# Learning Material Manifold for Efficient Space Exploration

CS 482 mid-term project presentation

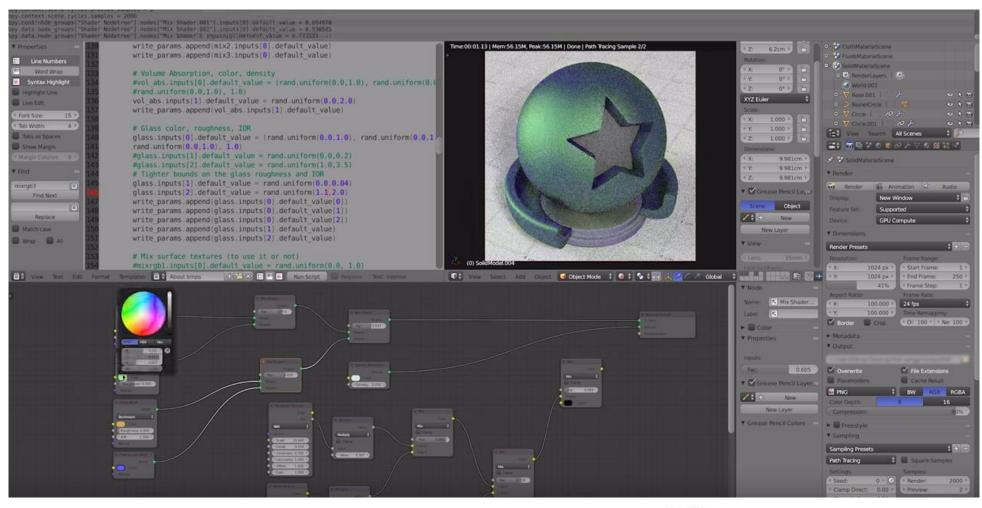
MinKu Kang

# Material Synthesis



a scene with metals and minerals, translucent, glittery and glassy materials more than a hundred synthesized materials and objects for the vegetation of the planet

### Manual Material Synthesis is Labor-intensive



It might be a well fit for an expert, but ...

 $\mathbf{x}_i \in \mathbb{R}^m$  Many parameters to tune.

From Authors Video: https://www.youtube.com/watch?v=6FzVhIV\_t3s

# Stage 1: A User Scores a Gallery







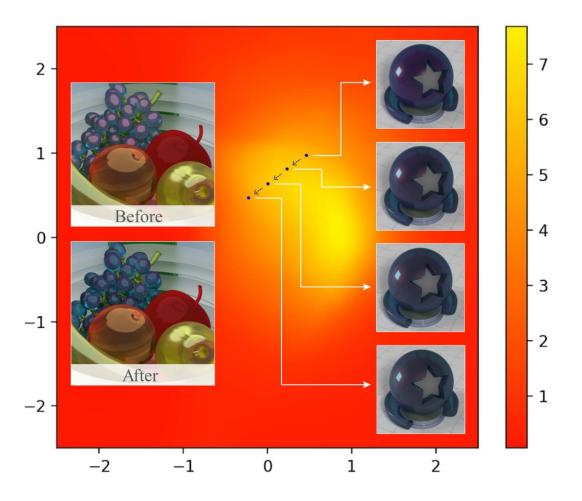
From Authors Video: https://www.youtube.com/watch?v=6FzVhIV\_t3s

Cons: It is hard for a user to assign dense scores to every candidates with high accuracy Improvement: Let the user just perform binary selections (select or not)

