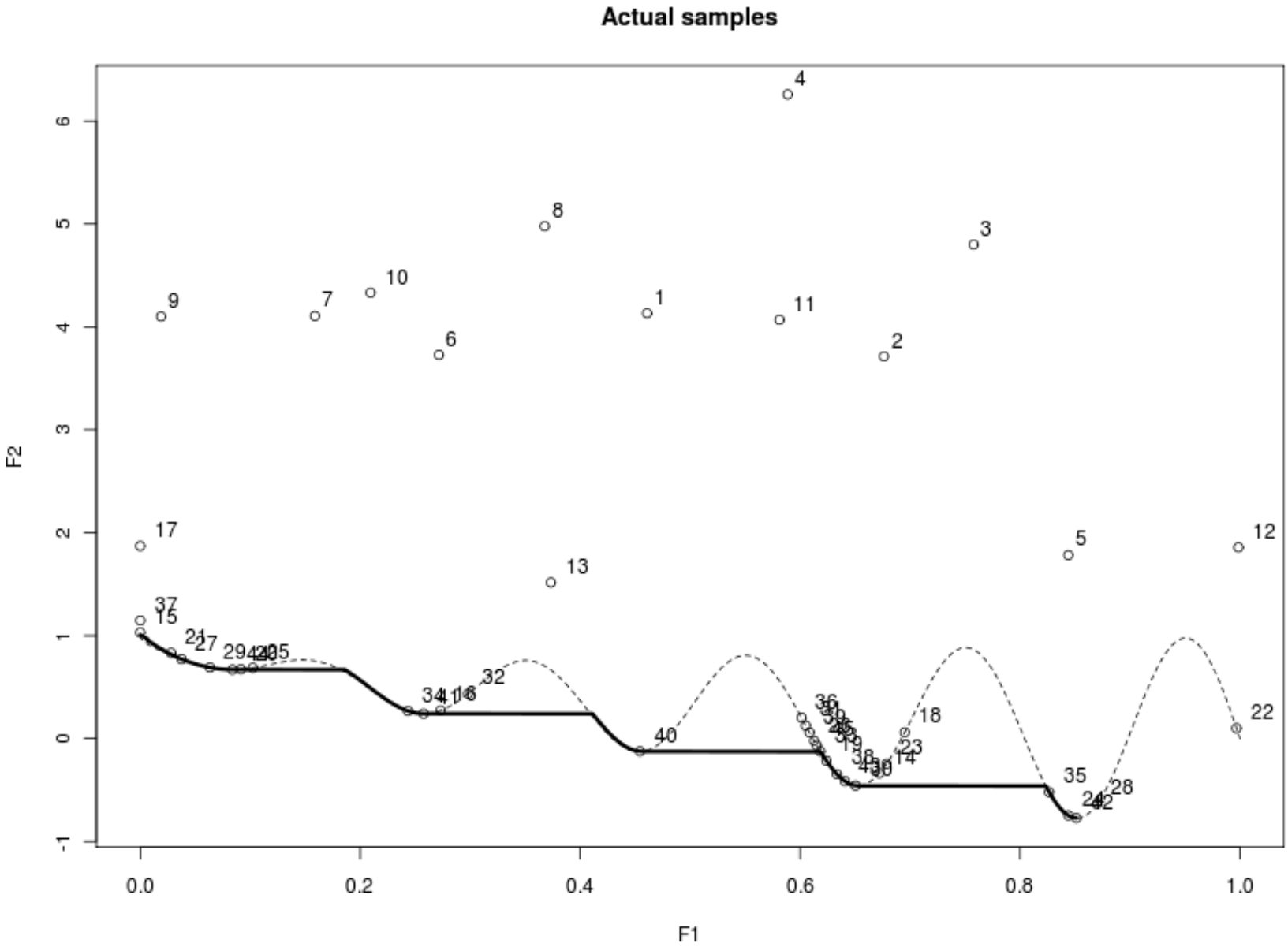
2nd iteration



3rd iteration



7th iteration



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