Bayesian Optimization on Large Graphs via a Graph Convolutional Generative Model: Application in Cardiac Model Personalization

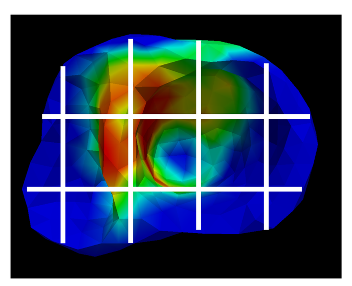
Jwala Dhamala[1], Sandesh Ghimire[1], John L. Sapp[2], B. Milan Horacek[2], and Linwei Wang[1]

Rochester Institute of Technology[1], New York, USA
Dalhousie University[2], Halifax, Canada

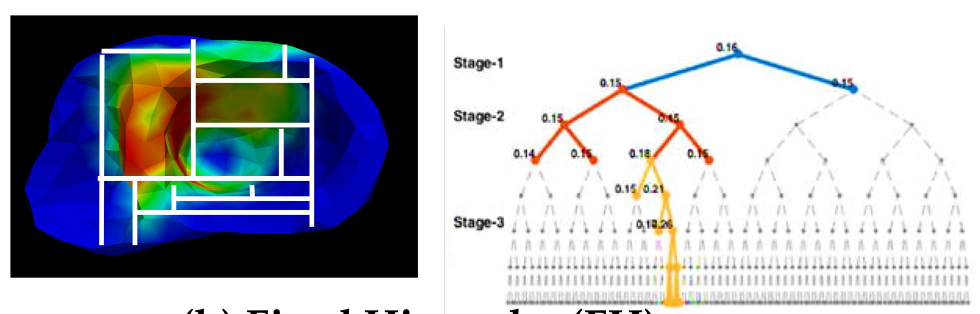
Overview

- Personalized virtual hearts are important for personalized medicine.
- Estimating **high dimensional (HD)** spatially distributed tissue properties from sparse, noisy, and indirect data is a challenge.
- **Novel framework:**
  - A novel graph convolutional variational auto-encoder (VAE) to allow generative modeling of non-Euclidean data
  - Embed a VAE into the objective function of Bayesian Optimization, providing an implicit low-dimensional (LD) search space that represents the generative code of the HD tissue properties defined over a graph.

Related Works

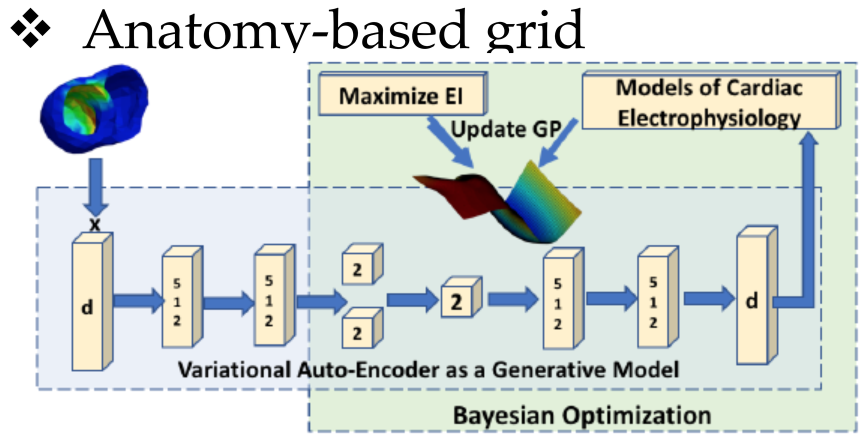


(a) Fixed segments (FS)



(b) Fixed Hierarchy (FH)

- Anatomy-based grid



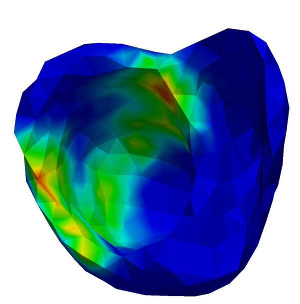
- **Incorporate anatomical knowledge in VAE**
- **Exploit spatial proximity and hierarchical composition information**