# Stage 2: Recommendations are Generated

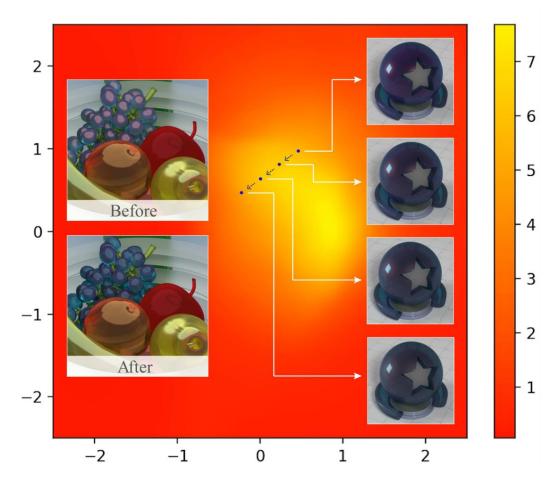


# Stage 3: Fine-searching in Latent Space



Cons: While GP-based methods are good in sample efficiency, the time complexity is high Improvement: Adopt recent manifold learning (dimensionality reduction) techniques (e.g., GAN)

# Latent Space Exploration



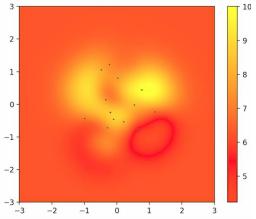
Low-dimensional latent space (m=2), with color representing score. GPLVM (Gaussian Process Latent Variable Model)

A few tens of high-scoring materials from the gallery are embedded into the low-dimensional latent space.

$$\mathbf{X} = \begin{bmatrix} \cdots \mathbf{x}_i \cdots \end{bmatrix}^T \text{ with } \mathbf{x}_i \in \mathbb{R}^m$$

$$\mathbf{L} = \begin{bmatrix} \cdots \mathbf{l}_i \cdots \end{bmatrix}^T \text{ with } \mathbf{l}_i \in \mathbb{R}^l$$

$$m \gg l$$



# GPR family requires kernel, and it is expensive

$$k(\mathbf{x}, \mathbf{x'}) = \sigma_f^2 \exp \left[ -\frac{(\mathbf{x} - \mathbf{x'})^2}{2l^2} \right] + \beta^{-1} \delta_{xx'}$$

$$\mathbf{K} = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & k(\mathbf{x}_1, \mathbf{x}_2) & \dots & k(\mathbf{x}_1, \mathbf{x}_n) \\ k(\mathbf{x}_2, \mathbf{x}_1) & k(\mathbf{x}_2, \mathbf{x}_2) & \dots & k(\mathbf{x}_2, \mathbf{x}_n) \\ \vdots & \vdots & \ddots & \vdots \\ k(\mathbf{x}_n, \mathbf{x}_1) & k(\mathbf{x}_n, \mathbf{x}_2) & \dots & k(\mathbf{x}_n, \mathbf{x}_n) \end{bmatrix}$$
Conditional distribution of the co

$$\mathbf{k}_* = \left[k(\mathbf{x}^*, x_1), k(\mathbf{x}^*, x_2), \dots, k(\mathbf{x}^*, x_n)\right]^T$$

Kernel function, Kernel matrix

**Joint** distribution over scores

$$\begin{bmatrix} \mathbf{U} \\ u(\mathbf{x}^*) \end{bmatrix} \sim \mathcal{N} \left( 0, \begin{bmatrix} \mathbf{K} & \mathbf{k}_*^T \\ \mathbf{k}_* & k_{**} \end{bmatrix} \right)$$

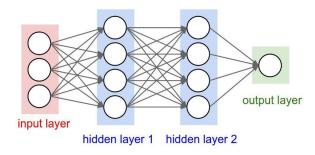
Conditional distribution over scores given observations

$$u(\mathbf{x}^*) = \mathbf{k}_*^T \mathbf{K}^{-1} \mathbf{U},$$
  
$$\sigma(u(\mathbf{x}^*)) = k_{**} - \mathbf{k}_* \mathbf{K}^{-1} \mathbf{k}_*^T$$

# Parametric vs. Non-parametric

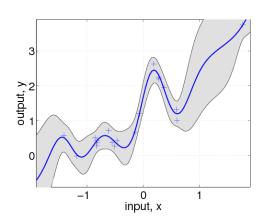
# observations is quite small (= # material-score pairs labeled by the user), which is in the order of a few of tens.

