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GrainLearning: A Bayesian uncertainty quantification toolbox for discrete and continuum numerical models of granular materials

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Summary

How to keep dikes safe with rising sea levels? Why are ripples formed in sand? What can we prepare for landing on Mars? At the center of these questions is the understanding of how the grains, as a self-organizing material, collide, flow, or get jammed and compressed. State-of-the-art algorithms allow for simulating millions of grains individually in a computer. However, such computations can take very long and produce complex data difficult to interpret and be upscaled to large-scale applications such as sediment transport and debris flows. GrainLearning is an open-source toolbox with machine learning and statistical inference modules allowing for emulating granular material behavior and learning material uncertainties from real-life observations.

Statement of need

Understanding the link from particle motions to the macroscopic material response is essential to develop accurate models for processes such as 3D printing with metal powders, pharmaceutical powder compaction, flow and handling of cereals in the alimentary industry, grinding and transport of construction materials. Discrete Element Method (DEM) has been used widely as the fundamental tool to produce the data to understand such link. However, DEM simulations are highly computationally intensive and some of the parameters used in the contact laws cannot be directly measured experimentally.

GrainLearning (Cheng et al., 2023) arises as a tool for Bayesian calibration of such computational models, which means the model parameters are estimated with a certain level of uncertainty, constrained on (noisy) real-world observations. Effectively, this makes the simulations digital twins of real-world processes with uncertainties propagated on model outputs, which then can be used for optimization or decision-making.

GrainLearning started in the geotechnical engineering community and was primarily used for granular materials in quasi-static, laboratory conditions (Cheng et al., 2018, 2019). These include triaxial (Hartmann et al., 2022; Li et al., 2024) and oedometric (Cheng et al., 2019) compressions of soil samples. In the particle technology community, attempts with GrainLearning have been made to identify contact parameters for polymer and pharmaceutical powders against angle-of-repose (Nguyen, 2022), shear cell (Thornton et al., 2023), and sintering experiments (Alvarez et al., 2022). Satisfactory results have been obtained in simulation cases where the grains were in dynamic regimes or treated under multi-physical processes.

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State of the field

Conventionally, the calibration of contact parameters at the grain scale is accomplished by trial and error, by comparing the macroscopic responses between simulation and experiments. This is due to the difficulty of obtaining precise measurements at the contact level and the randomness of grain properties (e.g., shape, stiffness, and asphericity). In the last decade, optimization (Do et al., 2018) and design-of-experiment (Hanley et al., 2011) approaches such as Latin Hypercube sampling and genetic algorithms have been used. However, the amount of model runs is still too large. For this reason, Gaussian process regression (Fransen et al., 2021) or artificial neural networks (Benvenuti et al., 2016) were tested as surrogate- or meta-models for the DEM. GrainLearning combines probabilistic learning of parameter space and sampling to achieve Bayesian optimization efficiently.

Functionality

- **Calibration**: By means of Sequential Monte Carlo filtering GrainLearning can infer and update model parameters. By learning the underlying distribution using a variational Gaussian model, highly probable zones are identified and sampled iteratively until a tolerance for the overall uncertainty is reached. This process requires the input of: a time series reference data, the ranges of the parameters to infer and a tolerance. The software iteratively minimizes the discrepancy between the model solution and the reference data.
- **Surrogate modeling**: Besides using direct simulation results (e.g. DEM) GrainLearning offers the capability of building surrogates (e.g. recurrent neural networks) as an alternative to computationally expensive DEM simulations, effectively reducing the cost by several orders of magnitude.

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