Dimensionality and Curvature Selection of Graph Embedding using Decomposed Normalized Maximum Likelihood Code-Length

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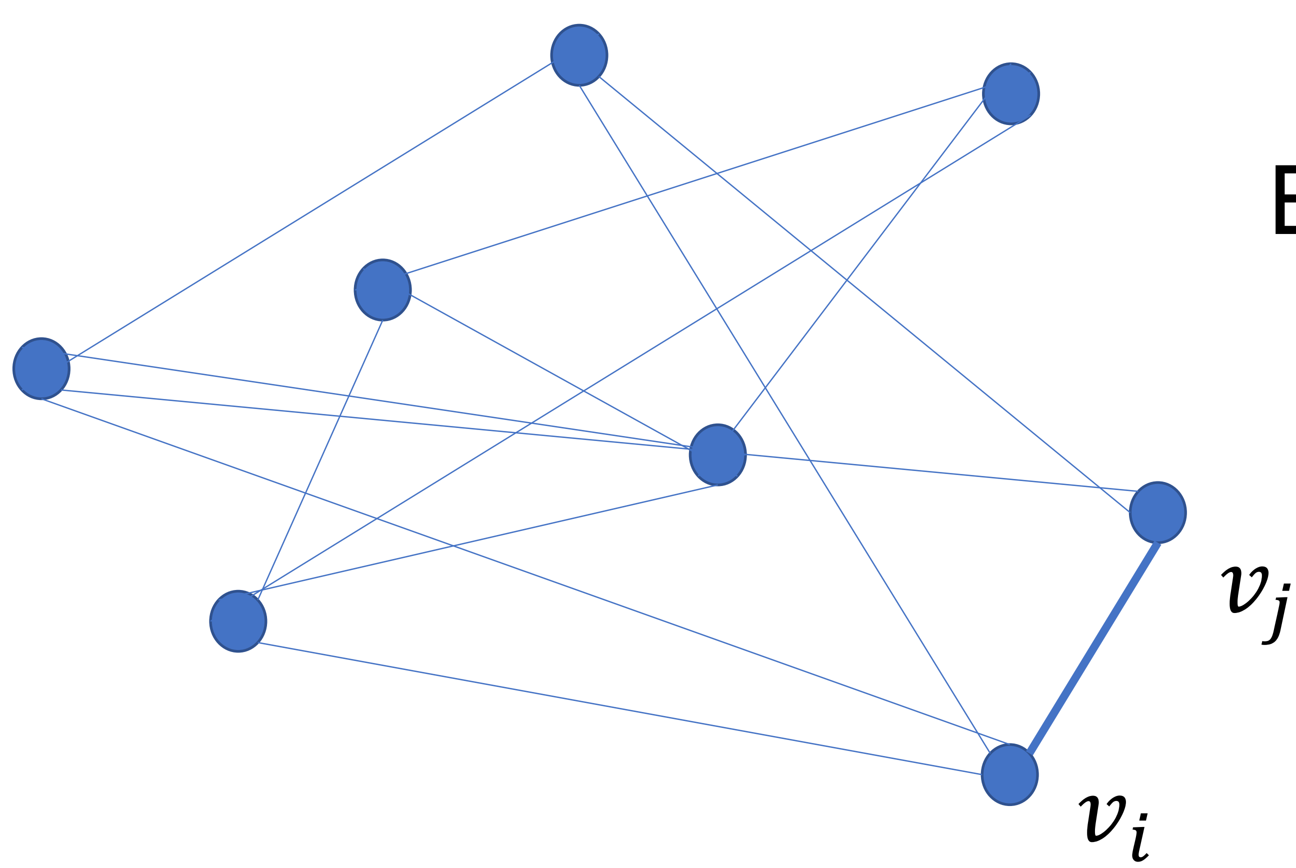
Agenda

1. Background

Graph Embedding

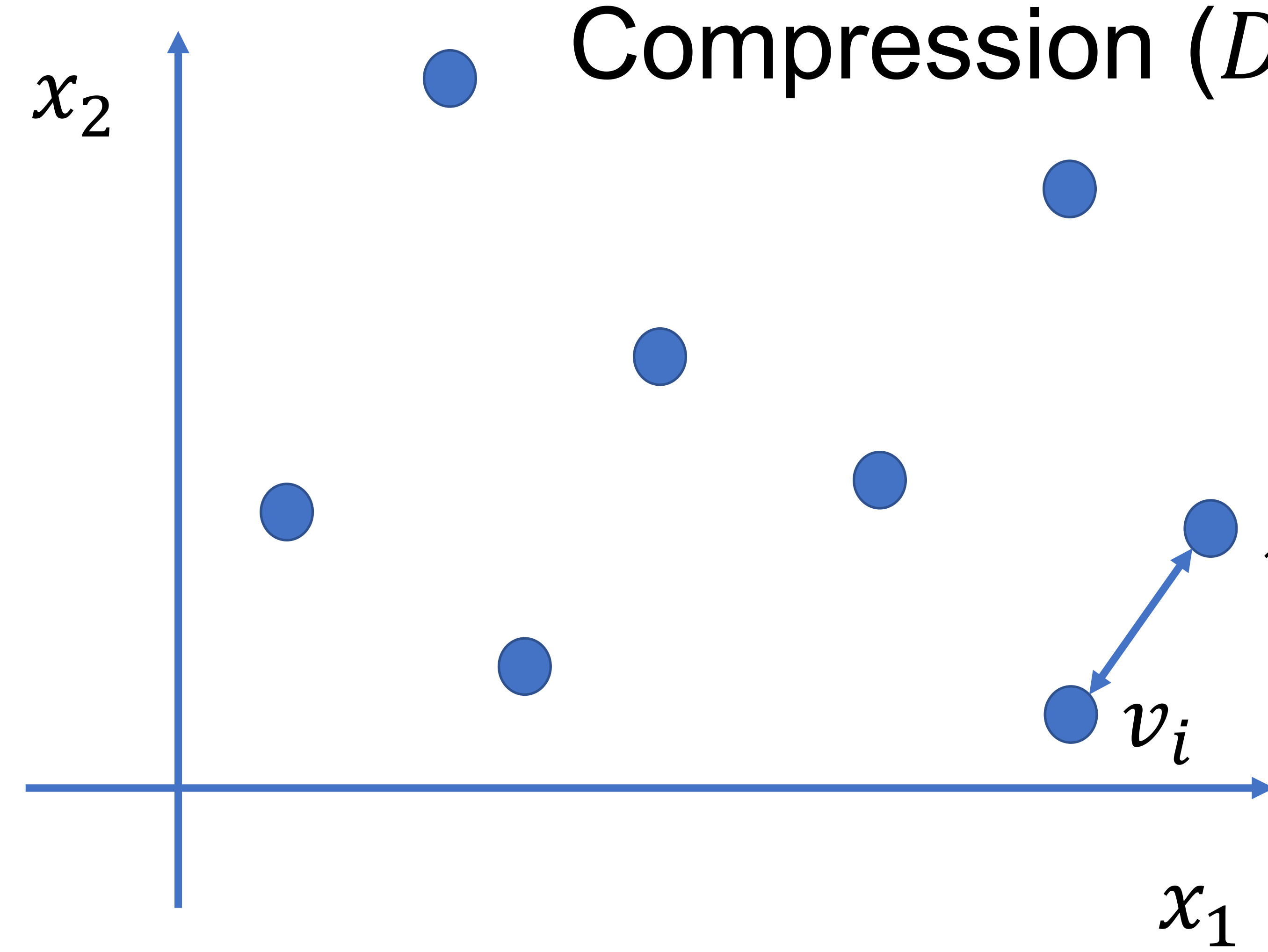
Convert discrete representation to continuous one.