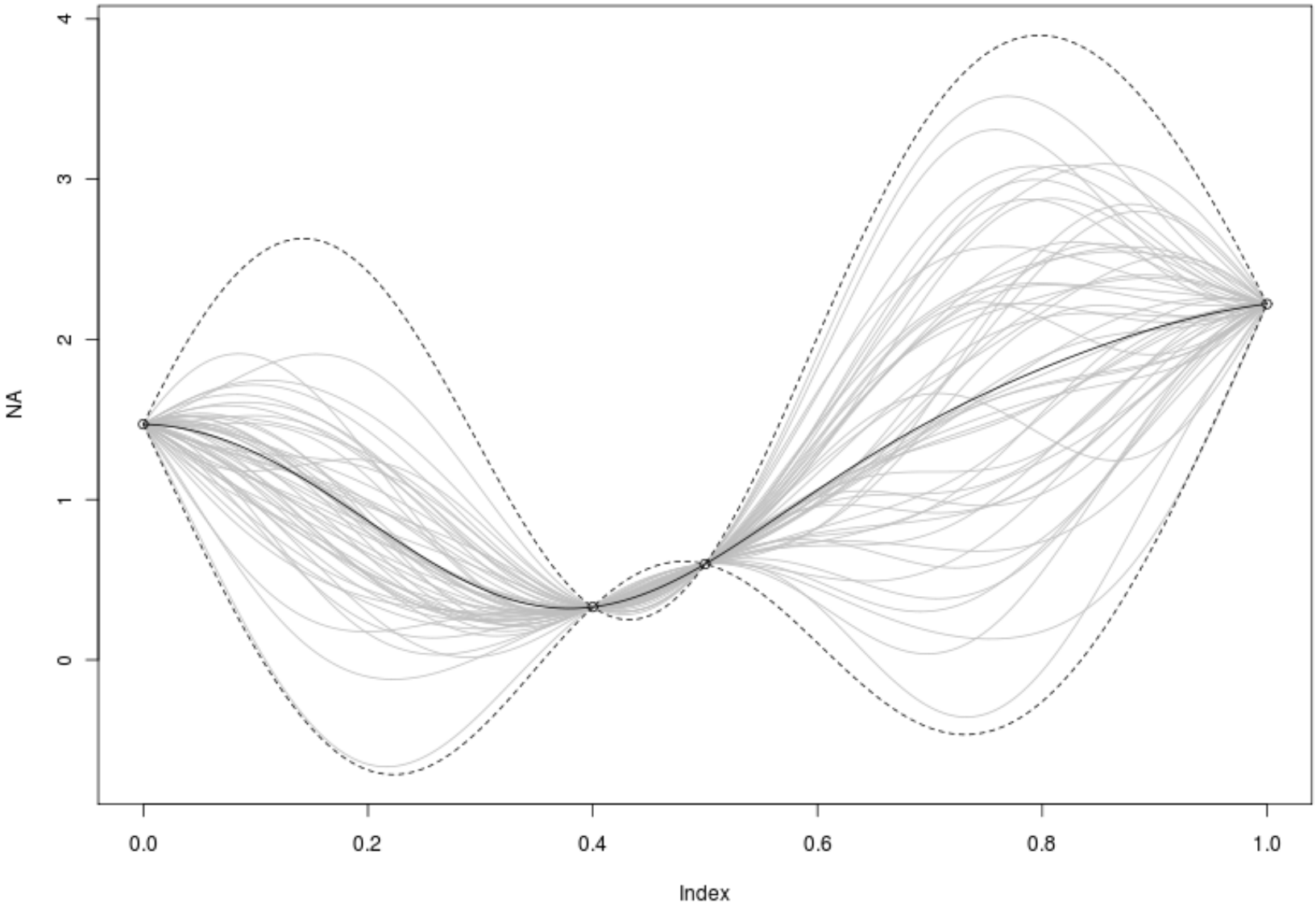
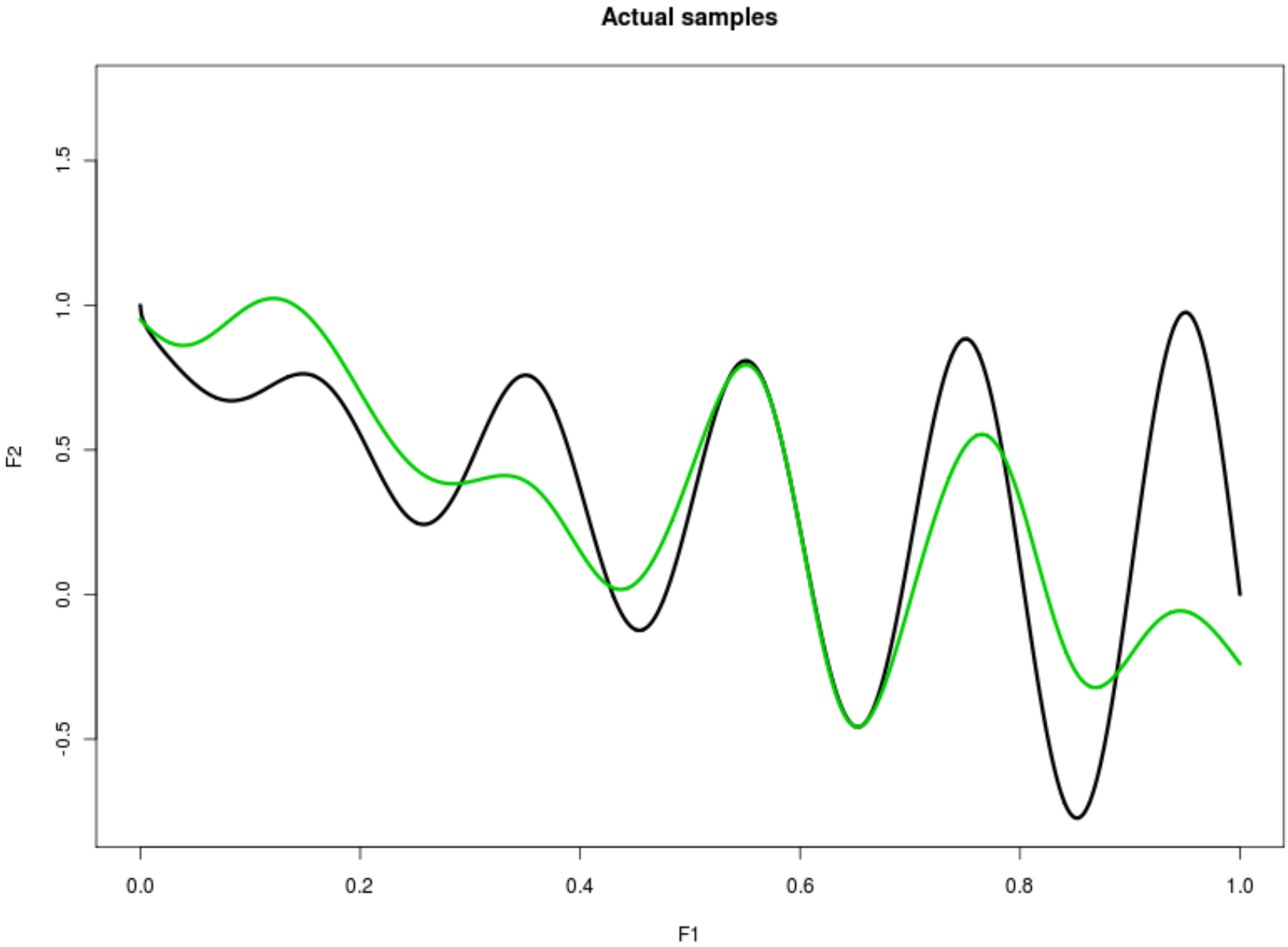
Main Question

How to select new sampling points?

