Gaussian Process based Surrogate Models for Polymer Rheology

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Objectives

Develop surrogate models (SMs) to emulate the input-output relationship of the molecular models (m) of polymer viscoelasticity (h), while requiring significantly less computational resources than m. Developed surrogate can be used for polymer design and characterisation under inverse problem setting. We *machine-learn* the SMs using Gaussian process (GP). Figure 1 illustrate the basis paradigm followed in this work.

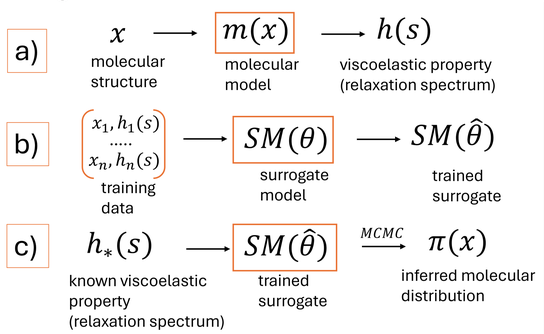

Figure 1: (a) Run the molecular model to gather the training data. (b) Build the surrogate model. (c) Use the trained surrogate to solve the inverse problem.

Gaussian Processes (GPs)

Gaussian process is a non-parametric non-linear regression/classification technique with built-in uncertainty quantification. In GP, any collection of random variable is specified by a Gaussian distribution. GP is specified by its mean $\mu(x)$ and kernel $k(x, x')$. The GP $f(x)$ is represented as,

$$f(x) \sim \mathcal{N}(\mu(x) = 0, k(x, x')). \quad (1)$$

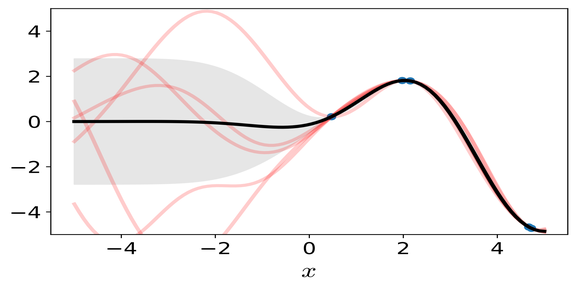

Figure 2: The figure shows a GP $f(x)$ fitted on input data (blue dots). The solid black line represents the predicted mean, and the shaded region indicates an interval of uncertainty around this mean. The red lines show five samples drawn from this GP.

Sparse Vector-Valued Data

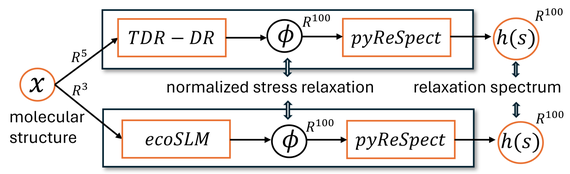

Figure 2: Physics based molecular models (TDD-DR and ecoSLM) used to generate vector-valued data.

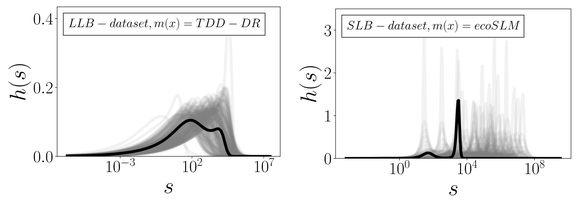

Figure 4: The dataset used in study: LLB (linear-linear polymer) and SLB(star-linear polymer).

Sparse : Dataset size is $\sim 10^2$ samples.

Surrogate Models (SMs)

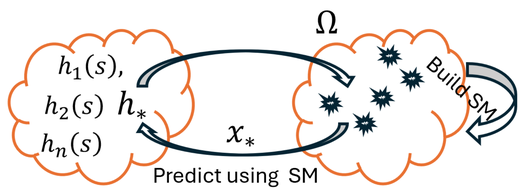

Figure 5: Using reduce order modelling $\boldsymbol{h}(\boldsymbol{s})$ is projected onto a lower-dimensional space Ω. The coefficients obtained from this projection act as inputs for a GP based surrogate. When a test point $\boldsymbol{x}_*$ is provided, the SM regress the corresponding coefficients and then converts them back to the initial space $\boldsymbol{h}_*(\boldsymbol{s})$.

