Generative adversarial reduced order modeling

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Abstract

In this work, we present GAROM, a new approach for reduced order modeling (ROM) based on generative adversarial networks (GANs). GANs attempt to learn to generate data with the same statistics of the underlying distribution of a dataset, using two neural networks, namely discriminator and generator. While widely applied in many areas of deep learning, little research is done on their application for ROM, i.e. approximating a high-fidelity model with a simpler one. In this work, we combine the GAN and ROM framework, introducing a data-driven generative adversarial model able to learn solutions to parametric differential equations. In the presented methodology, the discriminator is modeled as an autoencoder, extracting relevant features of the input, and a conditioning mechanism is applied to the generator and discriminator networks specifying the differential equation parameters. We show how to apply our methodology for inference, provide experimental evidence of the model generalization, and perform a convergence study of the method.

Background and Goals

Reduced Order Modelling

⇒ ROMs are a class of techniques aimed to reduce the computational complexity of mathematical models, widely used in industry

⇒ The data driven discriminative ROM approach lacks of uncertainty quantification!

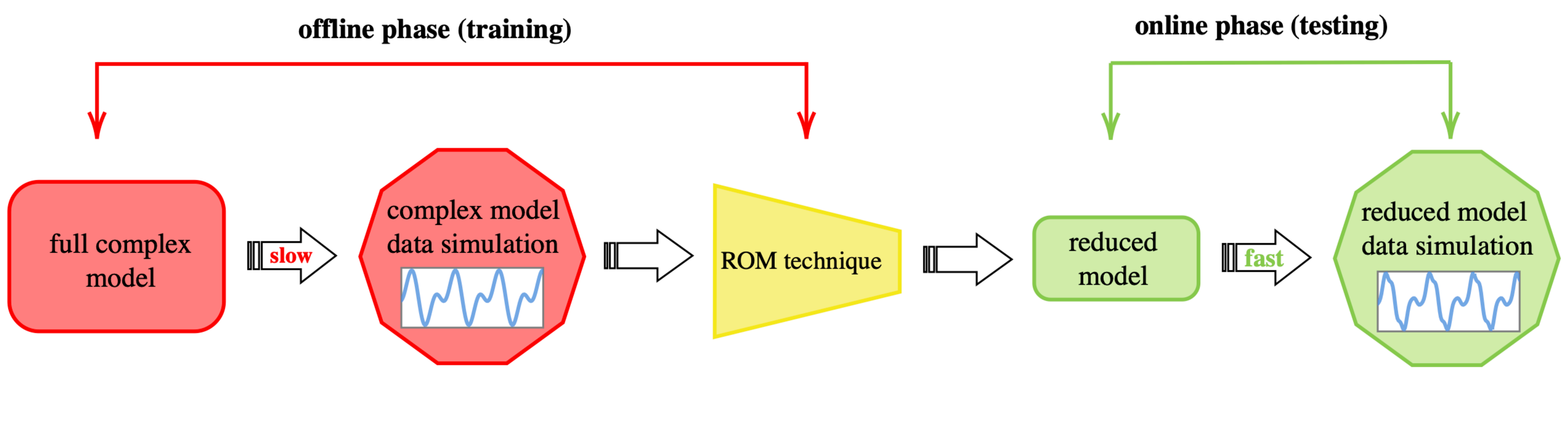


Figure 1: Data driven ROMs build a model by using only high fidelity data

Goal

⇒ Learn to a probabilistic reduced order model which can quantify the uncertainty for the generated snapshots while maintaining the accuracy of a discriminative model.