(Attributed/
non-attributed)

Embed

Compression ($D \ll |V|$)



Input

Graphs can represent

- Social networks (Freeman 2000)
- Lexical networks (Ferrer+ 2001)
- Protein-protein interaction networks (Theocharidis+ 2009)

etc...

→ **Practically important!**

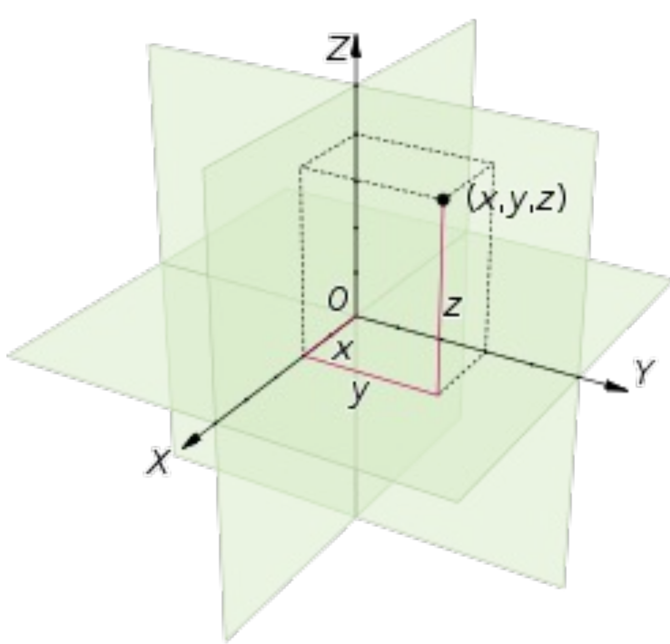
Downstream Tasks

- Node classification
- Link prediction
- Clustering
- Visualization (2-dimensional one)

Graph Embeddings on Riemannian Manifolds

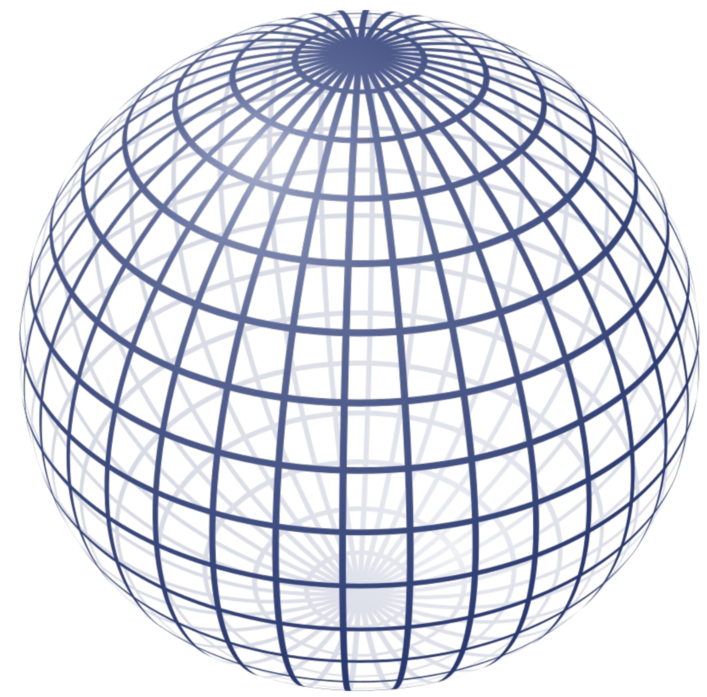
Recent Development of Graph Embeddings on Riemannian Manifolds.

Euclidean Space (Many studies)



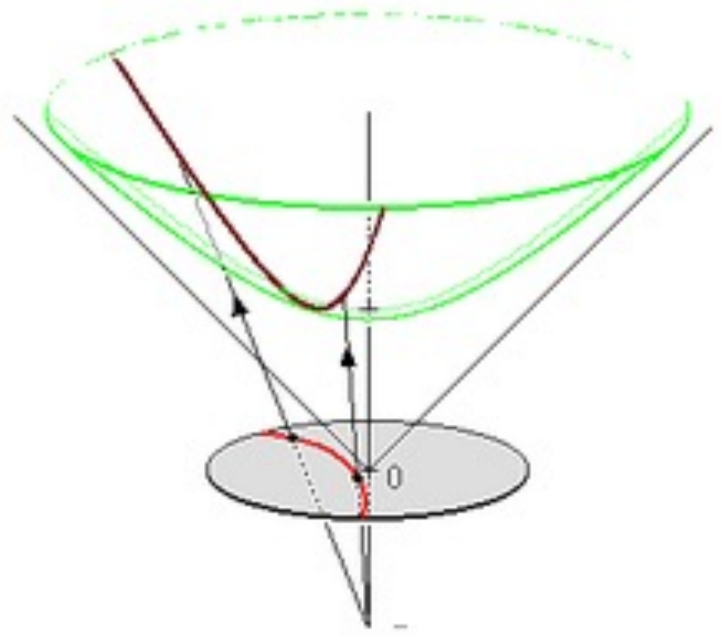
https://en.wikipedia.org/wiki/Euclidean_space

Spherical Space (Gu+ 2019)



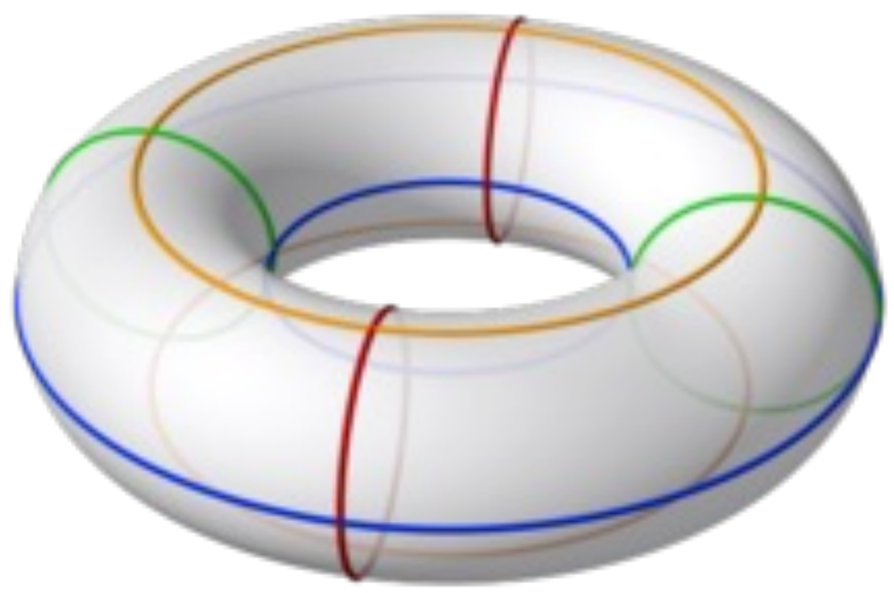
https://en.wikipedia.org/wiki/Sphere

Hyperbolic Space
(Nickel and Kiela 2017, 2018, etc)