- Data-driven generative model of HD tissue properties

Personalization of Model Parameters

- HD parameter estimation as optimization problem:

$$\hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} -||\mathbf{Y} - M(\boldsymbol{\theta})||^2$$



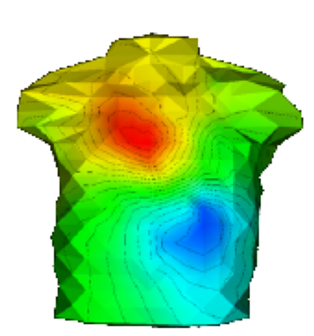
Cardiac Electrophysiological Model

$$\partial u/\partial t = \nabla(\mathbf{D}\nabla u) - cu(u-\theta)(u-1) - uv,$$
$$\partial v/\partial t = \varepsilon(u,v)(-v - cu(u-\theta-1)).$$

Here, u is the transmembrane action potential and $\boldsymbol{\theta}$ parameter being estimated is associated with ischemic severity.

Forward Model

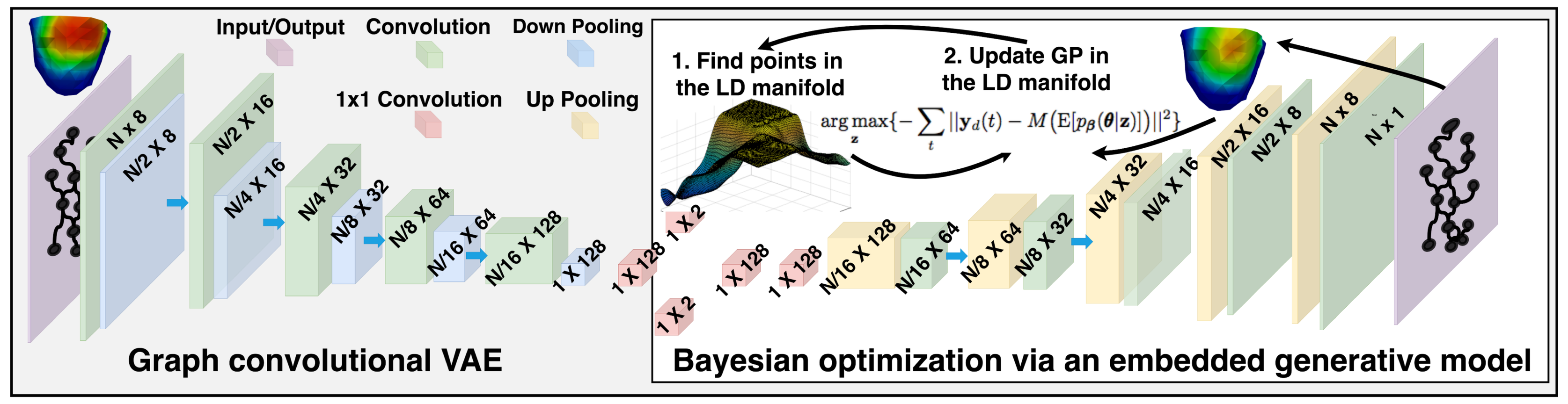
$$\mathbf{Y} = \mathbf{HU}(\boldsymbol{\theta}),$$



where H is transfer matrix, U is transmural action potential and Y is ECG signals.

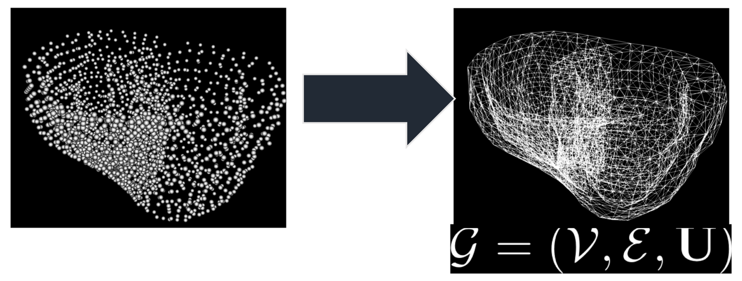
Complex objective function!