#### **Parametric Model**



Data is absobed into the weights: new prediction is affected by the estimated parameter. It requires many samples for an accurate parameter estimation

#### **Non-parametric Model**



'Let the data speaks'
: new prediction is
highly affected by the
past observations

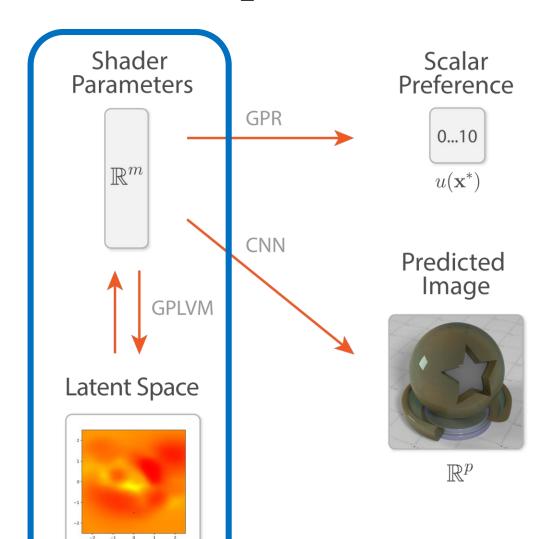
$$\mathbf{K} = \begin{bmatrix} k(\mathbf{x}_{1}, \mathbf{x}_{1}) & k(\mathbf{x}_{1}, \mathbf{x}_{2}) & \dots & k(\mathbf{x}_{1}, \mathbf{x}_{n}) \\ k(\mathbf{x}_{2}, \mathbf{x}_{1}) & k(\mathbf{x}_{2}, \mathbf{x}_{2}) & \dots & k(\mathbf{x}_{2}, \mathbf{x}_{n}) \\ \vdots & \vdots & \ddots & \vdots \\ k(\mathbf{x}_{n}, \mathbf{x}_{1}) & k(\mathbf{x}_{n}, \mathbf{x}_{2}) & \dots & k(\mathbf{x}_{n}, \mathbf{x}_{n}) \end{bmatrix}$$

$$\mathbf{k}_{*} = \begin{bmatrix} k(\mathbf{x}^{*}, x_{1}), k(\mathbf{x}^{*}, x_{2}), \dots, k(\mathbf{x}^{*}, x_{n}) \end{bmatrix}^{T}$$

$$u(\mathbf{x}^{*}) = \mathbf{k}_{*}^{T} \mathbf{K}^{-1} \mathbf{U},$$

$$\sigma(u(\mathbf{x}^{*})) = k_{**} - \mathbf{k}_{*} \mathbf{K}^{-1} \mathbf{k}_{*}^{T}$$

# The Component of Interest

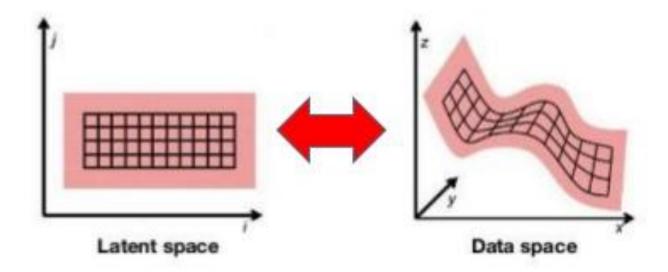


- 1. **GPR** is used to learn the user-specified material preferences
- 2. The system **recommends** new **materials** with **visualization**

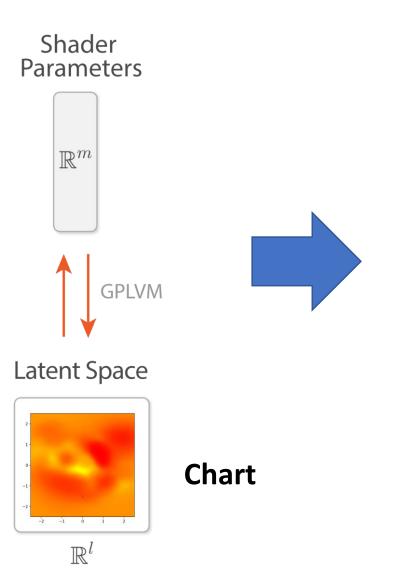
3. Optionally, GPLVM can be used to provide an intuitive 2D space for variant generation.