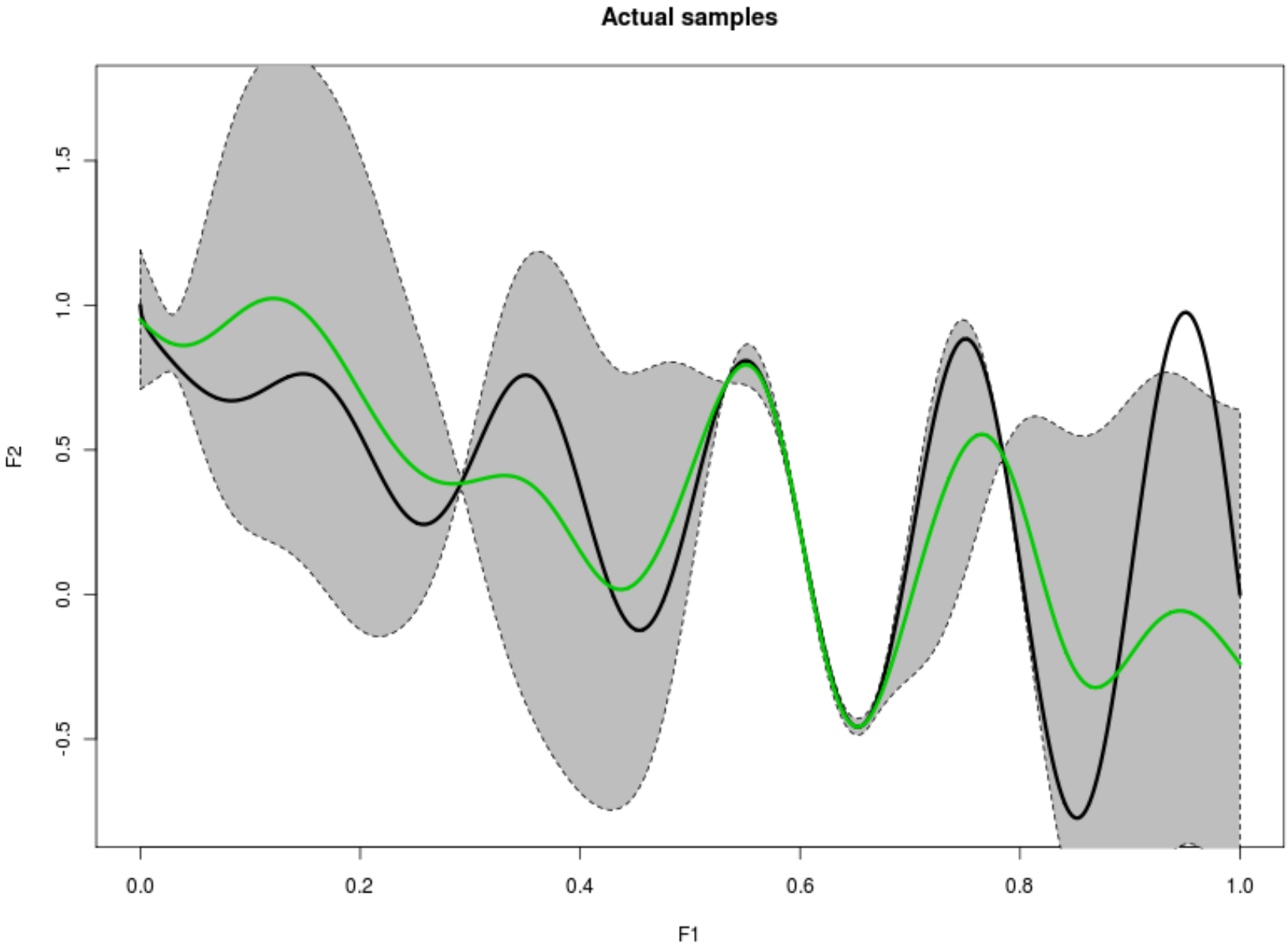
Kriging estimation example



Optimization trap



Optimization trap



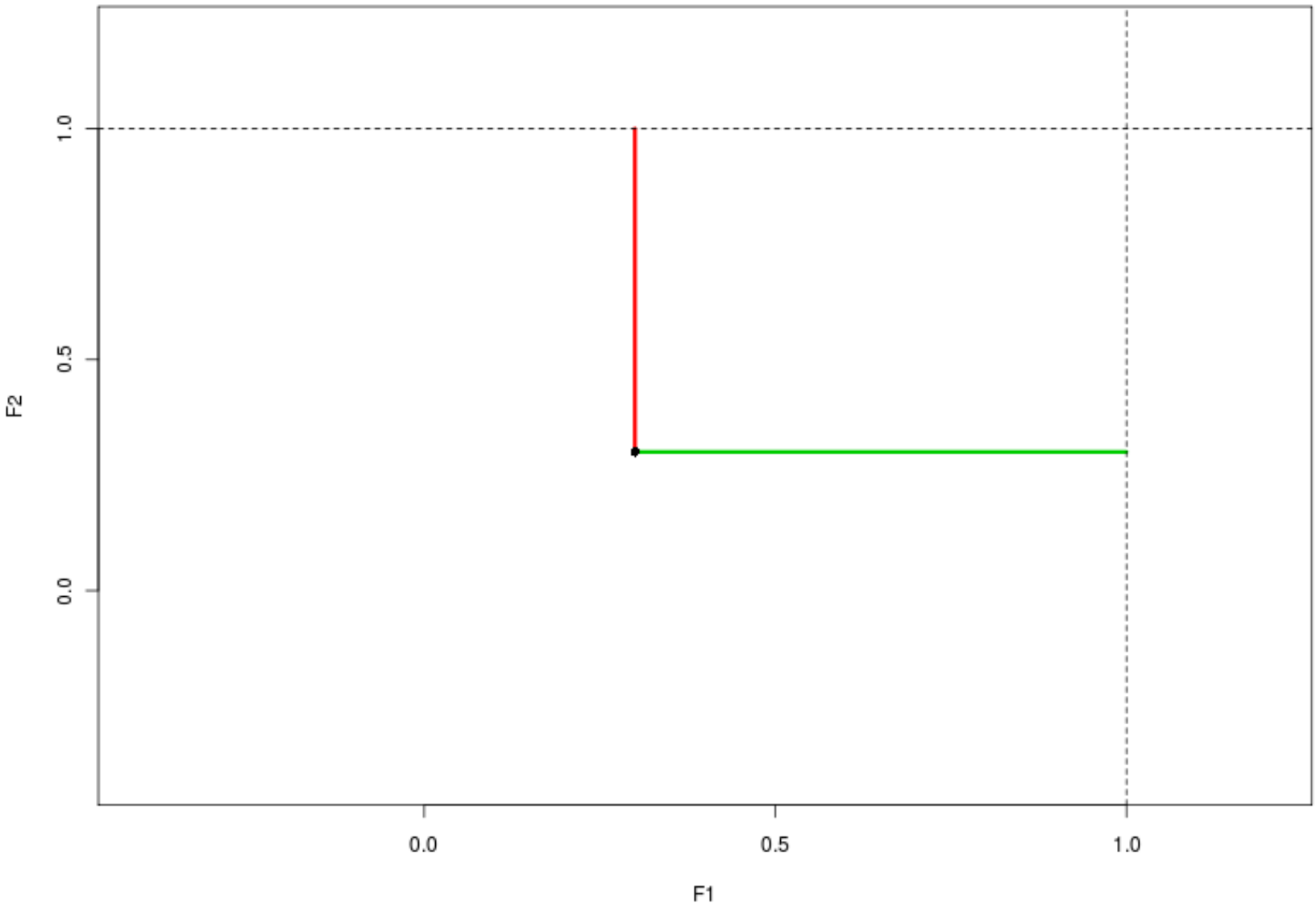
Explore and optimize

There are several concepts of balancing exploration and optimization. Widely used concept is Expected Improvement.

