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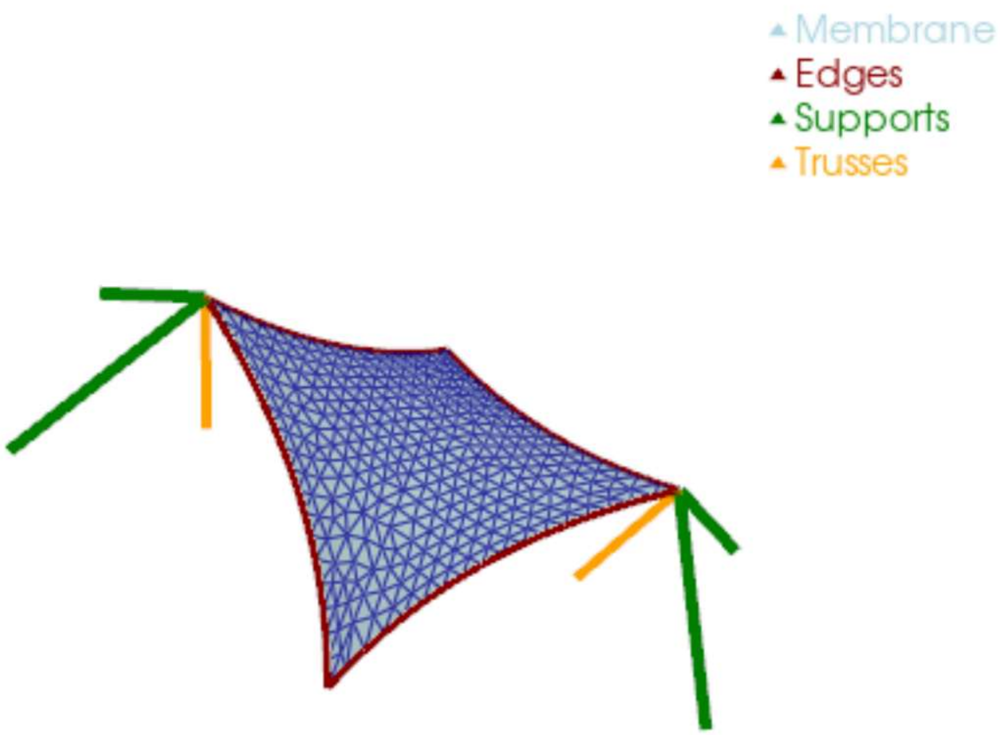
Case Study: Computer Experiments

Comparing Genetic Algorithms and LHS Designs

For the past few weeks, I have been working on a project "Computer Experiments" as part of my Case Studies course at TU Dortmund. We have delved into the world of structural analysis and the world of Finite Element Method analysis and surrogate models. This post aims to capture the ideas behind the project and an implementation of some [interesting research] I found.

Snow Load on a Sun-Sail

This is a sun-sail structure used for providing shade outdoors. It looks great, but what happens when a massive snowstorm hits? We need to know the exact load that will make it fail.



Sun-sail structure used for shade

To do this, engineers build a super-detailed virtual model of the sail. This is where Finite Element Method (FEM) Analysis comes in. We break this complex object into thousands of tiny, simple pieces (elements) and then use differential equations to model how each piece reacts to a force (like a snow load). Finite Element Method is a popular method for numerically solving differential equations arising in engineering and mathematical modeling. When you put all those little pieces together, you get the big picture of how the whole structure behaves.

The Computational Challenge

KratosMultiphysics provides specialized functions for implementing finite method analysis models. However, these simulations have a high computational cost. This is because it needs to solve ODEs for all particles and aggregate the results for each point. Thus, getting results for multiple snow loads for a complete analysis is not possible. Surrogate models come into the picture here; these are machine learning models whose job is to approximate the results of the expensive FEM model. These models can be anything - simple linear regressors, neural networks, random forests, etc.