### Manifold Assumption

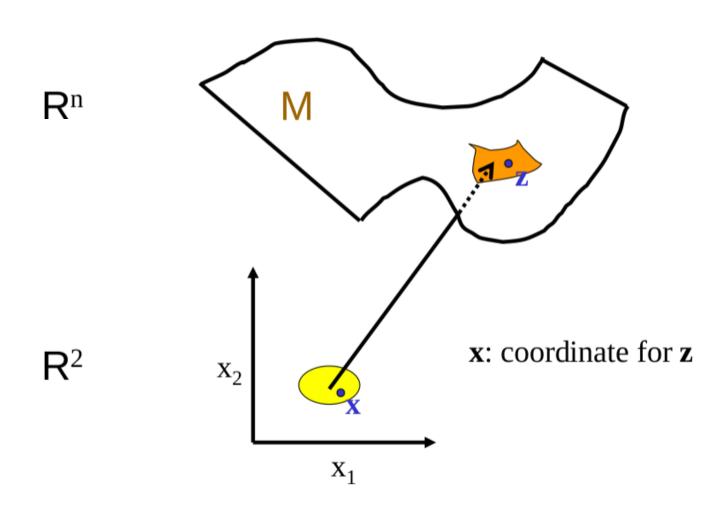
- Data lie approximately on a manifold of much lower dimension than the input space
- Mapping between two space is unique & reversible



# Goal of the Project



- 1. Find (learn) a meaningful manifold
- 2. Find (learn) a **mapping** between the lowdimensional chart and the manifold



# Manifold Learning

### Why Dimensionality Reduction?

- Most machine learning and data mining techniques may not be effective for highdimensional data
  - Curse of Dimensionality
  - Query accuracy and efficiency degrade rapidly as the dimension increases.
- The intrinsic dimension may be small.
  - For example, the number of genes responsible for a certain type of disease may be small.

### Why Dimensionality Reduction?

 Visualization: projection of high-dimensional data onto 2D or 3D.

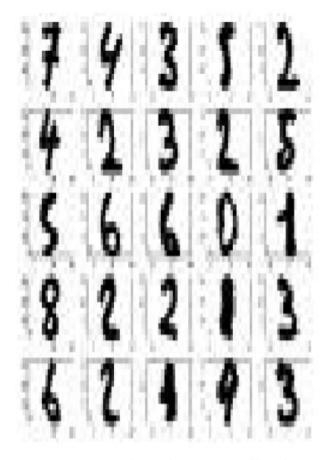
 Data compression: efficient storage and retrieval.

Noise removal: positive effect on query accuracy.

# Other Types of High-Dimensional Data



Face images



Handwritten digits

### Feature Reduction Algorithms

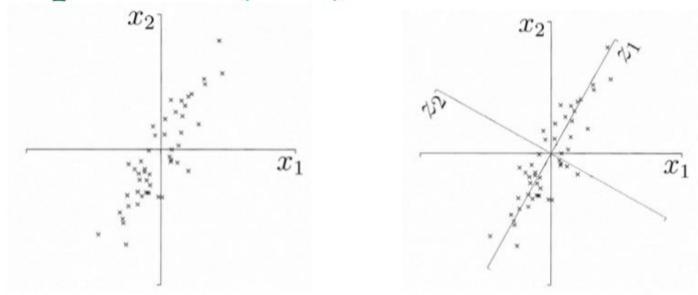
#### Linear

- Latent Semantic Indexing (LSI): truncated
   SVD
- Principal Component Analysis (PCA)
- Linear Discriminant Analysis (LDA)
- Canonical Correlation Analysis (CCA)
- Partial Least Squares (PLS)