GAROM

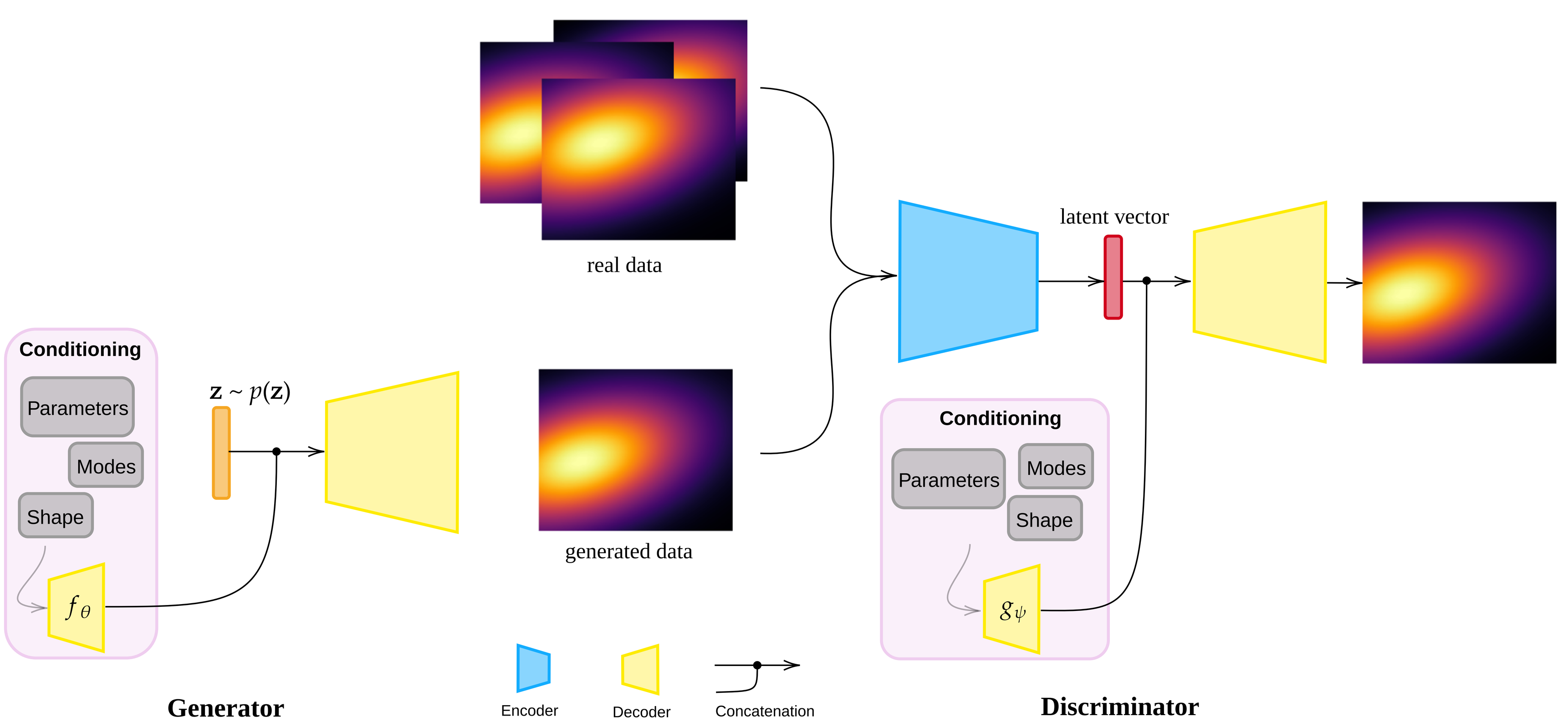
Distribution Learning

⇒ GAROM learns a distribution of numerical high fidelity solutions

- ⋆ $p(\mathbf{x}|\mathbf{c})$ distribution of high fidelity snapshots $\mathbf{x}$ given some conditioning $\mathbf{c}$
- ⋆ Generator $\mathcal{G}_\tau$ defines a probability distribution $p_{\mathcal{G}}(\mathbf{x}|\mathbf{z},\mathbf{c})$
- ⋆ Inference $\hat{\mathbf{x}} = \mathbb{E}_{\mathbf{x}\sim p_{\mathcal{G}}(\mathbf{x}|\mathbf{z},\mathbf{c})}[\mathbf{x}]$ is obtain by Monte Carlo approximation

⇒ Conditional BEGAN is used for adversarial learning

- ⋆ Generator $\mathcal{G}_\tau$ generates snapshots $\mathbf{x}$ given some conditioning $\mathbf{c}$
- ⋆ Discriminator $\mathcal{D}_\phi$ auto-encode snapshots given $\mathbf{c}$
- ⋆ Specific decoders f_θ and g_ψ for conditioning $\mathcal{G}_\tau$ and $\mathcal{D}_\phi$ respectively



Generative Adversarial Reduced Order Model

⇒ Autoencoder used as Discriminator $\mathcal{D}_\phi$, assigning low (high) reconstruction error to real (fake) ones. The objective is to learn the latent input representation only for real snapshots.

