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# Evaluating the performance of Latin Hypercube Sampling in hybrid modeling of the knee with contact surrogate

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**ABSTRACT:** Surrogate models are becoming popular in various areas science. To obtain them, costly iterations on complex models are required. Therefore, many studies employ Quasi-Monte Carlo (QMC) sequences, which can reduce the number of required samples. Latin Hypercube Sampling is one of the primary examples of such sequences. Nevertheless, the actual performance of QMC's can depend on the application. To the best of our knowledge, a test of LHS effectiveness was not done for a hybrid model of the knee. Therefore, this study focused on analyzing the LHS in surrogate training for hybrid knee modeling. In total 5 LHS sequences of varied size were generated. The largest sequence of 64 samples was used as validation. The remaining ones were employed for surrogate training and testing with Leave-One-Out cross-validation. The surrogates were also compared to actual Finite Element in the hybrid setting to assess the propagation of errors. The main findings were as follows: LOO-CV typically underestimated the worst-case performance of the surrogate, nonlinear propagation of errors was observed in the hybrid model – the best results in the surrogate space did not correspond to the ones in the hybrid space. These findings suggested that assessing the surrogate performance in hybrid scenarios was complex and required further study.

**KEYWORDS**: Polynomial Chaos Expansion, nRMSE, Quasi-Monte Carlo, Finite Element, Multibody

## 1. Introduction

In hybrid modeling in biomechanics, a multibody model of the joint or multiple joints is extended with a Finite Element (FE) model in some areas, such as contact mechanics. These FE models can be substituted with surrogates [1, 2], to further lower numerical complexity of the task and allow for complex simulations involving optimization and uncertainty quantification.

Surrogate models are becoming widely used in various area of engineering and science. Their main benefit lies in low computational complexity, when compared to more classical approaches in mechanics, such as the FE method. Nevertheless, a training dataset obtained from classical approaches is required to obtain the surrogate. Since FE models are expensive to solve, one of the fundamental problems lies in the design of the surrogate training set, so that it properly represents the original model and contains as few samples as necessary. Typically, Monte Carlo random sampling is not optimal for this purpose. Therefore, many other approaches were introduced: from Quasi Monte-Carlo sequences (QMC), such as Latin Hypercube Sampling (LHS) [3], to adaptive sampling and active learning. Many studies point out that using QMC sequences is beneficial, especially in low-dimensional models with limited number of samples. These sequences can also form a baseline for sequential sampling. While QMC's are known to improve the sample sets, their effectiveness is difficult to measure, as it may differ in various applications. To the best of our knowledge, such an analysis was not performed for hybrid biomechanical models of the knee.

Therefore, the aim of this study was to analyze the performance of LHS in hybrid modeling of the knee joint with surrogate contact mechanics.

## 2. Method

The hybrid model of the knee was assumed after [2, 4]. The model described the behavior of the tibio-femoral joint in dynamics and consisted of two rigid bodies, corresponding to the bones, four nonlinear cables, substituting the ligaments and two contact surrogate pairs, which mimicked the bimaterial contact of the bones through cartilage. The surrogate contact was trained on FE model, a spherical body was indented into a cuboid. Both bodies had two layers, with the outer one corresponding to cartilage and the inner representing the actual bone.

The contact surrogate was based on Polynomial Chaos Expansion (PCE) in ChaosPy [5] and had 5 parameters, representing the radius of the sphere and the material parameters of both bodies. In order to obtain a training set for it, several 4 LHS sequences were generated with 4, 8, 16 and 32 samples. Additionally, one large LHS set of 64 samples was generated as a reference for validation. Three polynomial orders were considered for the surrogate: 2, 3 and 4. The surrogate was trained on each of the sequences and validated with Leave-One-Out Cross-Validation (LOO-CV), additionally the surrogate model obtained for each step of LOO-CV was also tested on the 64-sample set. Normalized Root Mean Square Error (nRMSE) was computed to assess the performance of the surrogate. The final surrogate in each case was tested in the hybrid knee model and compared against the results obtained from the set of 64 samples with nRMSE as well. The full hybrid model was solved under external moment loads in dynamics with its angular displacement to moment serving as the output for surrogate assessment.

## 3. Results and discussion

The obtained results were presented in Fig. 1 and 2.

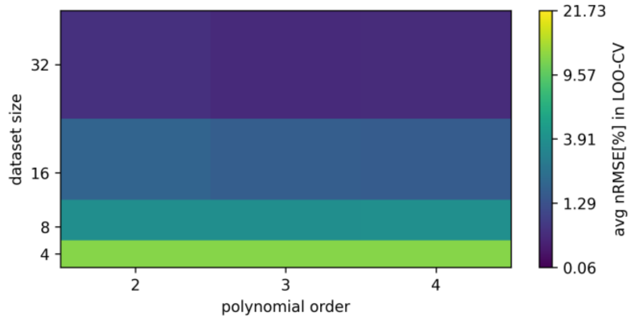


Fig. 1. The average nRMSE with regards to the dataset size (for training/testing within LOO-CV) and polynomial order.