#### Nonlinear

- Nonlinear feature reduction using kernels
- Manifold learning

# Geometric Picture of Principal Components (PCs)



- the 1<sup>st</sup> PC  $Z_1$  is a minimum distance fit to a line in X space
- the  $2^{nd}$  PC  $z_2$  is a minimum distance fit to a line in the plane perpendicular to the  $1^{st}$  PC

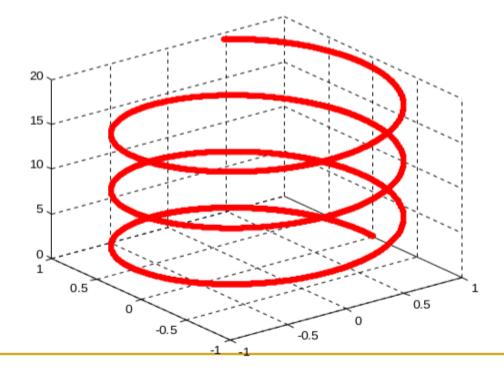
PCs are a series of linear least squares fits to a sample, each orthogonal to all the previous.

### **Deficiencies of Linear Methods**

 Data may not be best summarized by linear combination of features

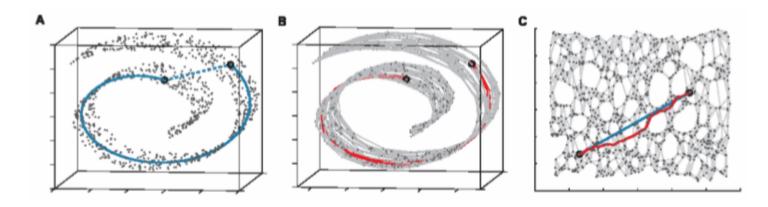
Example: PCA cannot discover 1D structure of a

helix



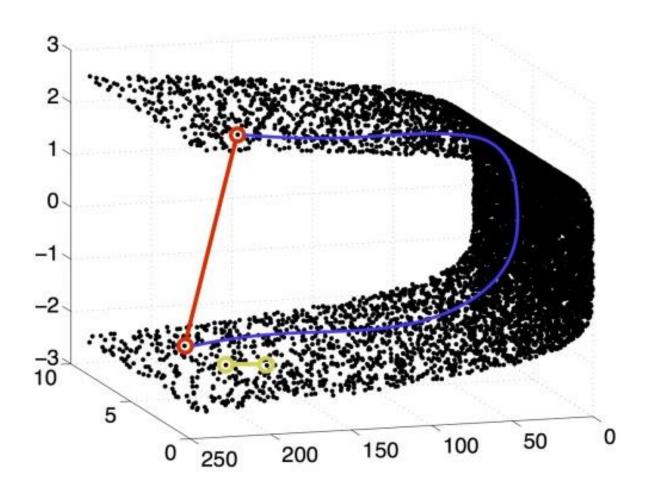
# Nonlinear Approaches- Isomap

Josh. Tenenbaum, Vin de Silva, John langford 2000



- Constructing neighbourhood graph G
- For each pair of points in G, Computing shortest path distances ---- geodesic distances.
- Use Classical MDS with geodesic distances.
   Euclidean distance → Geodesic distance