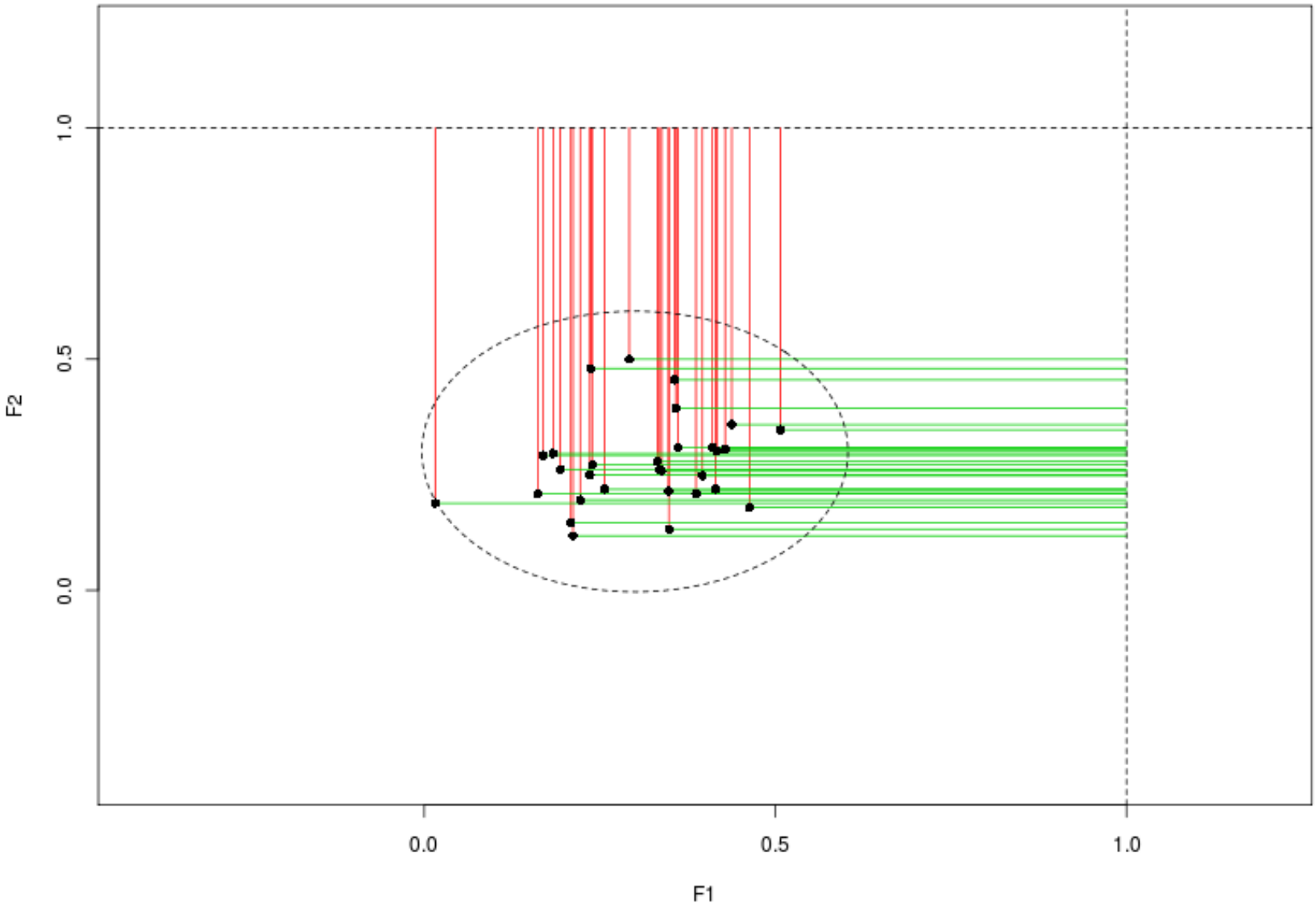
Extensions of Expected Improvement for multi-objective

- Expected Improvement (EI) with respect to a desired level of the objectives. (Jeong et al)
- Expected Hypervolume Improvement (EHVI) with respect to the dominated set.
- Probability of Improvement (PI) with respect to the dominated set. (Keane)

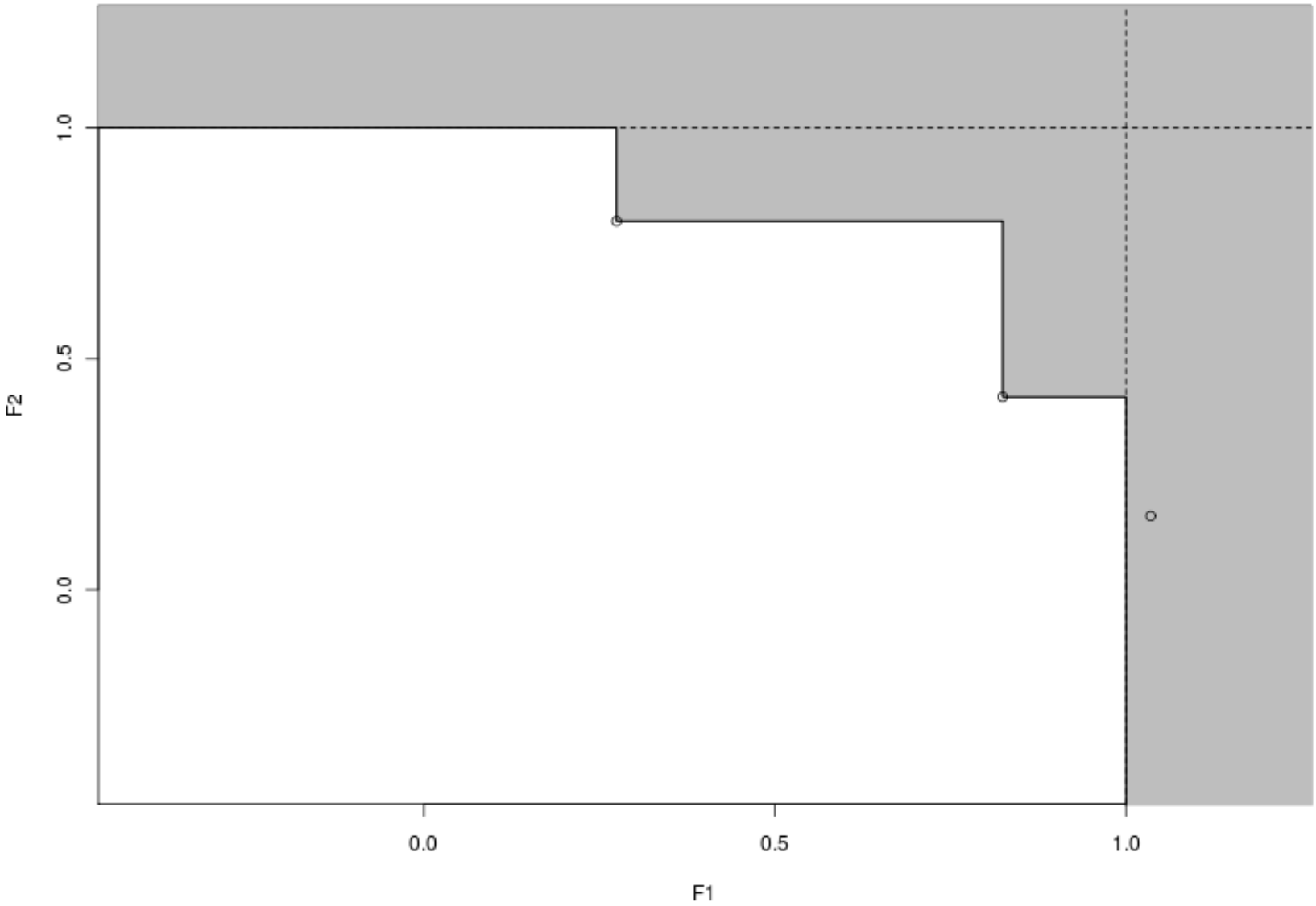
Improvement with respect to desired values