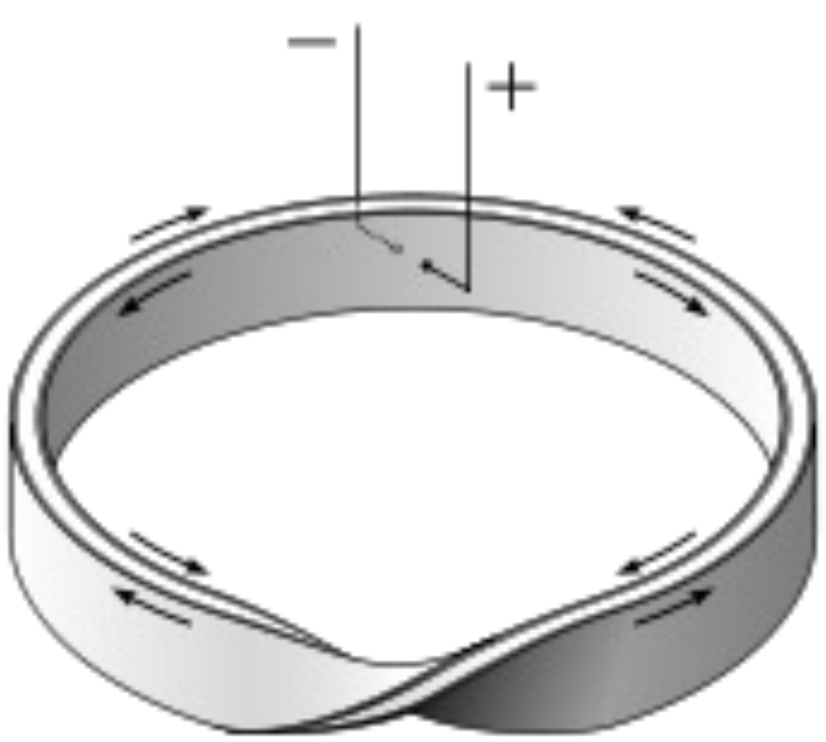
*https://en.wikipedia.org/wiki/Hyperboloid_model

Torus (Ebisu and Ichise 2018)



https://en.wikipedia.org/wiki/Torus

Möbius Ring (Chen+ 2021)

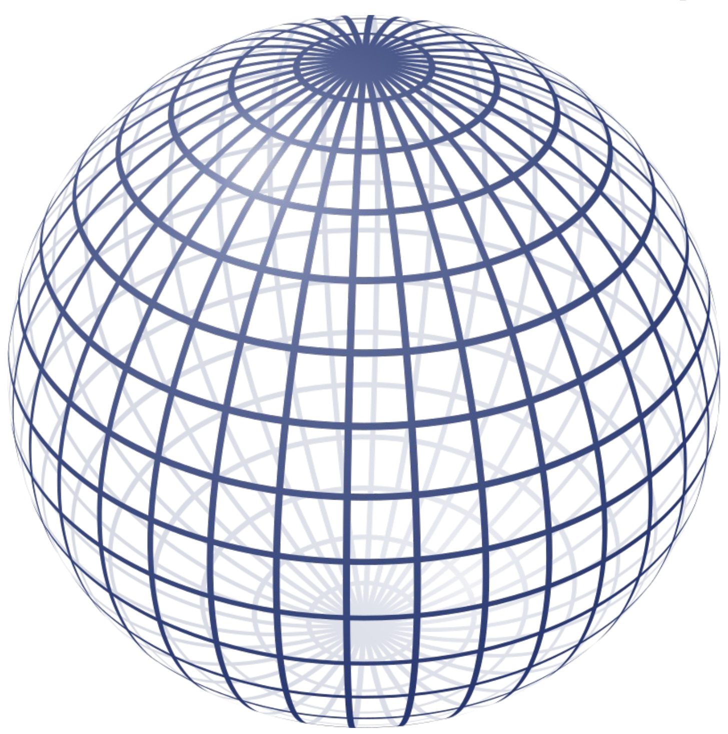


→How should we choose the best Riemmanian manifold associated with a given graph?

Model Spaces

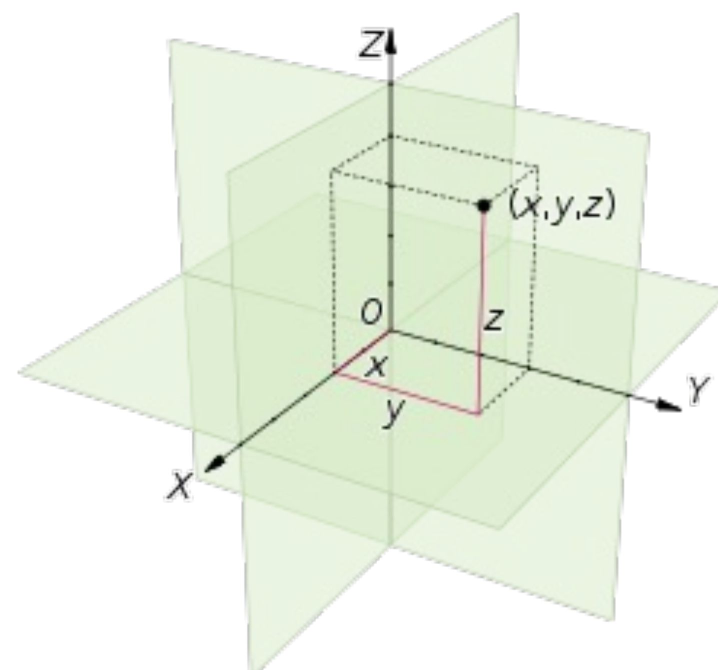
Spherical, Euclidean, and Hyperbolic spaces are chosen.