⇒ Final goal is to match the error distribution between real/fake reconstructed data

Autoencoder pixel-wise loss

$$\mathcal{L}(\mathbf{x} \mid \mathbf{c}) = |\mathbf{x} - \mathcal{D}_\phi(\mathbf{x} \mid \mathbf{c})|, \quad \mathbf{x} \text{ sample}$$

GAROM objective

$$\begin{cases} \mathcal{L}_{\mathcal{D}}(\phi) = \mathcal{L}(\mathbf{x} \mid \mathbf{c}) - k_t\, \mathcal{L}(\mathcal{G}_\tau(\mathbf{z} \mid \mathbf{c})) & \text{minimize } \phi \\ \mathcal{L}_{\mathcal{G}}(\tau) = \mathcal{L}(\mathcal{G}_\tau(\mathbf{z} \mid \mathbf{c})) + \eta|\mathbf{x} - \mathcal{G}_\tau(\mathbf{z} \mid \mathbf{c})| & \text{minimize } \tau \\ k_{t+1} = k_t + \lambda_k(\gamma\mathcal{L}(\mathbf{x} \mid \mathbf{c}) - \mathcal{L}(\mathcal{G}_\tau(\mathbf{z} \mid \mathbf{c}))) & \end{cases}$$

where $\gamma \in [0,1]$ is used to maintain an equilibrium between $\mathcal{G}_\tau$ and $\mathcal{D}_\phi$, and $\eta = \{0,1\}$ depending if the solution given a parameter is unique.

Numerical results

Uncertainty Quantification

⇒ The variance $Var(\mathbf{x}) = \mathbb{E}_{\mathbf{x}\sim p_{\mathcal{G}}(\mathbf{x}|\mathbf{z},\mathbf{c})}[(\mathbf{x}-\hat{\mathbf{x}})^2]$ gives an estimate of the model epistemic uncertainty and can be efficiently computed by Monte Carlo integration.

⇒ Analytical error bounds in probability can be computed using Markov Inequality or Probability Confidence Regions.

