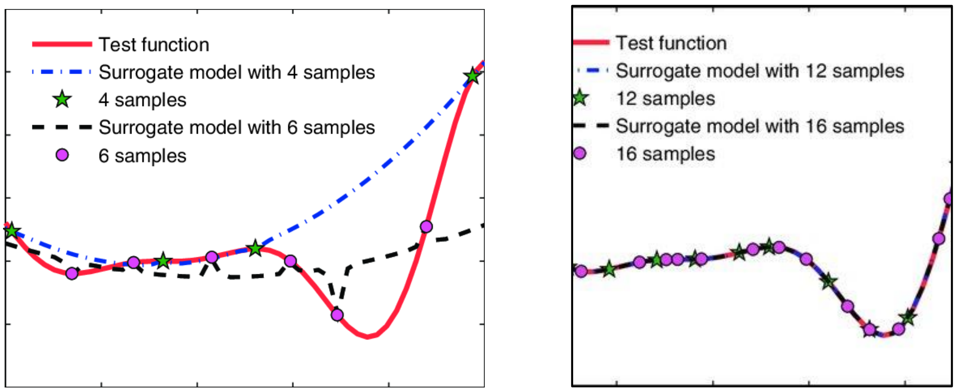
Surrogate-based Optimization

To optimise a design influenced by multiple parameters, each point in the multi-dimensional parametric space needs to be explored. This process is time consuming and computationally expensive. An efficient way to solve this issue is to develop low-fidelity surrogate models which mimic the actual experiment.

Surrogate models are low-fidelity regression models constructed using data drawn from high-fidelity models. These models can generate thousands of approximate results from a few samples, thereby simplifying the process of finding the optimal solution.



Surrogate modelling for a one variable function (effect of sample size)
Source: ResearchGate

Methodology:

The first step in surrogate modelling is the Design of Experiment, which consists of selecting sample points from the parametric space for the purpose of determining the relationship between the objectives and the variables. This step is the most crucial as it effects the overall output of the model. The objective function is evaluated at these sample points and this database is used to train the surrogates. Various surrogate models have been used by researchers and each of them is problem-dependent. A thorough discussion on Surrogate-Based Analysis and Optimisation (SBAO) is provided in the paper by Queipo et al. An excellent review of surrogate based optimisation of centrifugal pumps is given by Siddique et al.

Some surrogate modelling techniques are:

- Response surface approximation
- Kriging Model
- Radial Basis Neural Network

A multiple surrogate technique introduced by Goel et al. is used to improve the reliability and robustness of the surrogate approximation. This technique, termed as Weighted-average surrogate, assigns a weight (ω) to each surrogate model and then determines the approximate model based on the weights assigned to the individual models. The most commonly used weighing method is based upon the magnitude of the errors. This scheme can be expressed as

$$\omega_i = \frac{\sum_{j=1, j \neq i}^{m} e_j}{\sum_{j=1}^{m} e_j}$$

where e_j is the global database error measured for the j^{th} surrogate model and m is the no. of models.

Steps in Surrogate-based Optimization:

1. **Sampling** - Select a set of points in the parametric space to evaluate the objective function. (These points re chosen carefully to help the surrogate mimic the behavior of the simulator)
2. **Training the models -** Using the data from the selected points, train the surrogate model
3. **Verification -** Verify the surrogate model's prediction at the suggested (optimum) points.
4. **Sample update -** If there are discrepancies in the prediction, include these points and go back to step 2.

Once the results are verified, they can be taken as the global optimum.

References:

[1] Queipo, Nestor & Haftka, Raphael & Shyy, Wei & Goel, Tushar & Vaidyanathan, Rajkumar & Kevin Tucker, P. (2005). Surrogate-based analysis and optimization. Progress in Aerospace Sciences. 41. 1-28. 10.1016/j.paerosci.2005.02.001.

[2] Siddique, M Hamid & Shams, Murshid & Samad, Abdus. (2018). Surrogate Assisted Multi-objective Optimization of a Centrifugal Pump Impeller.

[3] Samad, Abdus & Kim, Kwang-Yong & Goel, Tushar & Haftka, Raphael & Shyy, Wei. (2008). Multiple Surrogate Modeling for Axial Compressor Blade Shape Optimization. Journal of Propulsion and Power. 24. 302-310. 10.2514/1.28999.