Spherical Space (K>0)



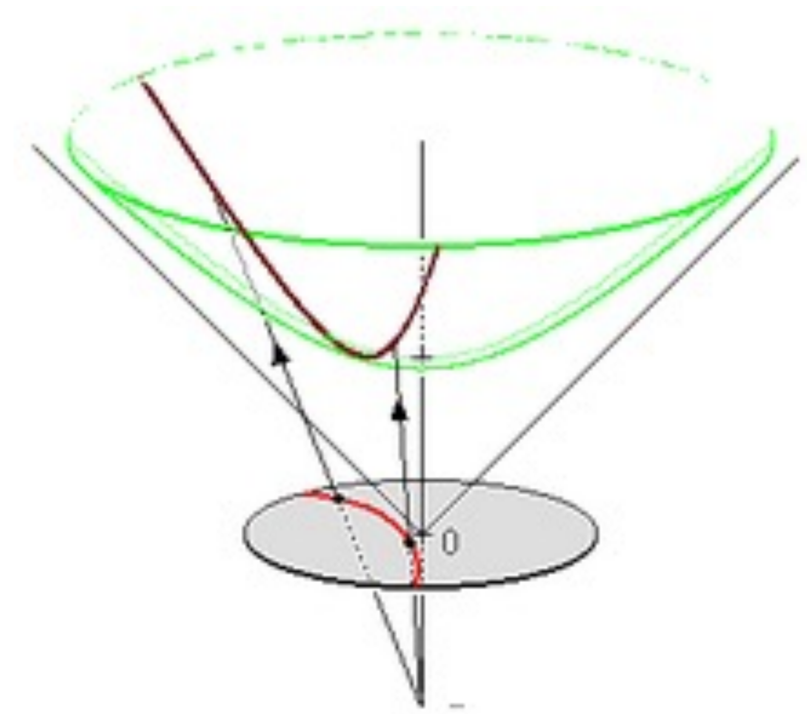
https://en.wikipedia.org/wiki/Sphere

Euclidean Space (K=0)



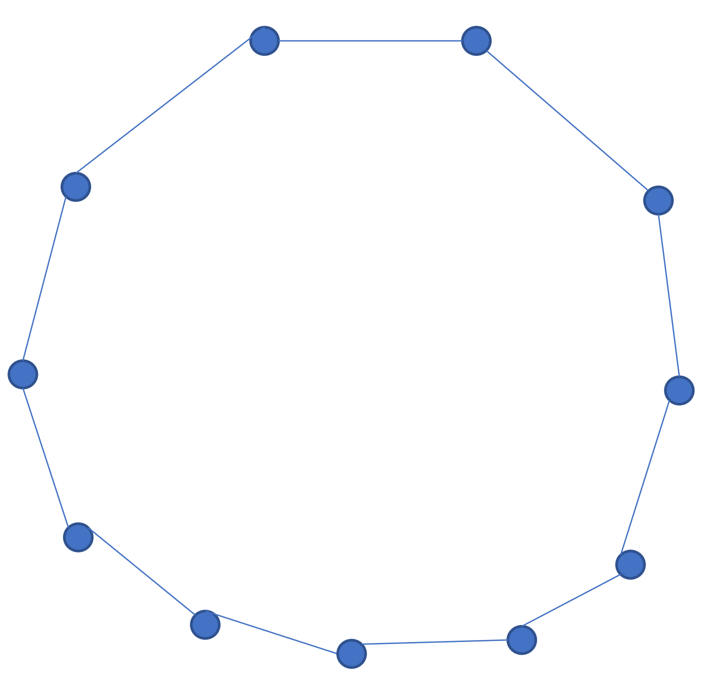
https://en.wikipedia.org/wiki/Euclidean_space

Hyperbolic Space (K<0)

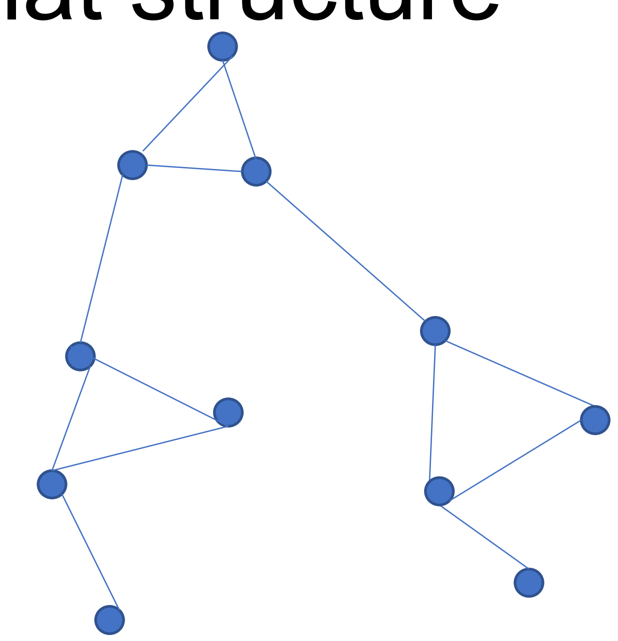


*https://en.wikipedia.org/wiki/Hyperboloid_model

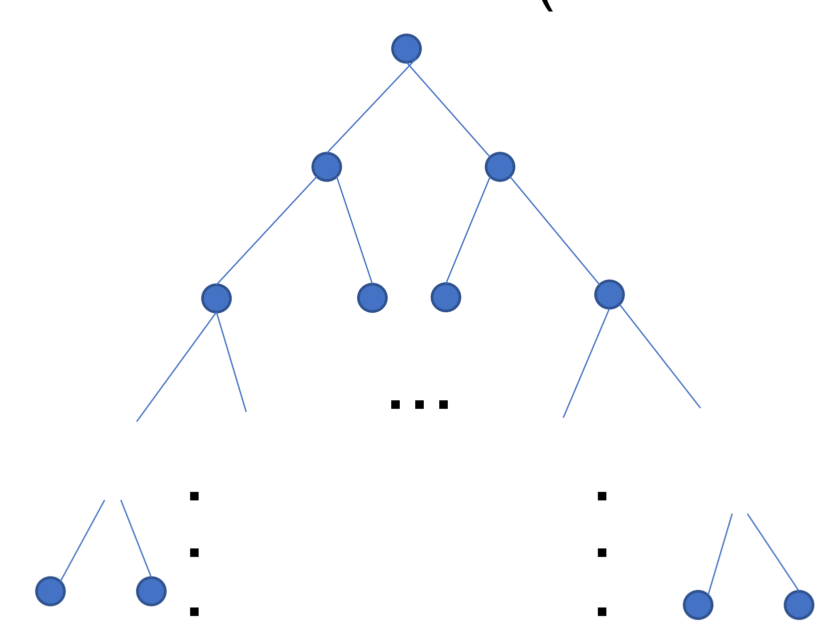
Cyclic structure (Gu+ 2019)



Flat structure



Tree-like structure (Krioukov+ 2010 etc)



Select D and K for the given graph.

MDL Principle (Rissanen 1978)

Select the model that minimizes the code-length.

Minimum Description Length (MDL) Principle

For data $x = x_1, \dots, x_n$ and model M, the MDL criterion is given by

$$MDL(x|M) = L(x|M) + L(M),$$

where $L(x|M)$ and $L(M)$ is encoding functions, and the best model is given by

$$\hat{M} = argmin_M \, MDL(x|M).$$

Example: Normalized Maximum Likelihood (NML) Code-Length (Shtarkov 1987)

For a parametric class of probability distributions $\mathcal{P}_M = \{p(x;\theta, M): \theta \in \Theta_M\}$, the NML code-length is given by

$$L_{NML}(x|M) = -\log p\left(x; \hat{\theta}(x), M\right) + \log C_n(M),$$

$C_n(M) = \sum_y p(y; \hat{\theta}(y), M)$: parametric complexity.