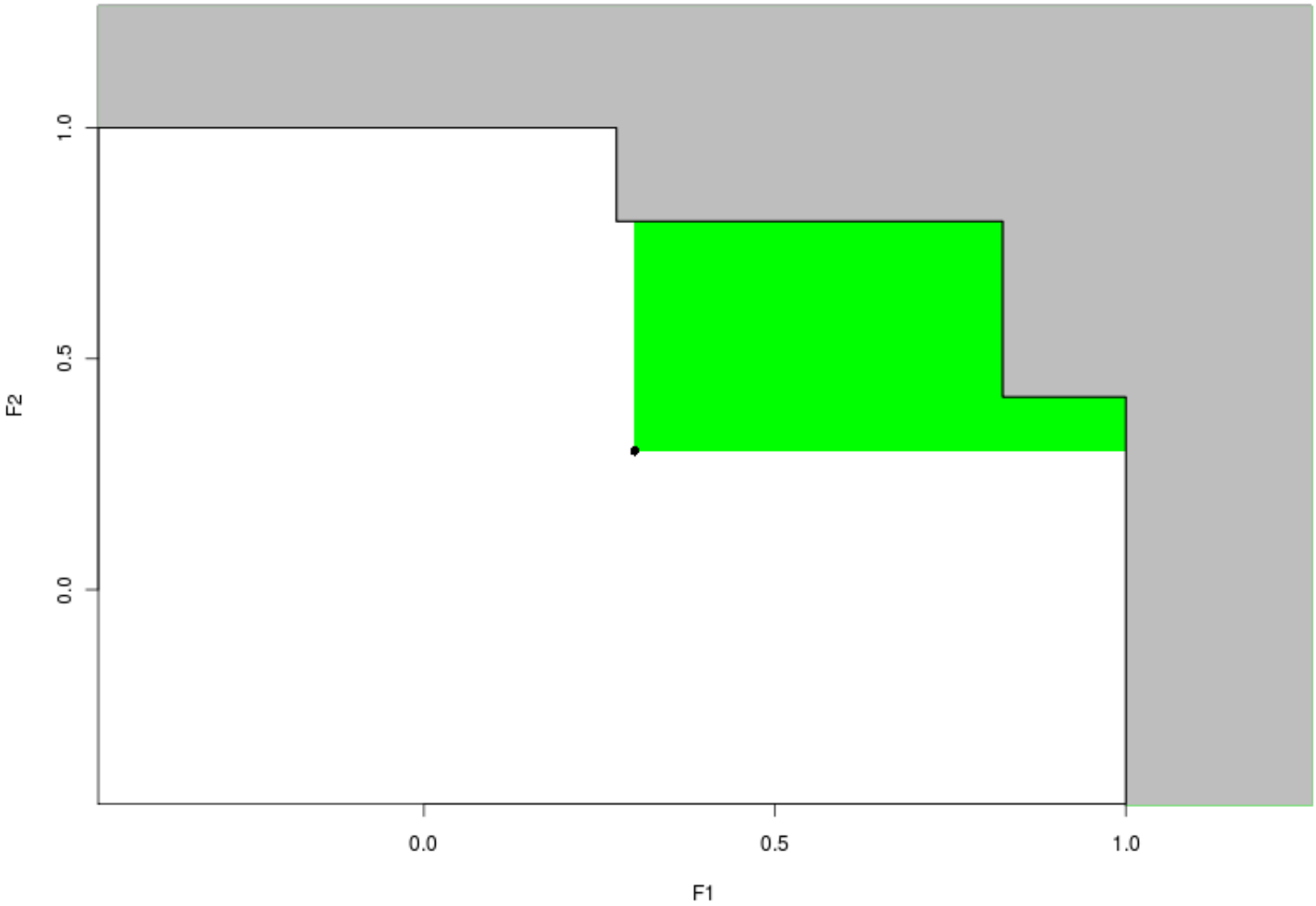
Expected Improvement



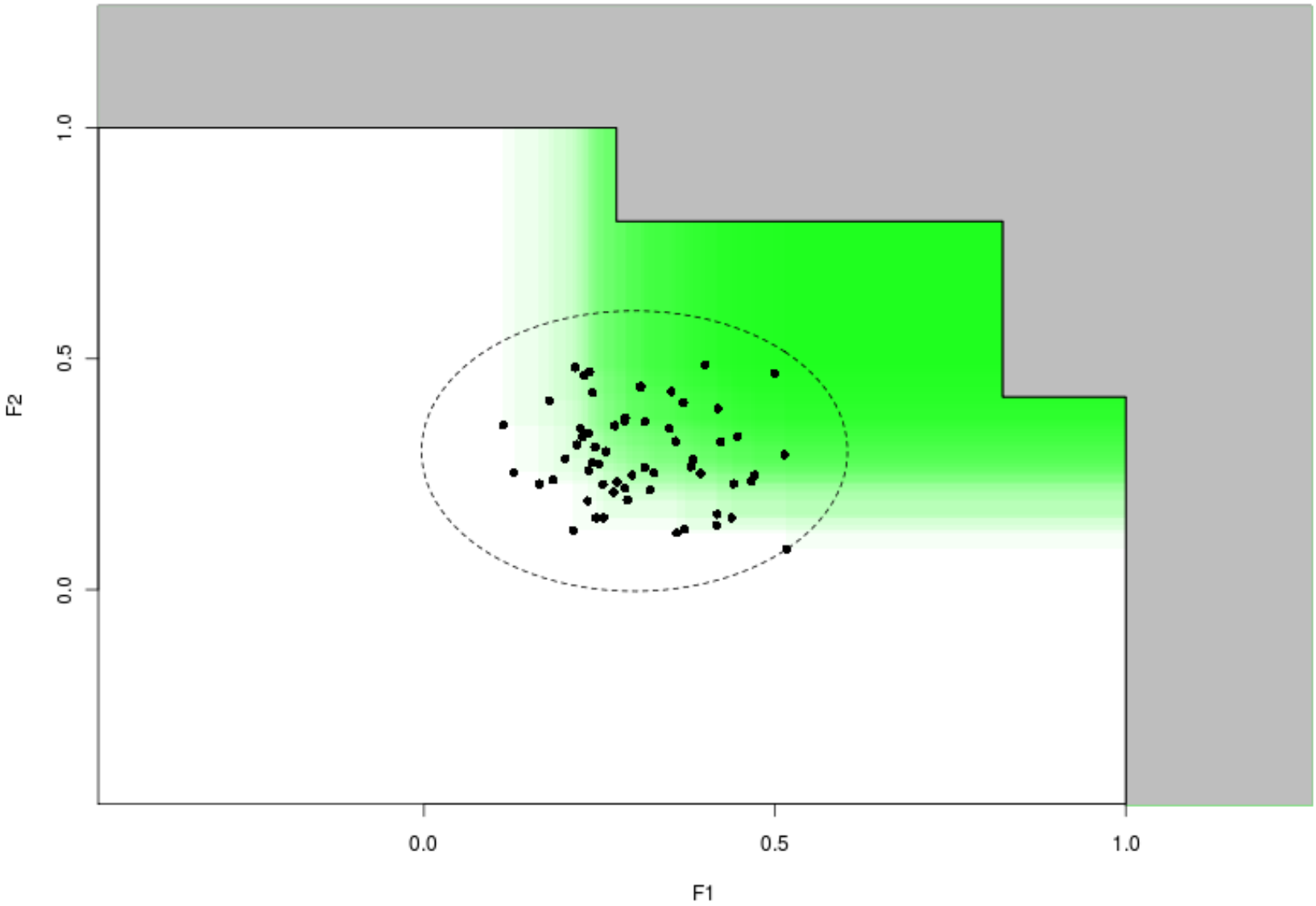
Dominated Set



Hypervolume Improvement



Expected Hypervolume Improvement



Sampling

We have then several quantities:

Functions

- Model estimator $\hat{f} : \Omega \to \mathbb{R}^2$.
- Model standard deviation $\hat{\sigma} : \Omega \to \mathbb{R}^2_+$.
- Expected Improvement: $EI : \Omega \to \mathbb{R}^2_-$
- Expected Hypervolume Improvement $EHVI : \Omega \to \mathbb{R}_+$.
- Probability of Improvement $PI : \Omega \to [0, 1]$.

From these we can construct several sampling criteria:

Sampling criterion (multidimensional)

- EI: (EI_1, EI_2)
- $EHVI$: $(\hat{f}_1, \hat{f}_2, -EHVI)$
- PI: $(\hat{f}_1, \hat{f}_2, -PI)$

Sampling

After we select the sampling criterion, we are performing these tasks:

1. Optimization of the criterion with NSGAII algorithm.
2. Clustering of the Pareto front of the criterion.
3. Selection of sampling points from the groups.

Cluster analysis

- *agnes* The Agnes agglomerative hierarchical clustering. We use a distance based on correlation obtained from the Kriging model.