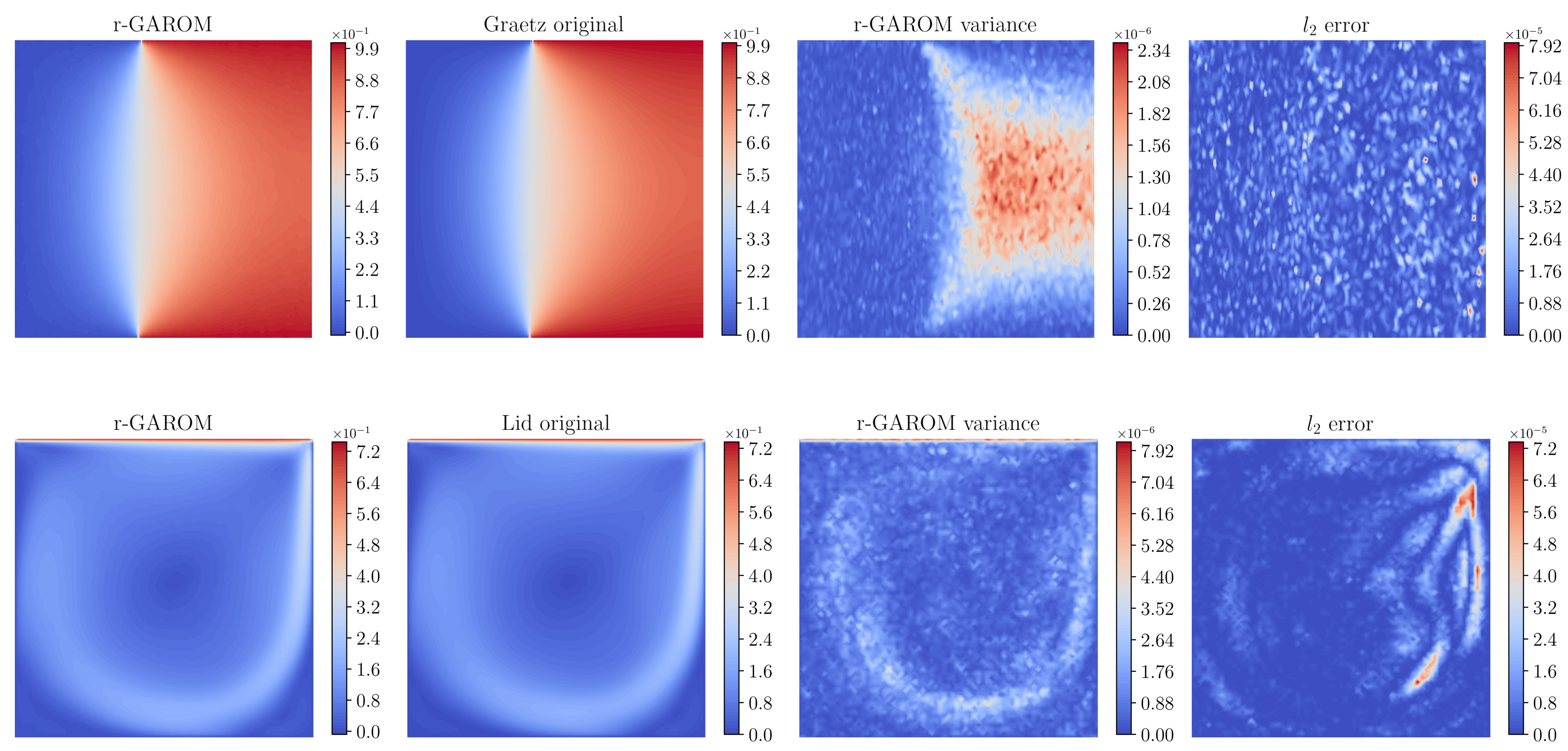


Figure 2: Image of the generated snapshot with its associated variance representing the magnitude of the unknown field for a testing parameter in a Lid Cavity experiment varying Re number, and Graetz Problem varying the geometry and Péclet number.

Predictive Distribution

⇒ GAROM performs similarly to SOTA methods, surpassing DL surrogate solvers in six out of nine tests.

⇒ Possibility to obtain an uncertainty to the results, while not possible with discriminative SOTA methods.

Method	Gaussian			Graetz			Lid Cavity		
	4	16	64	16	64	120	16	64	120
GAROM	(1.05 ± 0.17)	(0.77 ± 0.20)	(0.88 ± 0.16)	(0.58 ± 0.16)	(0.55 ± 0.14)	(0.51 ± 0.1)	(10.7 ± 0.22)	(9.50 ± 0.15)	(9.91 ± 0.17)
r-GAROM	$(\mathbf{0.80 \pm 0.15})$	(0.60 ± 0.14)	(0.65 ± 0.14)	$(\mathbf{0.32 \pm 0.09})$	$(\mathbf{0.22 \pm 0.05})$	$(\mathbf{0.20 \pm 0.04})$	(5.02 ± 0.11)	(3.41 ± 0.04)	(3.61 ± 0.06)
cGAN	(7.72 ± 0.30)	(7.72 ± 0.30)	(7.72 ± 0.30)	(21.3 ± 1.10)	(21.3 ± 1.10)	(21.3 ± 1.10)	(68.5 ± 1.55)	(68.5 ± 1.55)	(68.5 ± 1.55)
r-cGAN	(6.04 ± 0.27)	(6.04 ± 0.27)	(6.04 ± 0.27)	(1.65 ± 0.05)	(1.65 ± 0.05)	(1.65 ± 0.05)	(51.6 ± 1.11)	(51.6 ± 1.11)	(51.6 ± 1.11)
POD–RBF	15.4	**0.41**	**0.25**	0.48	0.48	0.49	**2.98**	**1.45**	**1.32**
POD–NN	15.4	1.30	1.12	0.41	0.47	0.44	3.02	2.73	3.20
AE–RBF	2.06	0.89	1.00	1.08	1.42	1.60	6.96	3.01	3.90
AE–NN	1.76	1.04	1.12	1.14	1.56	2.71	3.49	3.27	3.83
DeepONet	36.1	36.1	36.1	0.73	0.73	0.65	72.2	72.2	72.2
NOMAD	1.99	1.99	1.99	0.36	0.36	0.36	63.4	63.4	63.4

Table 1: Accuracy comparison for different test cases, methods, and latent dimensions. The table reports the mean l_2 relative error ϵ (in percent).

Conclusions

⇒ A generative model approach for reduced order modelling (GAROM) is presented

⇒ Conditional BEGAN used for adversarial learning, with the discriminator autoencoding high fidelity snapshots

⇒ Model epistemic uncertainty is easy quantifiable due to the probabilistic nature of the model

⇒ Results are comparable (and for some problems better) in accuracy to state of the art methods for a variety of benchmarks

⇒ Possibility to enhance the general method by: applying different conditioning mechanisms (modes, shapes), benchmarking the reconstruction capacity on noisy data, varying the generator and discriminator structure to handle scatter data points

References

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[3] David Berthelot, Thomas Schumm, and Luke Metz. Began: Boundary equilibrium generative adversarial networks. *arXiv preprint arXiv:1703.10717*, 2017.