Graph Convolutional Variational Autoencoder



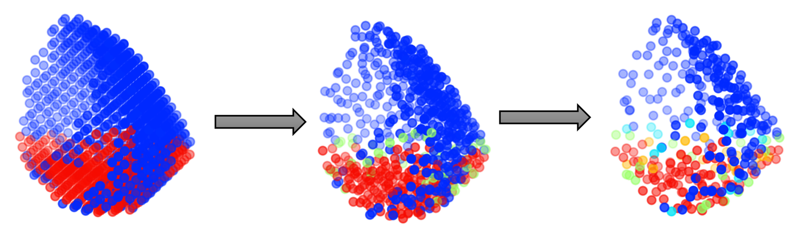
$$\mathcal{L}(\alpha;\beta;\boldsymbol{\theta}^{(i)}) = -D_{\mathrm{KL}}(q_{\boldsymbol{\alpha}}(\mathbf{z}|\boldsymbol{\theta}^{(i)})||p_{\boldsymbol{\beta}}(\mathbf{z})) + E_{q_{\alpha}(\mathbf{z}|\boldsymbol{\theta}^{(i)})}[\log p_{\boldsymbol{\beta}}(\boldsymbol{\theta}^{(i)}|\mathbf{z})]$$

Local Connectivity and Graph Convolution



Vertices : N nodes in the mesh
Edges : Using K nearest neighbors
Edge attribute: normalized $[x_i - x_j, y_i - y_j, z_i - z_j]$ or 0 if no edge

Hierarchical Compositionality and Pooling



Multilevel graph clustering with Graclus

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}_{N_1 \times N_2} \qquad \mathbf{P}_n = \begin{pmatrix} .5 & 0 & 0 & 0 \\ .5 & 0 & 0 & 0 \\ 0 & .5 & 0 & 0 \\ 0 & .5 & 0 & 0 \\ 0 & 0 & .5 & 0 \\ 0 & 0 & .5 & 0 \end{pmatrix}$$

Pooling: $\mathbf{F} = \mathbf{P}\mathbf{F}_c$ **Un-pooling:** $\mathbf{F}_c = \mathbf{P}_n^{T}\mathbf{F}$

Bayesian Optimization with Embedded VAE

Represent θ with the expectation of probabilistic generator :

$$\hat{\mathbf{z}} = \arg\max_{\mathbf{z}} -||\mathbf{Y} - M\left(\mathrm{E}[p_{\boldsymbol{\beta}}(\boldsymbol{\theta}|\mathbf{z})]\right)||^2$$

Embed HD search in LD latent space

$$\mathrm{EI}(\mathbf{z}) = (\mu(\mathbf{z}) - f_m)\Phi\left(\frac{\mu(\mathbf{z}) - f_m}{\sigma(\mathbf{z})}\right) + \sigma(\mathbf{z})\phi\left(\frac{\mu(\mathbf{z}) - f_m}{\sigma(\mathbf{z})}\right)$$

Summary

- Novel graph convolutional VAE for HD Bayesian optimization of model parameters
- **Future works:** incorporate uncertainty from probablistic generative model, training data from MRI and feature sharing across geometries.

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Synthetic Experiments

- Dataset synthetically generated by random region growing on patient-specific mesh
- Training data ~ 78, 208 & Testing/Validation data ~ 13,545
- B-spline basis of degree m=1 with kernel $k_1 = k_2 = k_3 = 5$
- Adam optimizer, initial learning rate = 0.001

gVAE as a Generative Model

	SSE					DC					Trainable parameters
Anatomy	1	2	3	4	5	1	2	3	4	5	
PCA	12.73	14.18	12.35	23.85	23.26	39.80	39.87	41.31	49.17	54.42	NA
fVAE-3h [6]	8.03	8.45	8.44	13.07	13.70	61.77	66.20	60.45	70.30	70.72	2,087,822
fVAE-4h	7.97	8.29	8.33	12.47	13.99	61.76	64.60	61.58	71.51	69.84	2,613,134
fVAE-5h	7.42	8.01	8.19	13.96	12.41	64.59	65.72	62.21	68.04	74.50	3,138,446
gVAE	**6.66**	**6.89**	**6.79**	**11.28**	**11.43**	**68.43**	**70.92**	**70.70**	**75.10**	**76.86**	2,778,069