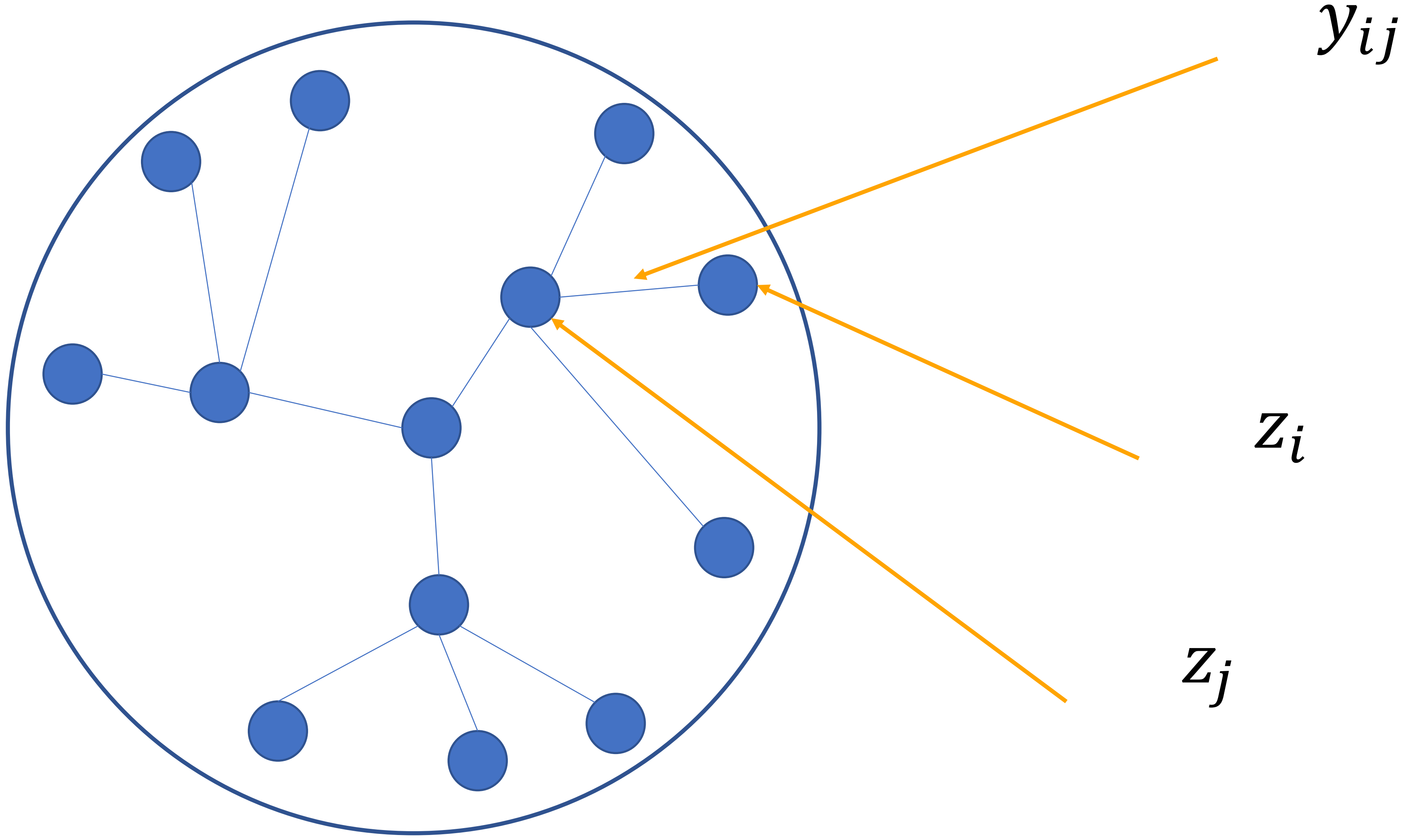
MDL model selection by regarding the dimensionality and similarity as a model.

Agenda

2. Formulation of Graph Embedding

Conventional Formulation of Graph Embedding (Nickel and Kiela 2018)

Connect points with logistic function.



$$p_K(\boldsymbol{y}; \boldsymbol{z}, \gamma) := \prod_{(i,j)\in\Lambda_n} p_K(y_{ij}; z_i, z_j, \gamma),$$

$$p_K(y_{ij}; z_i, z_j, \gamma) := \begin{cases} \frac{1}{1+\exp(d^K_{z_i z_j} - \gamma)} & (y_{ij} = 1), \\ 1 - \frac{1}{1+\exp(d^K_{z_i z_j} - \gamma)} & (y_{ij} = 0). \end{cases}$$

$\gamma > 0$

Logistic function.

Non-Identifiability Problem

Non-identifiability problem

Non-identifiability refers to a situation where there is no one-to-one correspondence between parameters and probability distributions. For all x, there exist $\theta_1 \neq \theta_2$ such that the following equation holds.

$$p(x;\theta_1) = p(x;\theta_2).$$

- The asymptotic normality for the maximum likelihood estimate does not hold.
- Conventional information criteria such as AIC (Akaike 1974), BIC (Schwarz 1978), etc… do not guarantee their rationales because their derivation depend on asymptotic theory.
- Calculation of the NML code-length is also difficult.

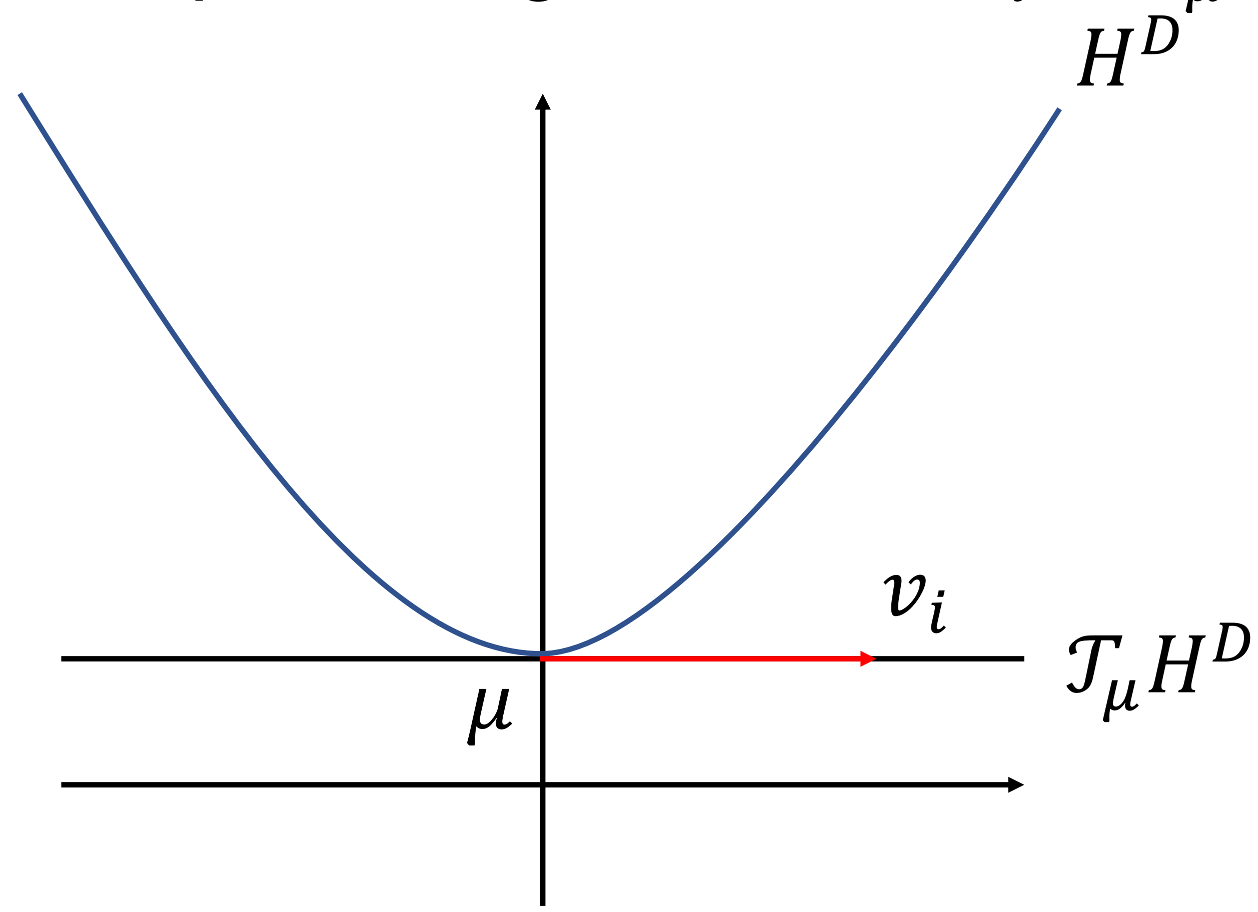
The conventional formulation of hyperbolic embedding is non-identifiable. Thus, we use latent variable models.