- *kmeans* K-Means algorithm performed in parameter space ($k = 4$).
- *one* Place whole Pareto front in one group.

Selection

- *parmean* New point in the mean of parameters of the group
- *valmean* New point in a point from the group that is nearest to the mean of values of the group
- *var* We select from the group the point with the highest variance.
- *crit EHVI* and *PI* respectively.

Kriging Model

- *km* Kriging model with 0-degree polynomial as mean
- *lkm* Kriging model with 1-degree polynomial as mean

Methodology

Computer experiments

Full-factorial experiment.

- 66 possible settings.
- 3 test-case functions (Zitzler et al. (2000)).
- 50 runs of the algorithm.
- Stopping when achieving 80 sample points.

Performance metric: Hypervolume Ratio

$$HVR = \log \frac{|Q|}{|P^*|}$$

Where $|Q|$ hypervolume of dominated set, $|P^*|$ hypervolume of the real Pareto front.

Results. Cluster Analysis.

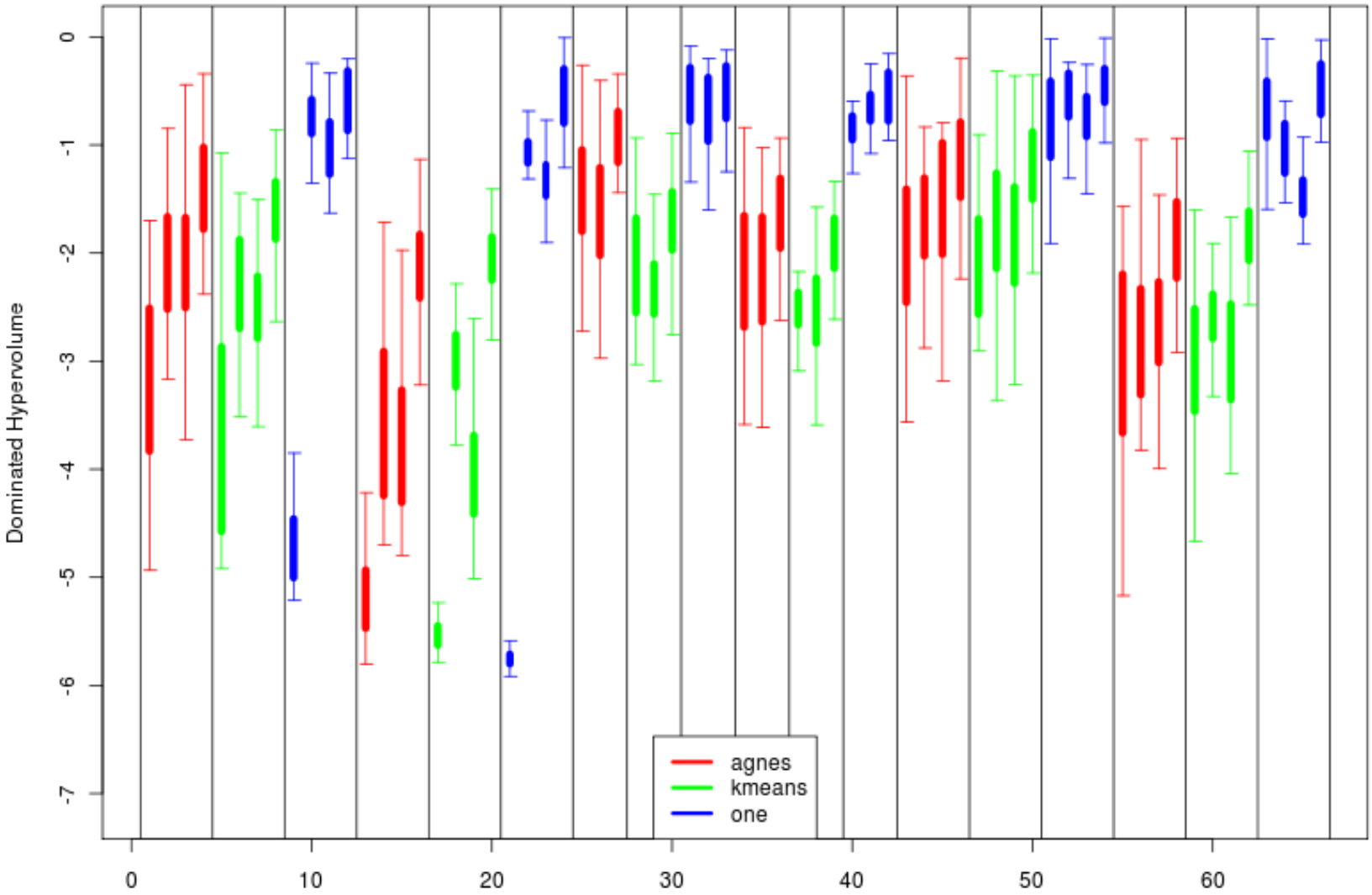


Fig.1: Boxplot of results for ZDT3 testcase with 80 sample points.