Our process involves:

- Run the expensive FEM analysis on a small budget (n=200 points)
- Train the surrogate model based on these results.
- Use the surrogate model for near-instant inference.

Design of Experiments

Since we have to run the FEM model for the data points, we have a choice to make: Which 200 Points to Pick?

This is the make-or-break part of our whole plan. Our fast model is only as good as the 200 training points we feed it. We have a huge "design space" (material properties, etc.), and we need to choose the points that represent that space as best as possible.

We can pick our points either:

- **Statically:** Select all 200 points at the start, run them, and then train the model.
- **Sequentially:** Select a few, run them, analyze the results to see where we need more information, and then pick the next few points smartly.

In this blog, we're focusing on the static design selection and picking all 200 points upfront. We're going to compare two methods: Latin Hypercube Sampling (LHS) and Genetic Algorithms. How do these three methods work?

- **Latin Hypercube Sampling (LHS):** A technique that ensures each variable is sampled equally across its range, preventing clusters of points.
- **Genetic Algorithms (GA):** An evolutionary optimization method that "breeds" and "mutates" sets of points to achieve an optimal distribution based on a mathematical criterion.

Model Parameters and Optimality

The following parameters define the structural properties of our sun-sail. We need to find the best way to sample the non-deterministic parameters to train our surrogate models effectively:

Part	Parameter	Symbol	Unit	Distrib.	Mean	Std.
Membrane	Young's modulus	E_{mem}	GPa	Lognormal	0.6	0.09
Membrane	Poisson's ratio	ν_{mem}		Uniform	0.4	0.0115
Membrane	Thickness	t_{mem}	mm	Deterministic	1	
Membrane	Pre-stress	σ_{mem}	MPa	Lognormal	4	0.8
Membrane	Surface loading	f_{mem}	kPa	Gumbel	0.4	0.12
Membrane	Rupture stress	$\sigma_{mem,y}$	MPa	Lognormal	11	1.650
Truss	Young's modulus	E_{tru}	GPa	Deterministic	205	
Truss	Cross sectional area	A_{tru}	cm^2	Deterministic	25	
Edge Cable	Young's modulus	E_{edg}	GPa	Deterministic	205	
Edge Cable	Diameter	d_{edg}	mm	Deterministic	12	
Edge Cable	Pre-stress	σ_{edg}	MPa	Lognormal	353.678	70.735
Support Cable	Young's modulus	E_{sup}	GPa	Deterministic	205	
Support Cable	Diameter	d_{sup}	mm	Deterministic	12	
Support Cable	Pre-stress	σ_{sup}	MPa	Lognormal	400.834	80.166

Here, $\sigma_{mem,y}$ is the maximal rupture stress and is not an input to the model.

Based on these distributions, we need to sample 200 points based on our design. We use the scipy.stats.qmc.LatinHypercube module for building an LHS sample out of the box. We then use this sample as input for the genetic algorithm. The file lhs_optimizer.py contains the code.

To optimize the point distribution, we use the **Force Criterion** $G(L)$. This treats sample points as electrically charged particles, minimizing the sum of their repulsive forces:

$$G(L) := \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{1}{||x_i - x_j||^2}$$

The initial Latin Hypercube Sample (LHS) is fed into a **Genetic Algorithm (GA)**, which constructs a population of **50 LHS samples** and evolves them over **5000 iterations**.

Out-of-the-box LHS

```
Minimum Distance Squared (d(L)) : 0.046
Min Distance Occurrences (n(L)): 1
Force Criterion (G(L))         : 22149.1128
```

Genetic Algorithm Optimization

```
Initial G(L): 21900.851242

Stopping criterion met at generation 2290

Final G(L): 20421.162951
Minimum Distance Squared (d(L)) : 0.234
Min Distance Occurrences (n(L)): 8
Force Criterion (G(L))         : 20421.163
```

Maximin LHS (Best of 50 Runs)

```
Minimum Distance Squared (d(L)) : 0.068
Min Distance Occurrences (n(L)): 1
Force Criterion (G(L))         : 22154.941
```

Here we can see that the Genetic Algorithm gives a sample with the largest minimum distance between the closest points and the lowest $G(L)$ value, indicating a more optimal spread of points in the design space.