Agenda

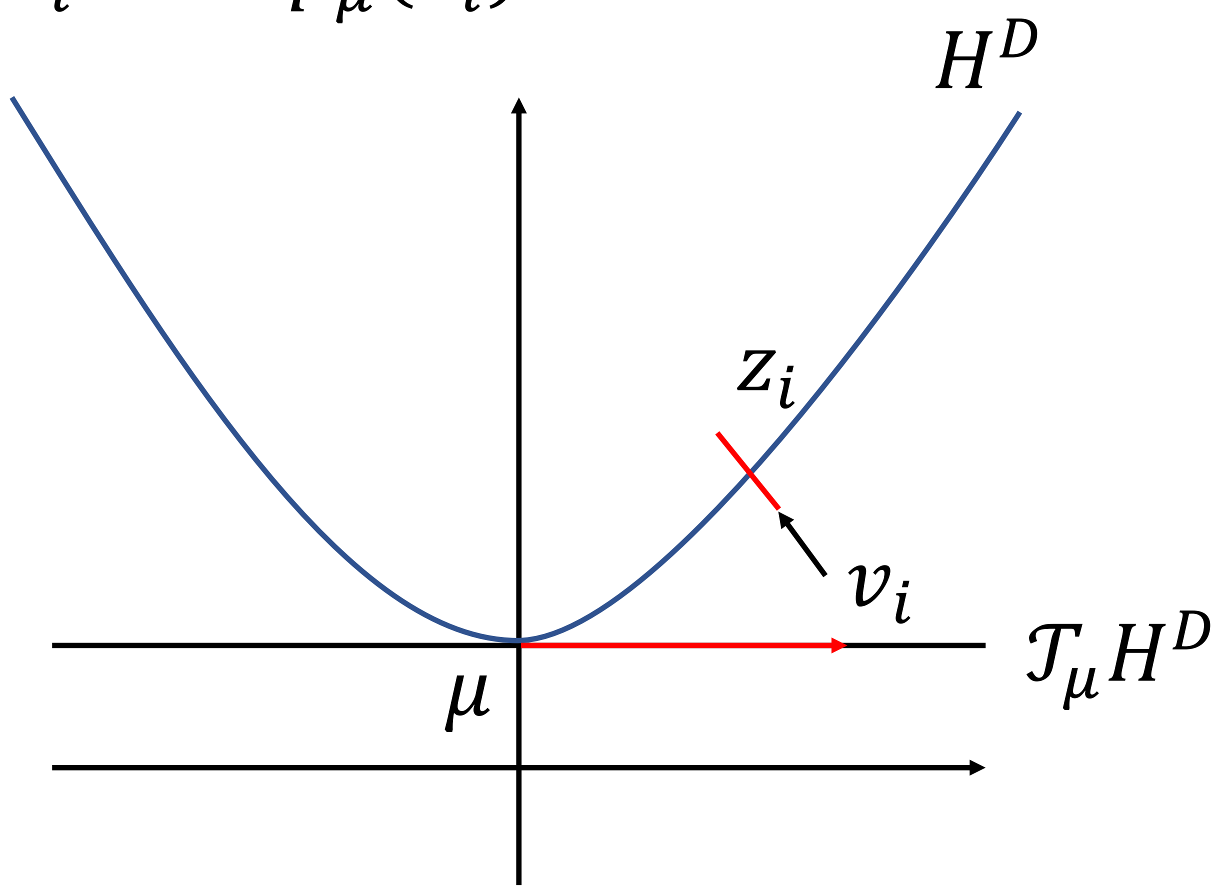
3. Dimensionality and Curvature Selection using DNML code-length

Wrapped Normal Distribution on Hyperbolic Space (Nagano+ 2019)

1. Sample a tangent vector v_i in $\mathcal{T}_\mu H^D$.



2. $z_i = Exp_\mu(v_i)$.



$$p(\boldsymbol{v}; \Sigma) := \prod_{i \in [n]} p(v_i; \Sigma),$$

$$p(v_i; \Sigma) := \frac{1}{(2\pi)^{\frac{D}{2}} |\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2} v_i^\top \Sigma^{-1} v_i\right).$$