GP based surrogates:

1. KLGP: GPR based on KL-expansion basis.
2. BSGP: GPR based on B-spline basis.
3. GPsep: GPR assuming a separable kernel. The co-variance between two points $\boldsymbol{x}$ and $\boldsymbol{x}'$, and at grid ($\boldsymbol{s}$) index i and j is simplified to: $k(\boldsymbol{x}, \boldsymbol{x}')_{ij} = k_s(i, j) \cdot k_x(\boldsymbol{x}, \boldsymbol{x}')$

Neural Network (MLP) based surrogates:

1. KLNN: NN based on KL expansion basis.
2. BSNN: NN based on B-spline basis.

Results-LLB

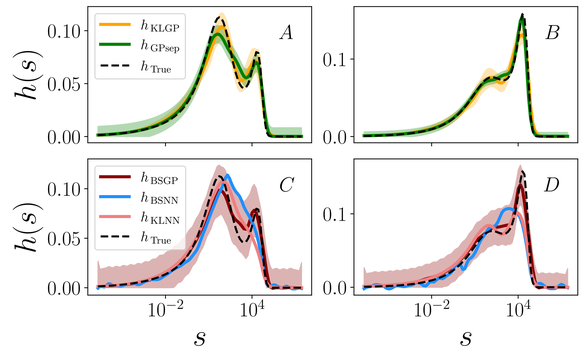

Figure 4: The predicted means (lines) and 95% confidence intervals (shaded regions) using GPsep (green), KLGP (orange) and BSGP (red) are compared with the true RS (dashed black line). The predicted mean is also shown for KLNN and BSNN. The two columns correspond to two different test points. KLGP offers the most calibrated confidence intervals. They reflects greater uncertainty in interesting regions relative to the smoother regions.

	$n_{\text{train}} = 101$
RMSE (KLGP)	$(2.95 \pm 0.10) \times 10^{-3}$
RMSE (GPsep)	$(2.93 \pm 0.13) \times 10^{-3}$
RMSE (BSGP)	$(3.86 \pm 0.14) \times 10^{-3}$
RMSE (BSNN)	$(9.79 \pm 0.27) \times 10^{-3}$
RMSE (KLNN)	$(6.14 \pm 0.27) \times 10^{-3}$
-	$n_{\text{train}} = 200$
RMSE (KLGP)	$(1.98 \pm 0.08) \times 10^{-3}$
RMSE (GPsep)	$(2.13 \pm 0.09) \times 10^{-3}$
RMSE (BSGP)	$(2.84 \pm 0.12) \times 10^{-3}$
RMSE (BSNN)	$(9.60 \pm 0.23) \times 10^{-3}$
RMSE (KLNN)	$(6.67 \pm 0.15) \times 10^{-3}$

Table 1: Average RMSE for test data using different SMs for the LLB dataset. n_{train} is training dataset size, and $n_{\text{test}} = 249$. Among GP-based SMs, KLGP performs relatively better (although statistical confidence is weak). All GP-based methods outperform the NN-based method with statistical significance.

Future Research

The surrogate model struggled with sharp peaks in the data. Consider exploring wavelet-based methods, which can adapt to such features. Explore B-spline methods that efficiently select node positions for bases. Additionally, explore neural network-based approaches for potential SMs.

Results-SLB

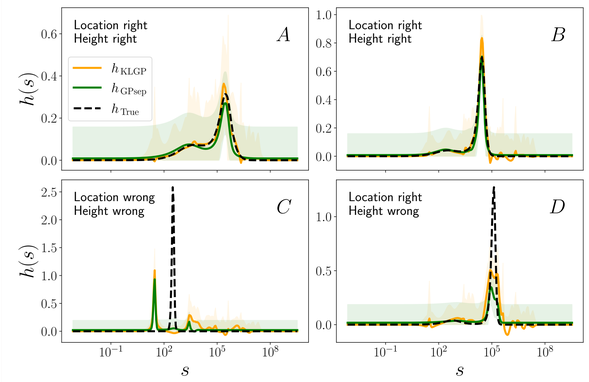

Figure 5: The predicted mean and 95% confidence intervals for GPsep and KLGP at four different test points are compared with the true RS (dashed black line). In the top row the location in height of the peak(s) are captured. In the bottom row, either location or height is captured as noted, but not both.

GPsep	$(7.68 \pm 1.42) \times 10^{-2}$
KLGP	$(7.01 \pm 1.80) \times 10^{-2}$
BSGP	$(6.25 \pm 1.55) \times 10^{-2}$
KLNN	$(9.81 \pm 1.88) \times 10^{-2}$
BSNN	$(8.53 \pm 1.65) \times 10^{-2}$

Table 2: Average RMSE for SLB test data using different SMs. $n_{\text{test}} = 16$.

prediction quality	KLGP		GPsep		BSGP	
	nsp	*sp*	*nsp*	*sp*	*nsp*	*sp*
good	9	-	4	-	9	-
fair	-	2	3	2	1	3
bad	3	2	5	2	2	1

prediction quality	KLNN		BSNN	
	nsp	*sp*	*nsp*	*sp*
good	1	-	-	-
fair	4	-	4	-
bad	7	4	8	4

Table 3: Qualitative assessment of different SM on a SLB test dataset with $n_{\text{test}} = 16$ samples. *sp* and *nsp* denote the presence or absence of sharp peaks in the test RS

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