Fitting a Gaussian Process

To enable efficient inference, we now construct a surrogate model of the system. We use **Gaussian Process Regression (GPR)**, a probabilistic and non-parametric method that places a distribution over functions rather than fitting a single deterministic model.

An **RBF kernel**, scaled by a constant factor, is employed, and the kernel hyperparameters are optimized during training. In addition to point predictions, GPR provides an associated *predictive standard deviation*, which is particularly valuable for quantifying uncertainty and assessing confidence in individual predictions.

The model is fitted using the GaussianProcessRegressor class from `scikit-learn`.

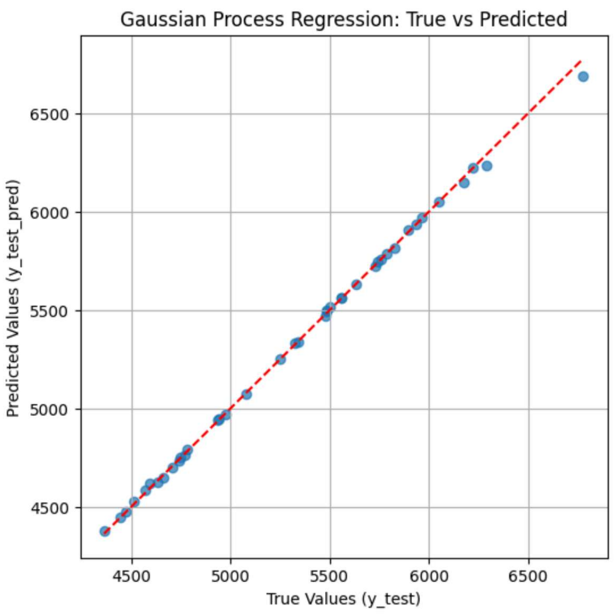
Model Performance

GA-Optimized Design

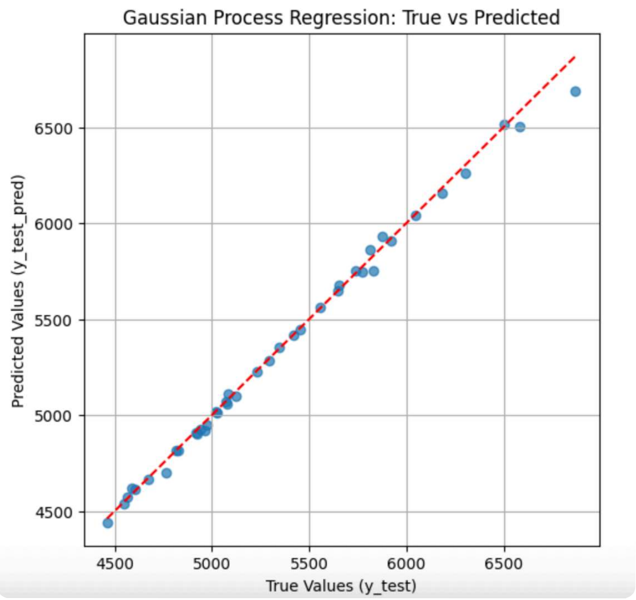
```
R² (Train) : 1.000000
R² (Test)  : 0.999011
MSE (Train): 6.232487e-11
MSE (Test) : 364.330749
```

Simple LHS Design

```
R² (Train) : 1.000000
R² (Test)  : 0.995251
MSE (Train): 1.152095e-10
MSE (Test) : 1752.885582
```



Gaussian Process Regression — True vs Predicted (GA-optimized)



Gaussian Process Regression — True vs Predicted (Simple LHS)

This study confirms that optimizing the design of experiments using Genetic Algorithms can substantially improve the accuracy and reliability of surrogate models for complex structural engineering problems.