Surrogate Modeling and Uncertainty Quantification of Maximum Cauchy Stress in Solar Sail Membranes

Case Studies II - Computer Experiments

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Introduction

- Sunsail structure - provides shade;
  - weakness : snow load
- Need to model structure behaviour
  - Solving large global system of linear equations on *Kratos*[1,2].
  - Time consuming and costly.
- Surrogate model uses a limited set of outputs from the costly FEM model and tries to approximate it for the entire domain.

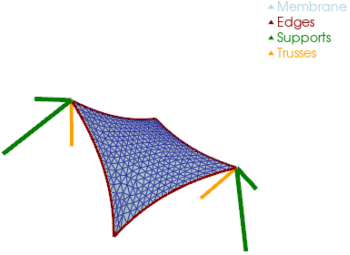

Figure 1: The sunsail mesh is made with 690 elements

1: [Dadvand et al., 2010] 2: [Ferrándiz et al., 2023]

Table 1: Kratos model input parameters and response

Quantity	Unit	Distribution	Mean	Std.
Young's Modulus E_{mem}	kPa	Lognormal	600000	90000
Poisson's Ratio ν_{mem}		Uniform	0.40	0.01
pre-stress σ_{mem}	kPa	Lognormal	4000	800
surface loading f_{mem}	kPa	Gumbel	0.40	0.12
pre-stress σ_{edg}	kPa	Lognormal	353677.65	70735.53
pre-stress σ_{sup}	kPa	Lognormal	400834.67	80166.93
Maximal Cauchy stress σ_{memmax}	kPa			

Research Objectives

How accurately do surrogate models approximate the maximum Cauchy stress in a sun-sail membrane?

How does uncertainty in the inputs induce uncertainty in the output?

Research Objectives

How accurately do surrogate models approximate the maximum Cauchy stress in a sun-sail membrane?
We look at the accuracy across Support Vector Regression, Polynomial Chaos, and Gaussian Process Regression models.

How does uncertainty in the inputs induce uncertainty in the output?
Given uncertainty in the input features, we want to find the distribution of the output Maximal Cauchy Stress.

Key Assumptions: Input features are independent and FEM model results are deterministic.

Design of Experiment

Optimized LHS using a genetic algorithm [Liefvendahl and Stocki, 2006].

Force Criterion or fitness for each LHS is simply inverse of distance:

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

Initialize with $N_{pop} = 50$ LHS models, each consisting of 200 samples. Then:

- Select 'survivors' - best $N_{pop}/2$ LHS based on fitness score and discard rest
- Cross-over: For each pair of survivors, create 2 children
- Mutate: Swap elements in each child randomly according to probability $p_{mutate} = 0.1$
- Calculate fitness of the resulting population and if stopping condition is reached, then select the best LHS from the population.

Support Vector Regression (SVR)

SVR finds a function $f(x) = w^T x + b$ that approximates the data with minimal error [Awad and Khanna, 2015].

$$\min_{w,\, \xi_i,\, \xi_i^*} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{N}(\xi_i + \xi_i^*)$$

subject to

$$\begin{cases} y_i - w^T x_i - b \leq \varepsilon + \xi_i, & i = 1, 2, \ldots, N \\ w^T x_i + b - y_i \leq \varepsilon + \xi_i^*, & i = 1, 2, \ldots, N \\ \xi_i,\ \xi_i^* \geq 0 \end{cases}$$

- ε-insensitive loss allows small prediction errors
- $C > 0$ controls the bias–variance trade-off
- Nonlinearity captured using a **Radial Basis Function (RBF):** $k(x_i, x_j) = \exp\left(-\gamma \|x_i - x_j\|^2\right)$
- Only requires feature independence.

Polynomial Regression (PLY)

Polynomial regression models nonlinear relationships by including polynomial terms to extend linear regression [James et al., 2021].

