Surrogate modelling for GISAXS reconstruction

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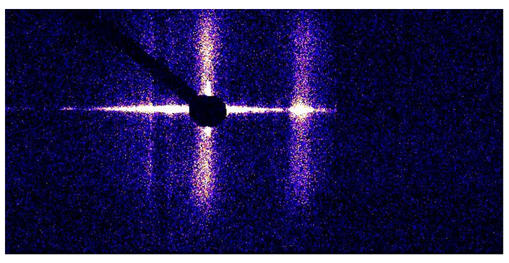
Experimental setup

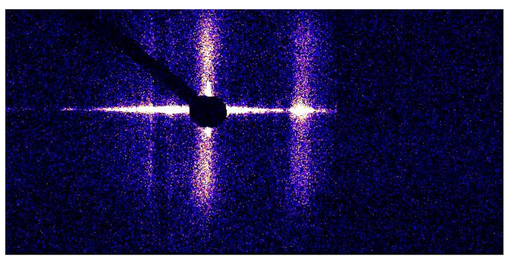
sample with parameters **y**

GISAXS experiment



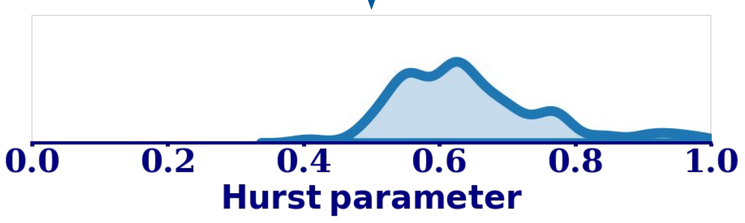
Experimental image $\mathbf{X}_{exp}$

Inverse problem



Experimental image $\mathbf{X}_{exp}$

estimate $\mathbf{p_f}(\mathbf{y}|\mathbf{X} = \mathbf{X_{exp}})$



Challenges

Inverse problem is **ill-posed**

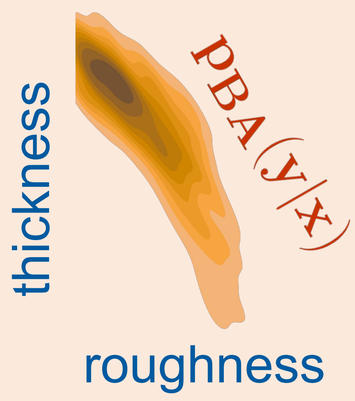
Posterior distribution is **complex** due to ambiguities

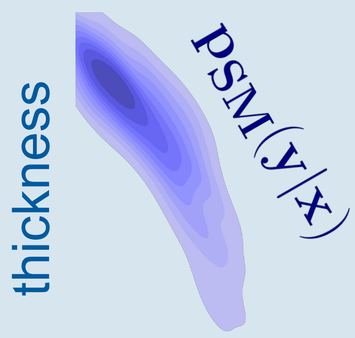
Reconstruction via simulation is highly **time-consuming**

Uncertainty estimation is desired

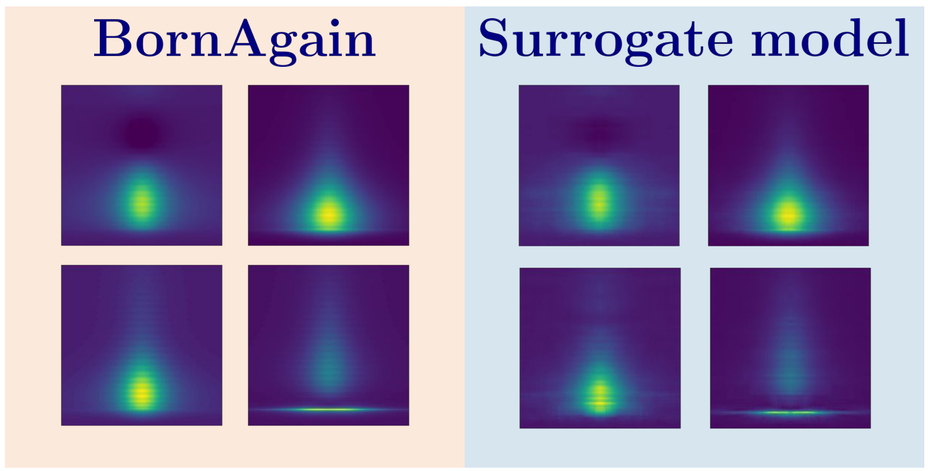
Solution: Approximate Bayes Computation + Surrogate model

Prior	Acceptance criterion	Posterior	Time
$\mathbf{y} \sim \mathbf{Uniform}(0, \mathbf{I})$	$\mathbf{BornAgain}\ [1]$ $\mathbf{f} : \mathbf{y} \rightarrow \mathbf{X}$	$\mathbf{p_{BA}}(\mathbf{y}\|\mathbf{x})$	50k samples **32 hours**
sample N times	$\|\mathbf{f}(\mathbf{y}) - \mathbf{X_{exp}}\| < \epsilon$		
	$\mathbf{Surrogate\ model}$ $\mathbf{f} : \mathbf{y}, \theta \rightarrow \mathbf{X}$	$\mathbf{p_{SM}}(\mathbf{y}\|\mathbf{x})$	50k samples **1 minute**





Simulation



Surrogate model

Convolutional neural network

Optimized via MSE loss

Wasserstein distance $\mathbf{W}_{|\mathbf{y}|}(\mathbf{p_{BA}}, \mathbf{p_{SM}}) = 0.03$

Summary

Interpretable and **trustworthy** reconstruction

Remarkable computation **time reduction** w.r.t. BornAgain

[1] Pospelov, Gennady et al. “BornAgain: software for simulating and fitting grazing-incidence small-angle scattering.” *Journal of Applied Crystallography* 53 (2020): 262 - 276.

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DRESDEN concept