Results. Selection Method

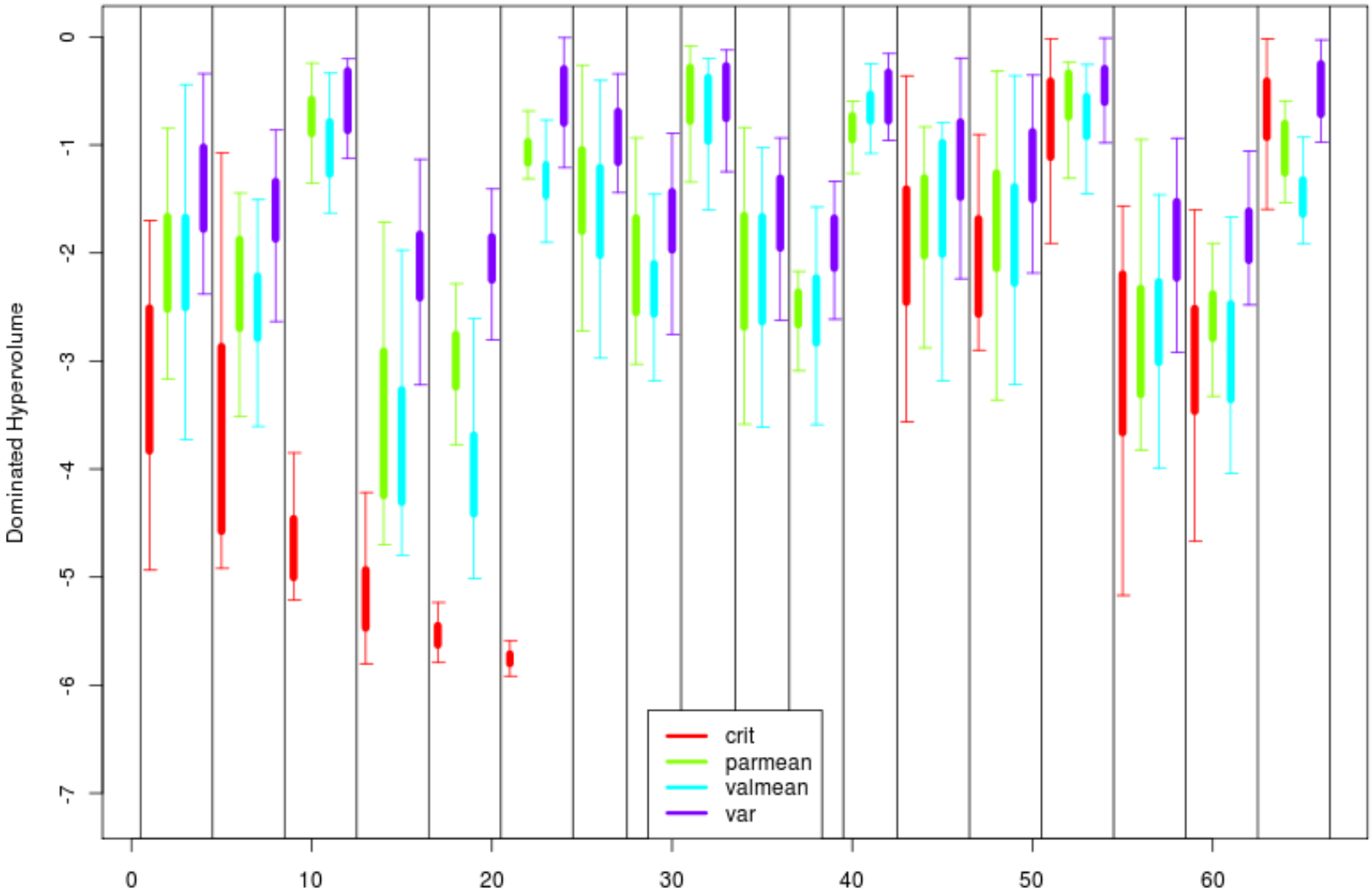


Fig.1: Boxplot of results for ZDT3 testcase with 80 sample points.