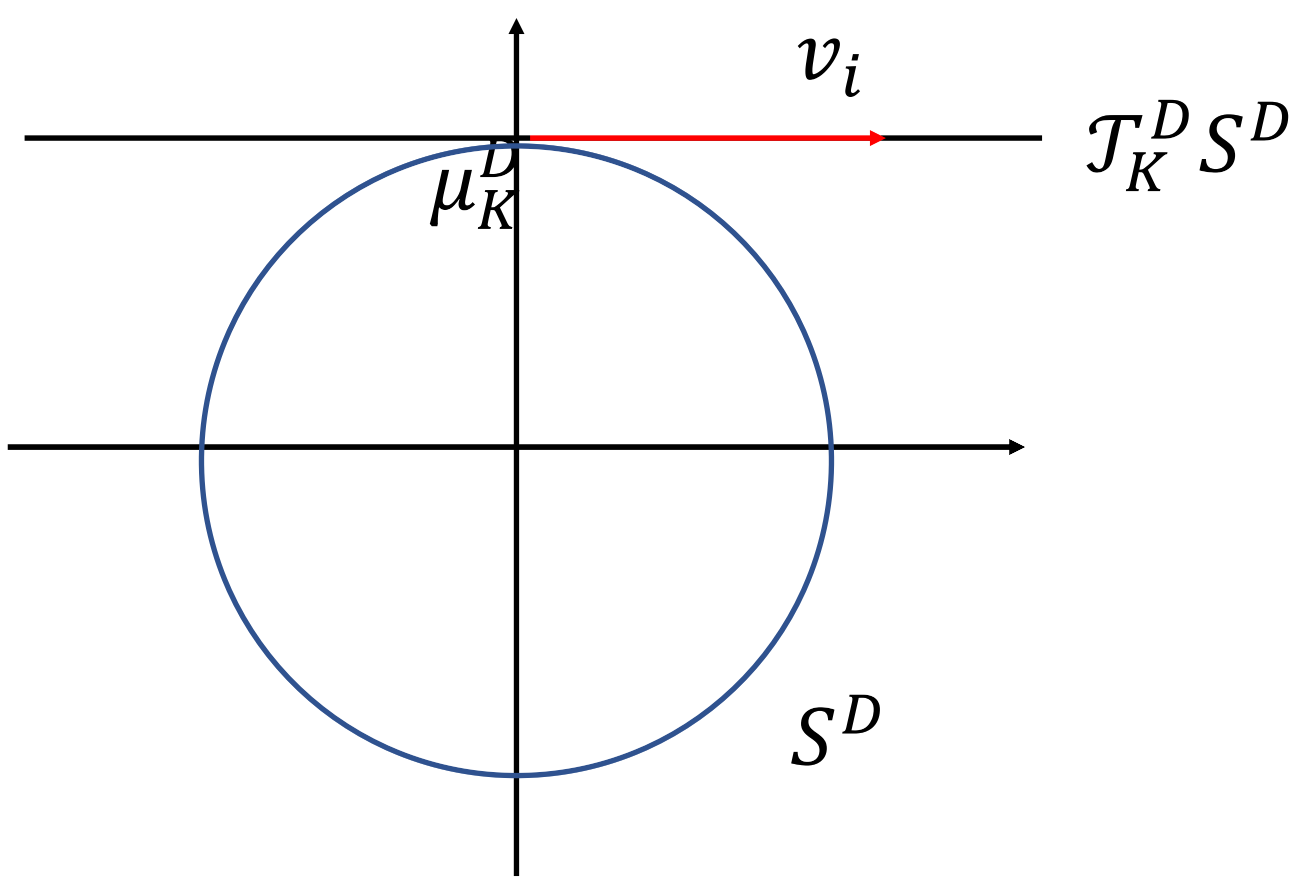
Gaussian distribution
for each tangent vector

$$p(z_i; \Sigma) := \underbrace{\frac{1}{J(z_{i,1:D} : v_i)}}_{\text{Jacobian}} \underbrace{p(v_i, \Sigma)}_{\text{Probability density of each tangent vector.}},$$

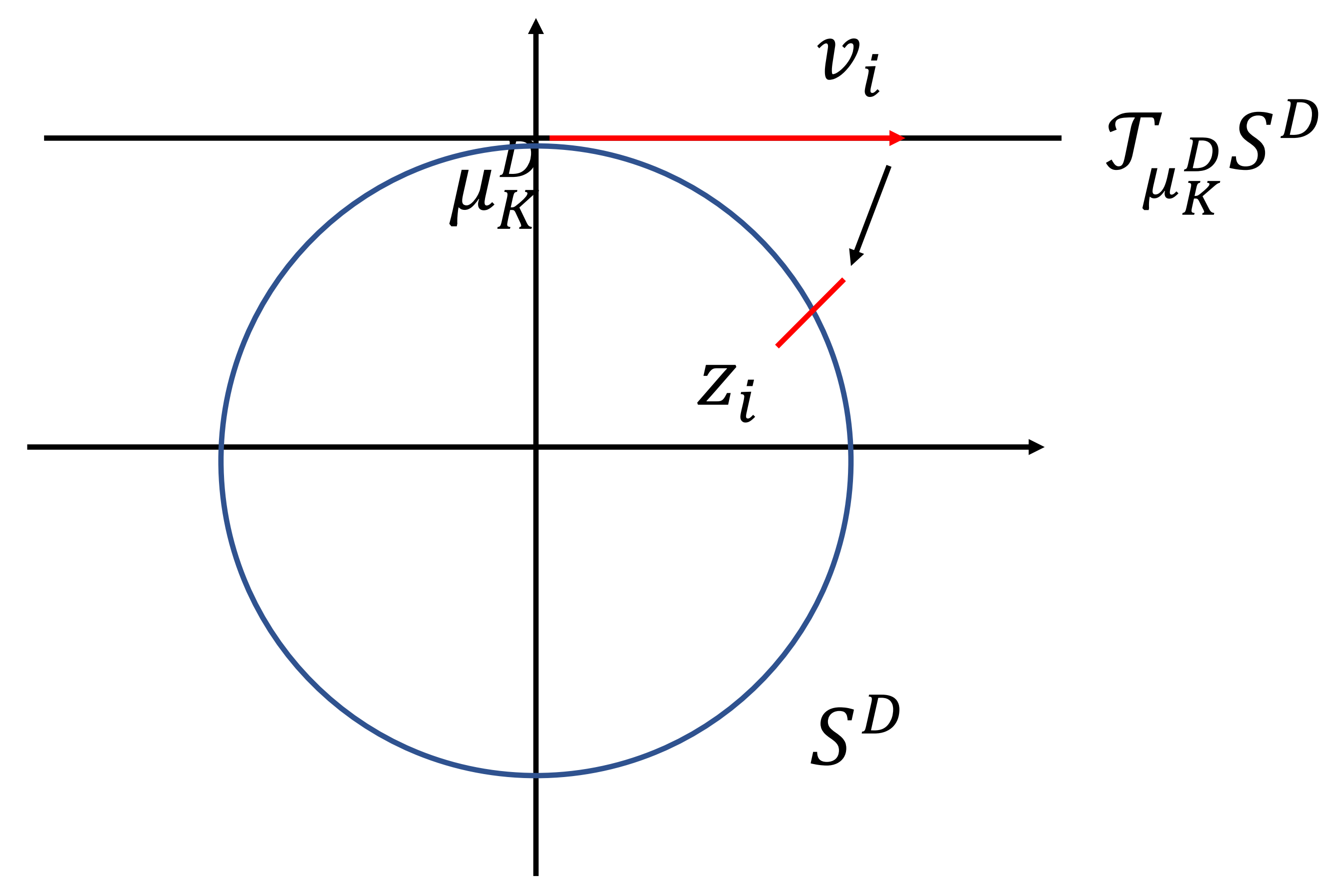
$$J(z_{i,1:D} : v_i) = \left\{ \frac{\sinh \|v_i\|_{\mathcal{L}}}{\|v_i\|_{\mathcal{L}}} \right\}^{D-1}.$$

WNDs on Spherical Space

1. Sample a tangent vector v_i in $\mathcal{T}_{\mu_K^D} S^D$.



2. $z_i = Exp_\mu^K(v_i)$.



$$p_K(v_i;\ \Sigma) := \frac{f(\tilde{v}_i;\ \Sigma)}{W_K(\Sigma)}.$$

Multivariate truncated normal dist.