Table 1: Comparison of reconstruction accuracy

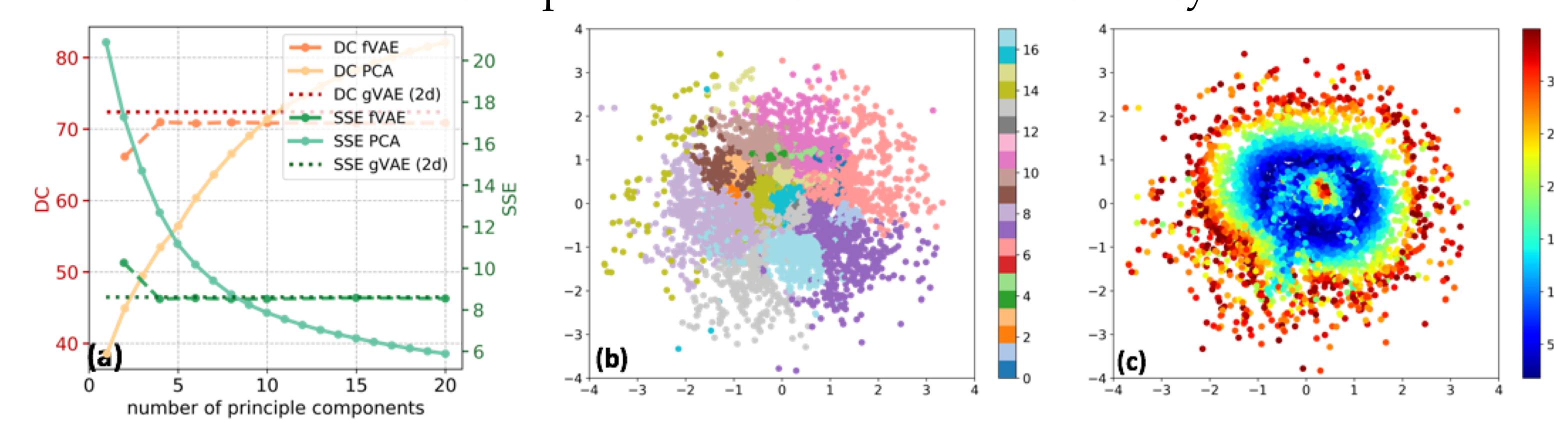
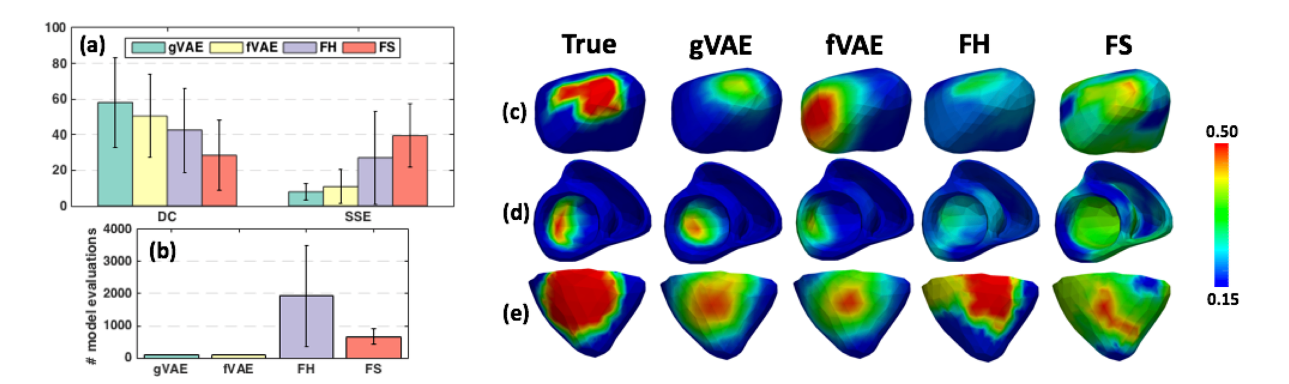
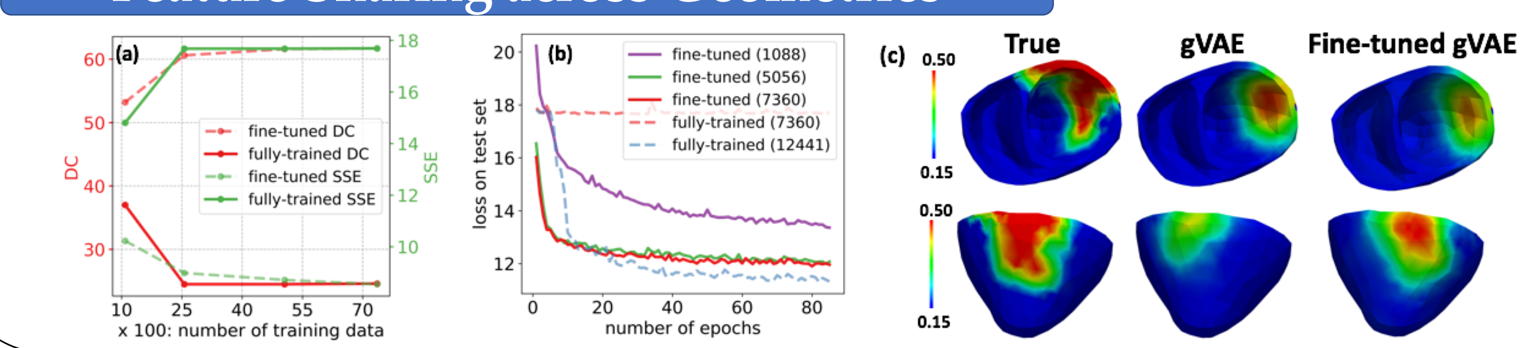