Results. Sampling Criterion

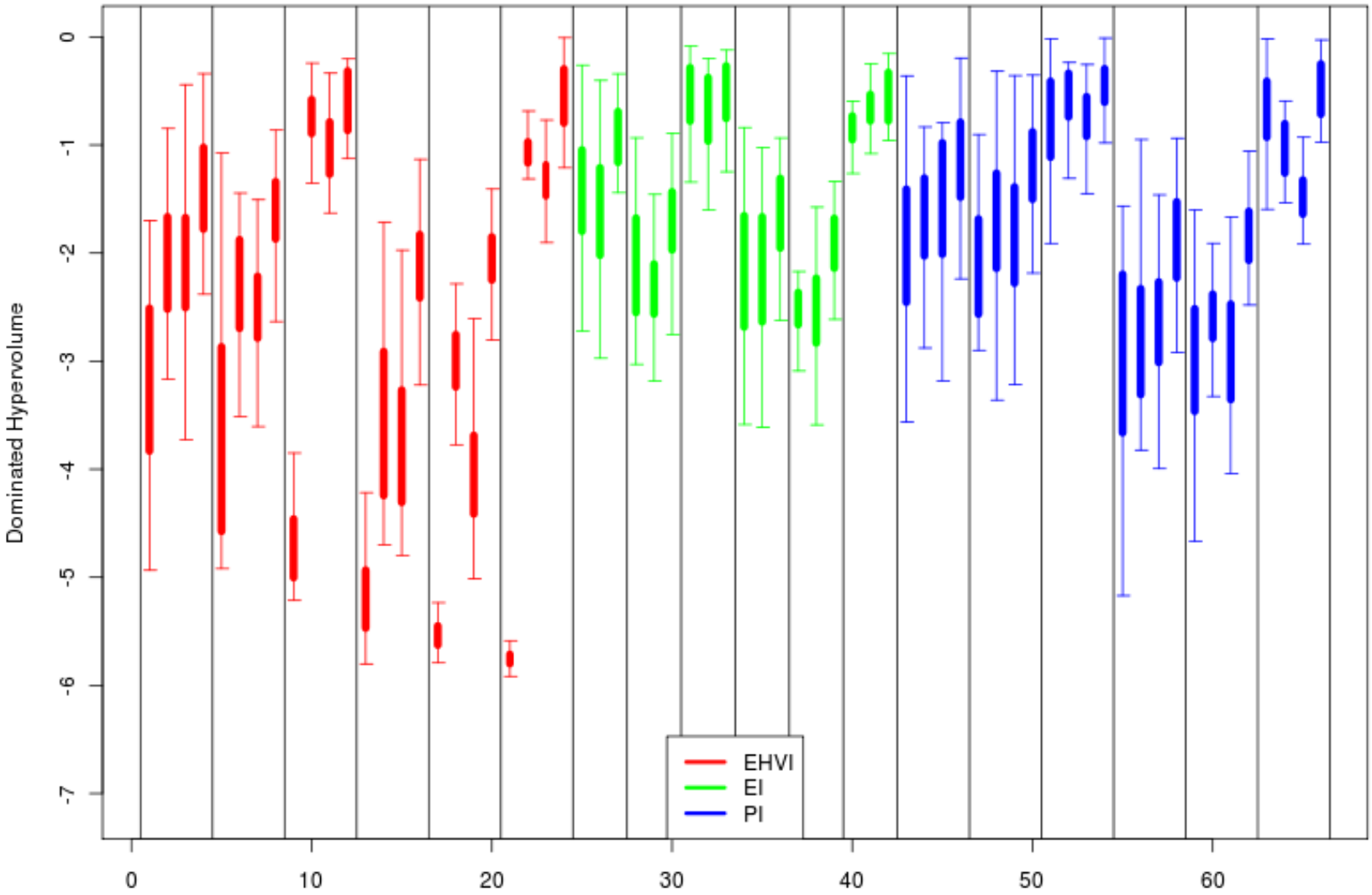


Fig.1: Boxplot of results for ZDT3 testcase with 80 sample points.

Results. Kriging Model

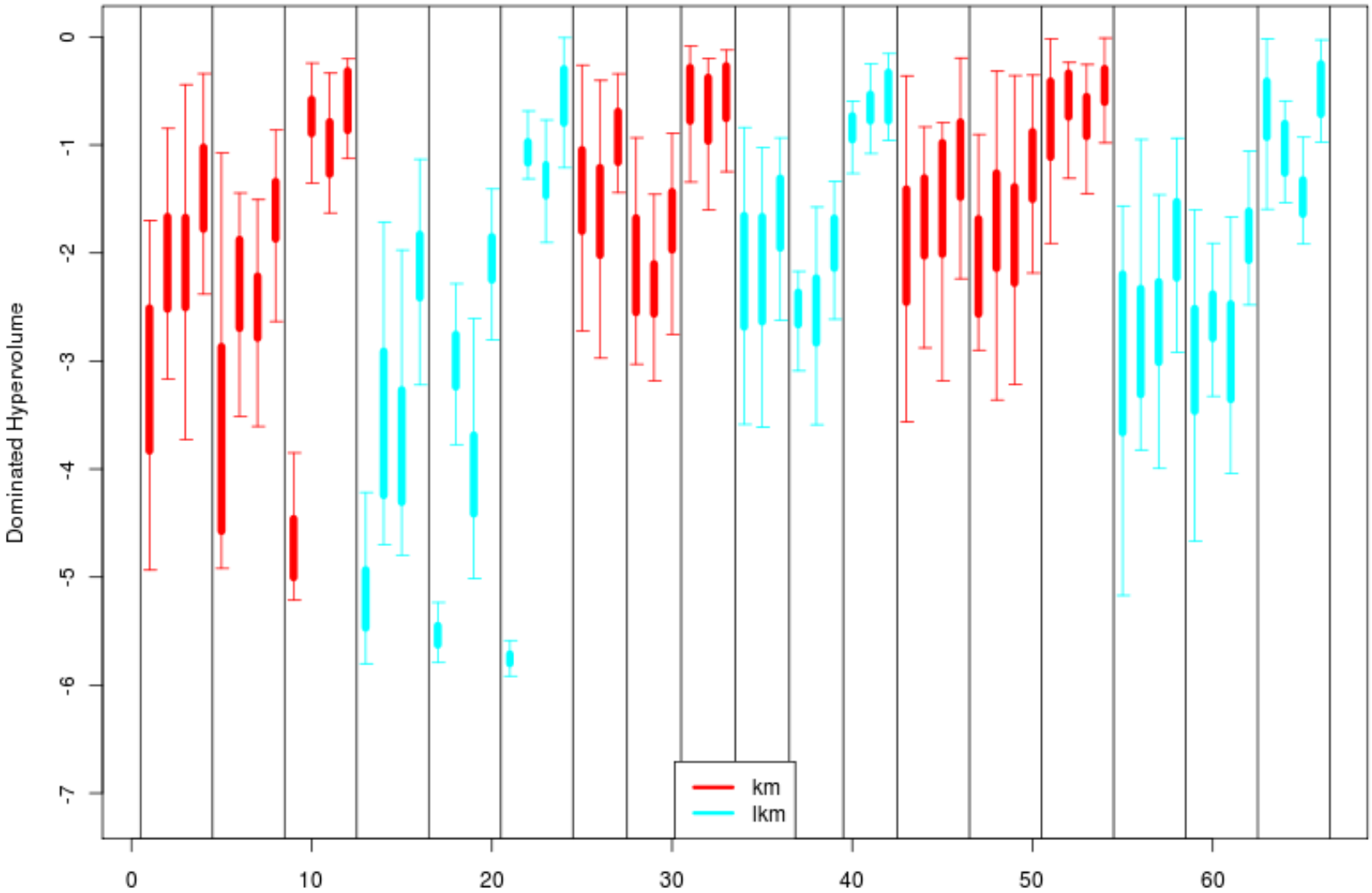


Fig.1: Boxplot of results for ZDT3 testcase with 80 sample points.

Summary of results:

Model

The model has constant and high influence on convergence of the algorithm.

Sampling Criterion

EHVI performed best in these experiments, and outpaced other criteria in the multi-modal ZDT3 test-case.

Best performing

The best performing algorithm selected one sampling at a iteration, basing on *EHVI*.

Research

Further developments

- Extension of *EHVI* calculation algorithm on arbitrary number of objective functions.
- Incorporation of constrains into the algorithm.
- Testing on engineering problems.

Thank You for your attention.