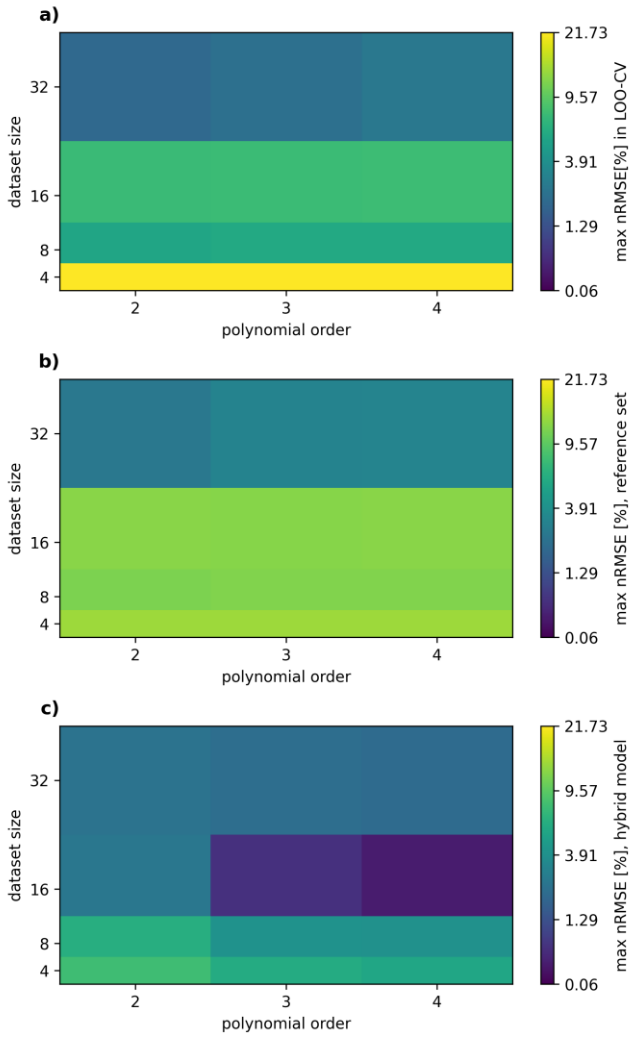


Fig. 2. The max nRMSE with regards to the dataset size (for LOO-CV) and polynomial order in three cases: a) considering only LOO-CV, b) on a reference set of 64 samples, and c) within the full hybrid model of the knee.

As seen in Fig. 1, when considering the average nRMSE, the performance of the surrogate steadily improved with larger datasets. The worst results were obtained for the set with 4 samples. In terms of the max nRMSE, the best results were obtained for the largest dataset of 32 samples – Fig. 2a.

Nevertheless, as seen in Fig. 2b, LOO-CV underestimated the worst-case performance of the surrogate on almost all of the tested datasets, except the 4-sample one. In the remaining sets, the relative difference between the actual max nRMSE and the one from LOO-CV could be as high as 100 %. It is worth pointing out, that the results from LOO-CV and the reference set started to converge at 32 samples.

Interestingly, as seen in Fig. 2c, the results obtained from the full hybrid knee model were not compatible with those from LOO-CV and reference set using the contact surrogate in isolation. In this case, the lowest max nRMSE was obtained for the 16-sample set, instead of the larger 32-sample set, which was the case with the isolated contact model. Furthermore, within the hybrid model test, the benefit of using higher polynomial orders was clear, which was not apparent with the isolated contact surrogate. Additionally, the nRMSE values were generally lower in the full model, which suggested that the hybrid model was not sensitive to the errors in the surrogate contact prediction. This signified the need for a comprehensive test procedure for surrogates in hybrid models, involving both testing in isolation, as well as, in the complete model. That being said, with higher number of training samples, the results seemed to be more consistent.

## 4. Conclusion

The study focused on analyzing the performance of Latin Hypercube Sampling in surrogate training for hybrid knee modeling. The two main findings were as followed:

1) LOO-CV typically underestimated the worst-case performance of the surrogate,
2) nonlinear propagation of errors was observed when using the hybrid model – the best results within the surrogate space did not correspond to the best results in the hybrid model space.

The results suggest that the problem of assessing surrogates performance, especially in a hybrid setting, is very complex and requires further study.

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