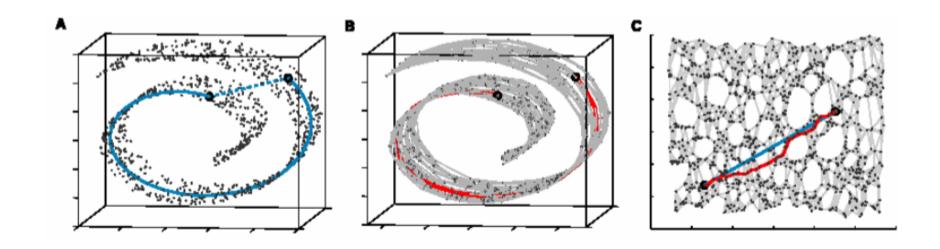
# Intrinsic Geometrical Property



# Construct Neighborhood Graph G

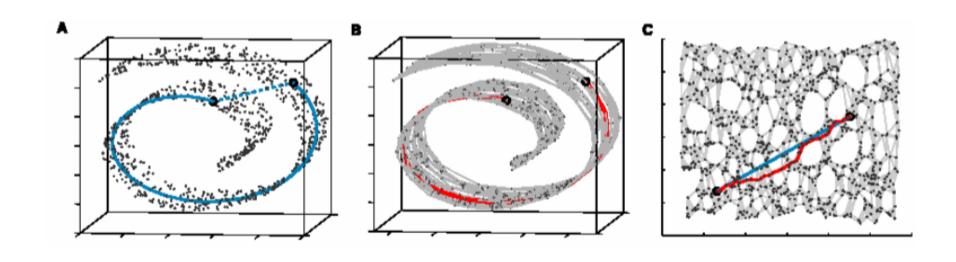
K- nearest neighborhood (K=7)

D<sub>G</sub> is 1000 by 1000 (Euclidean) distance matrix of two neighbors (figure A)



# Compute All-Points Shortest Path in G

Now  $D_G$  is 1000 by 1000 geodesic distance matrix of two arbitrary points along the manifold (figure B)



# Isomap: Advantages

- Nonlinear
- Globally optimal
  - Still produces globally optimal low-dimensional Euclidean representation even though input space is highly folded, twisted, or curved.
- Guarantee asymptotically to recover the true dimensionality.

# Isomap: Disadvantages

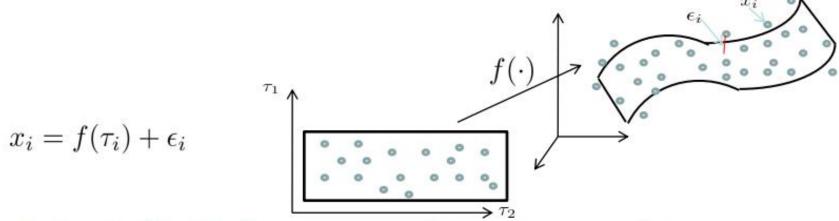
May not be stable, dependent on topology of data

- Guaranteed asymptotically to recover geometric structure of nonlinear manifolds
  - As N increases, pairwise distances provide better approximations to geodesics, but cost more computation
  - If N is small, geodesic distances will be very inaccurate.

# More formally,

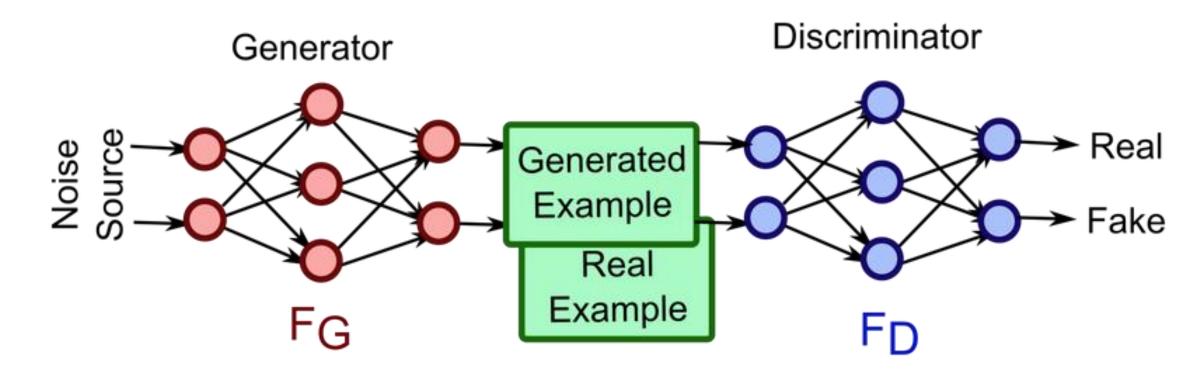
# What is manifold learning?