Linear model:

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

Polynomial regression (degree d):

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \cdots + \beta_d x_i^d + \varepsilon_i$$

- Nonlinearity introduced through polynomial feature expansion
- Model parameters estimated using OLS & degree via CV
- Simple and interpretable model structure
- Computationally efficient and serves as a baseline nonlinear surrogate

Gaussian Process Regression (GPR)

Purpose: Probabilistic surrogate modeling with uncertainty estimation.

A Gaussian process (GP) is a collection of random variables such that any finite subset has a joint Gaussian distribution [Rasmussen and Williams, 2006].

Gaussian process prior:

$$f(x) \sim \mathcal{GP}\big(m(x),\ k(x, x')\big)$$

Predictive distribution:

$$f_* \mid X_*, X, y \sim \mathcal{N}(\mu_*, \sigma_*^2)$$

Predictions are obtained by conditioning the GP prior on the observed data.

- Kernel-based regression model for learning smooth nonlinear relationships
- Hyperparameters learned automatically by maximizing the marginal likelihood
- Provides predictive mean and variance for each input
- Kernel-based covariance defines uncertainty across the input space

Hyperparameters

Training data: 160 samples; testing data: 40 samples (80% - 20% split)

Model	Hyperparameter	Opt. Value	Role
SVR	C	1000	Regularization.
SVR	ϵ	0.001	Width of ε tube.
SVR	γ	0.01	RBF parameter.
PLY	d	2	Degree of polynomial.
GPR	l	13.6	Length scale (RBF Kernel).
GPR	α	0.001	Noise level (RBF Kernel).

Table 2: Model Hyperparameters

Q1 : Models' Performance

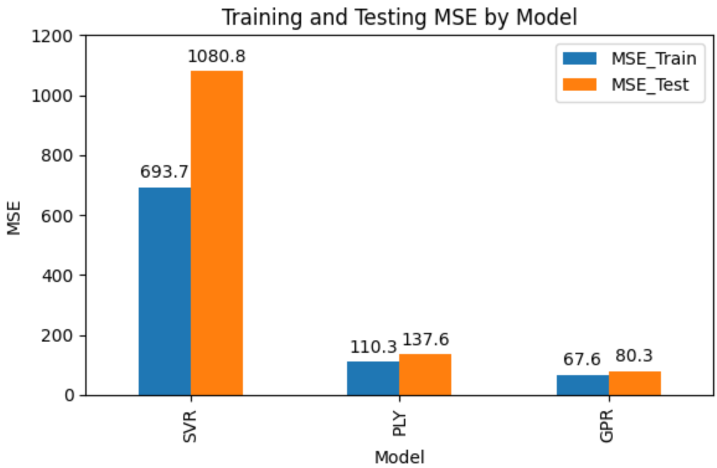

Figure 2: MSE comparison of SVR, polynomial regression, and GPR models on training and test data sets.

Residual Plots : SVR

- Very large residuals → strongly mispredicted points.
- At low predicted values → residuals are mostly negative (overestimation).
- At high predicted values → residuals are mostly positive (underestimation).

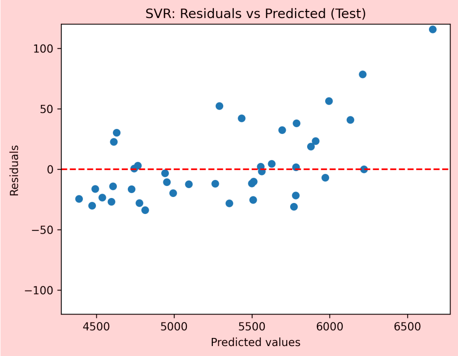

Figure 3: Residual Plot of SVR Model on Test Set

Residual Plots : PLY

- Residual well around the center.
- But now overestimating for two highest points.

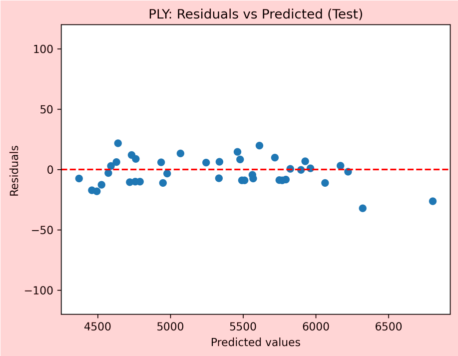

Figure 4: Residual Plot of PLY Model on Test Set

Residual Plots : GPR

- GPR residuals are the smallest and centered around zero → best fit.
- At the highest predicted values → GPR predicts these points accurately.