Fig. 2: (a) Comparison of reconstruction accuracy using gVAE with a 2d manifold vs. PCA and fVAE with various-dimensional manifolds. (b)-(c): Plots of 2d latent codes from gVAE colored by infarct location (b) and infarct size (c).

gVAE-based Parameter Optimization

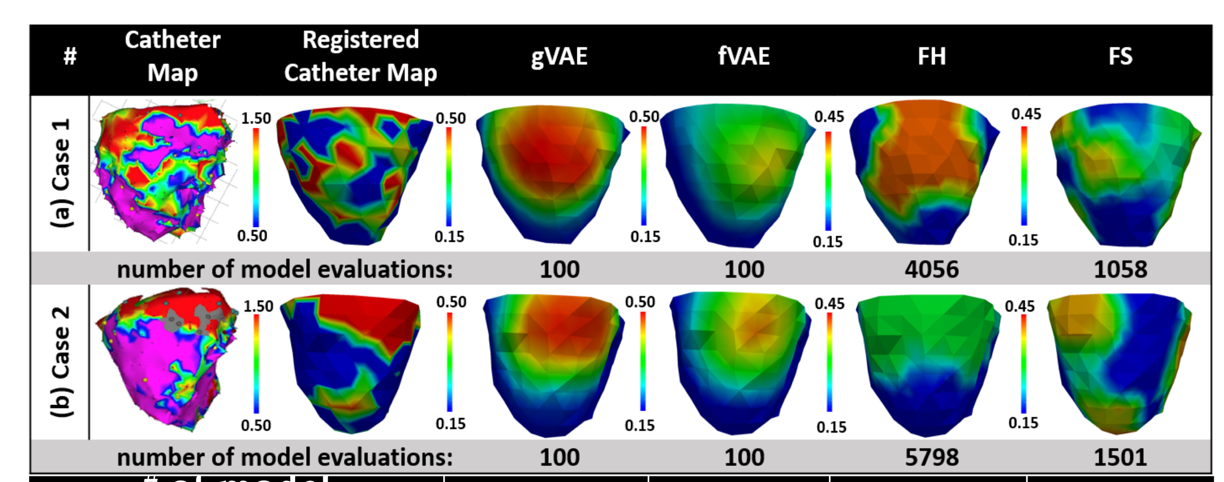


Feature Sharing across Geometries



Real-data Experiments

- Two patients with previous myocardial infraction
- Data: 120-lead ECG data.



# of model evaluations	gVAE	fVAE	FH	FS
Case 1	100	100	5798	1501
Case 2	100	100	4056	1058