• A d dimensional manifold  $\mathcal M$  is embedded in an m-dimensional space, and there is an explicit mapping  $f:\mathcal R^d\to\mathcal R^m$  where  $d\le m$ . We are given samples  $x_i\in\mathcal R^m$  with noise .



•  $f(\cdot)$  is called *embedding function*, m is the *extrinsic dimension*, d is the *intrinsic dimension* or dimension of the latent space.

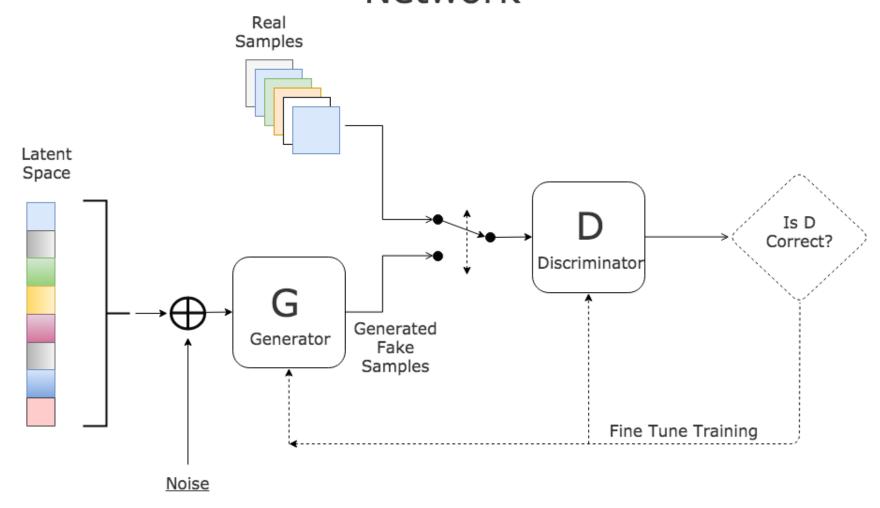
### Generative Adversarial Networks



https://akshaynathr.wordpress.com/2018/01/02/gan-generative-adversarial-network/

Goodfellow, Ian; Pouget-Abadie, Jean; Mirza, Mehdi; Xu, Bing; Warde-Farley, David; Ozair, Sherjil; Courville, Aaron; Bengio, Yoshua (2014). "Generative Adversarial Networks".

### Generative Adversarial Network

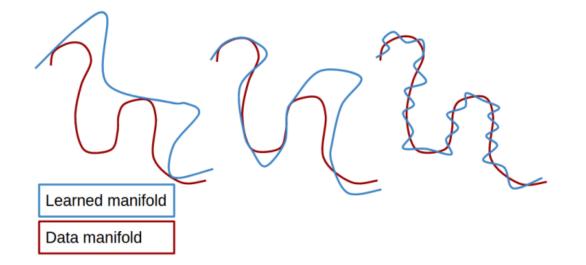


https://stats.stackexchange.com/questions/277756/some-general-questions-on-generative-adversarial-networks

# Manifold Learning through GAN?

#### **Implicit Manifold Learning on Generative Adversarial Networks**

Kry Yik Chau Lui <sup>1</sup> Yanshuai Cao <sup>1</sup> Maxime Gazeau <sup>1</sup> Kelvin Shuangjian Zhang <sup>1</sup>

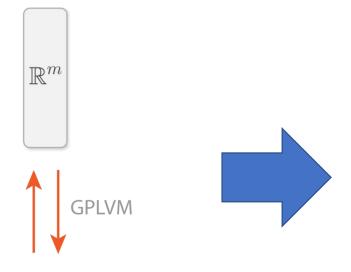


<sup>&</sup>lt;sup>1</sup>Borealis AI, Toronto, Canada. Correspondence to: Kry Yik Chau Lui <yikchau.y.lui@rbc.com>.

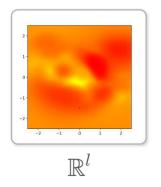
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# Goal of the Project

Shader Parameters



**Latent Space** 



- 1. Find (learn) a meaningful manifold
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