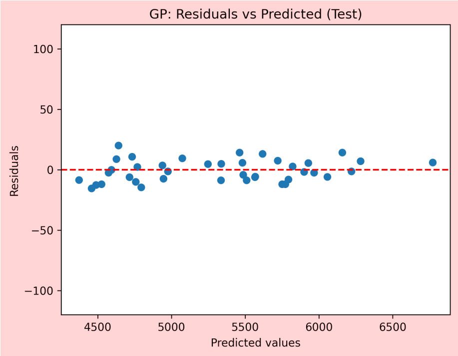

Figure 5: Residual Plot of GPR Model on Test Set

Q2 : Distribution of Maximal Cauchy Stress ($\sigma_{\text{mem,max}}$)

Using Monte Carlo Simulation [Sudret et al., 2017] on 10,000 samples:

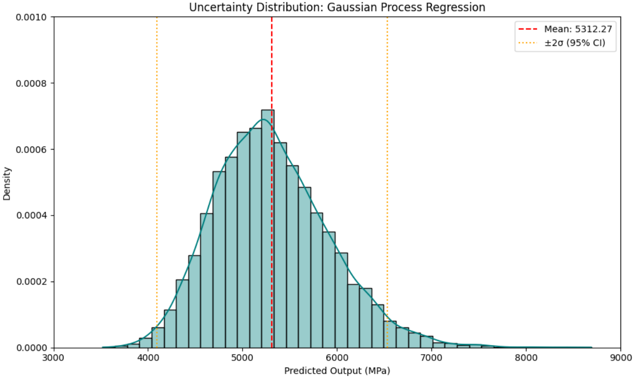

Figure 6: Empirical Distribution of $\sigma_{\text{mem,max}}$ from GPR Predictions

Mean: 5312.26 kPa, Std.: 609.9 kPa, COV: 11.5%
95% CI: 4092.28 kPa - 6532.24 kPa

Findings

Distributional assumptions

- For a pre-stressed membrane, $\sigma_{\text{mem,max}} > 0$.
- The empirical distribution is right-skewed.
- It is natural to model it with a continuous distribution whose support is $\mathbb{R}^+$ (e.g. lognormal or gamma).
  - AIC or Akaike Information Criterion is a metric used to compare different statistical models; the lower the AIC, the better the model balances fit and complexity.

Findings

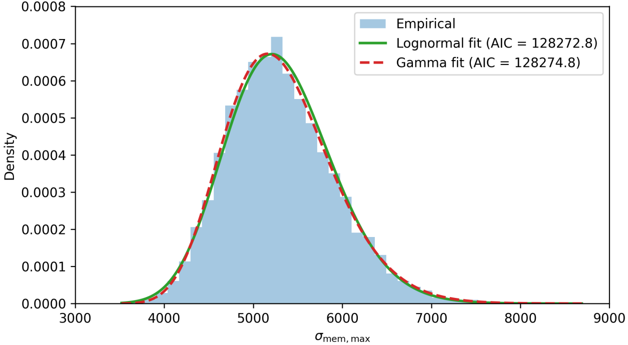

Figure 7: Empirical Distribution of $\sigma_{\text{mem,max}}$ from GPR Predictions with overlaid lognormal and gamma PDFs

- The $\Delta\mathrm{AIC} \approx 2$ is small $\rightarrow$ a slight advantage for the lognormal fit.

Conclusion

- Gaussian Process Regression gives the best accuracy to approximate to the FEM model to compute maximal Cauchy stress on the membrane.
- Got the distribution of the maximal Cauchy stress and also fit a theoretical lognormal and gamma distribution over the empirical one.

Possible improvements:

- Space-filling or optimized LHS can be used for MC simulations.
- SVR model seems to be overfitting and can be improved.

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