$$W_K(\Sigma) := \int_{\|\tilde{v}'\|_2 \le \frac{\pi}{\sqrt{|K|}}} f(\tilde{v}';\ \Sigma) d\tilde{v}'$$

$$f(\boldsymbol{x};\ \Sigma) := \frac{1}{\sqrt{(2\pi)^D |\Sigma|}} \exp\left(-\frac{1}{2}\boldsymbol{x}^\top \Sigma^{-1} \boldsymbol{x}\right).$$

$$p_K(\boldsymbol{z}_i;\ \Sigma) := \frac{1}{J_K(\boldsymbol{z}_i;\ \boldsymbol{v}_i)}\ p_K(\boldsymbol{v}_i;\ \Sigma),$$

$$J_K(\boldsymbol{z} : \boldsymbol{v}) := \begin{cases} 1 & (K = 0), \\ \left(\frac{|\sin_K(\sqrt{|K|}\|\boldsymbol{v}\|_K)|}{\sqrt{|K|}\|\boldsymbol{v}\|_K}\right)^{D-1} & (K \neq 0). \end{cases}$$

* Wrapped normal distributions for Euclidean space is standard Gaussian distributions.

2. Decomposed Normalized Maximum Likelihood (DNML) Code-Length

Use DNML code-length for LVMs.

DNML Code-Length (Yamanishi+ 2019)

Assume that observable variable y and latent variable z follow

$$p(\boldsymbol{y}, \boldsymbol{z}; \boldsymbol{\theta}, M) := p(\boldsymbol{y} \mid \boldsymbol{z}; \boldsymbol{\theta}_1, M)p(\boldsymbol{z}; \boldsymbol{\theta}_2, M),$$

Then, DNML code-length is defined as

$$L_{\mathrm{DNML}}(\boldsymbol{y}, \boldsymbol{z}) := L_{\mathrm{NML}}(\boldsymbol{y} \mid \boldsymbol{z}) + L_{\mathrm{NML}}(\boldsymbol{z}),$$

where

Negative logarithm of the maximum likelihood

$$L_{\mathrm{NML}}(\boldsymbol{y} \mid \boldsymbol{z}) := \boxed{-\log p(\boldsymbol{y} \mid \boldsymbol{z}; \hat{\boldsymbol{\theta}}_1(\boldsymbol{y}, \boldsymbol{z}))} + \boxed{\log \sum_{\boldsymbol{y}'} p(\boldsymbol{y}' \mid \boldsymbol{z}; \hat{\boldsymbol{\theta}}_1(\boldsymbol{y}', \boldsymbol{z})),}$$

$$L_{\mathrm{NML}}(\boldsymbol{z}) := \boxed{-\log p(\boldsymbol{z}; \hat{\boldsymbol{\theta}}_2(\boldsymbol{z}))} + \boxed{\log \sum_{\boldsymbol{z}'} p(\boldsymbol{z}'; \hat{\boldsymbol{\theta}}_2(\boldsymbol{z}')).}$$

Penalty term (parametric complexity).

Our contribution: derived an explicit form of the approximation of each penalty term.

(Yamanishi+ 2019).

→Derive $L_{NML}(y \mid z)$ and $L_{NML}(z)$ for two priors.

1. Derivation of $L_{NML}(y \mid z)$

NML is approximated using Fisher information.
(Rissanen 1996, Grunwald et al., 2015)

1. Derivation of $L_{NML}(y \mid z)$

$L_{NML}(y \mid z)$ is approximated by

$$L_{\mathrm{NML}}(\boldsymbol{y} \mid \boldsymbol{z}, D, K) \approx -\log p(\boldsymbol{y} \mid \boldsymbol{z}; \hat{\gamma}(\boldsymbol{y}, \boldsymbol{z})) + \log \frac{n(n-1)}{4\pi} + \underline{\log \int_{\gamma_{\min}}^{\gamma_{\max}} \sqrt{|I_n(\gamma)|}\, d\gamma},$$

Integral over the parameter domain.

$$I_n(\gamma) = E_\gamma \left[-\frac{2}{n(n-1)} \underline{\frac{\partial^2 \log p(\boldsymbol{y} \mid \boldsymbol{z}; \gamma)}{\partial \gamma^2}} \right]$$

Fisher information

Likelihood

With some calculation, we have

$$I_n(\gamma) = \frac{2}{n(n-1)} \sum_{(i,j) \in \Lambda_n} \frac{1}{4} \cosh\left(\frac{d^K_{z_i z_j} - \gamma}{2} \right)^{-2}.$$

Numerical integration with the Gaussian quadrature (Vetterling+ 1992).

2. Derivation of $L_{NML}(z)$

2. Derivation of $L_{NML}(z)$

For **Euclidean and Hyperbolic** cases, $L_{NML}(z)$ is given by

$$L_{\mathrm{NML}}(\boldsymbol{z} \mid D, K) = -\log p_K(\boldsymbol{z}; \hat{\boldsymbol{\sigma}}(\boldsymbol{z})) + D \log \frac{1}{\Gamma(\frac{n}{2})} \left(\frac{n}{2e}\right)^{\frac{n}{2}} + \sum_{i \in [D]} \log \log \frac{\sigma_i^{\max}}{\sigma_i^{\min}}.$$

The derivation mainly depends on Rissanen's g-function (Rissanen 2012).

For **spherical** case, parametric complexity of multivariate truncated normal distribution is not trivial to obtain. Thus, we use the importance sampling:

$$\begin{aligned} \int p_K(\boldsymbol{v};\ \hat{\boldsymbol{\sigma}}(\boldsymbol{v})) d\boldsymbol{v} &= \int \frac{p_K(\boldsymbol{v};\ \hat{\boldsymbol{\sigma}}(\boldsymbol{v}))}{q(\boldsymbol{v})} q(\boldsymbol{v}) d\boldsymbol{v} \\ &= E\left[\frac{p_K(\boldsymbol{v};\ \hat{\boldsymbol{\sigma}}(\boldsymbol{v}))}{q(\boldsymbol{v})}\right] \\ &\approx \sum_{\boldsymbol{v}} \frac{p_K(\boldsymbol{v};\ \hat{\boldsymbol{\sigma}}(\boldsymbol{v}))}{q(\boldsymbol{v})}, \end{aligned}$$

where $q(\boldsymbol{v})$ is a sampling distribution of $\boldsymbol{v}$.

Agenda

4. Experimental Results

Experimental Results

DNML can identify the curvature sign and dimensionality with sufficient amount of data, whereas accurate estimation of curvature is still challenging.

Table 5.1. Accuracy of curvature sign estimation.

Dataset	# of nodes	DNML	AIC	BIC
E-8	400	**0.08**	0.00	0.00
	800	0.67	**0.75**	0.00
	1600	**1.00**	**1.00**	0.67
	3200	**1.00**	**1.00**	**1.00**
H-8	400	**1.00**	**1.00**	**1.00**
	800	0.92	**1.00**	**1.00**
	1600	0.83	**1.00**	**1.00**
	3200	**1.00**	**1.00**	**1.00**
S-8	400	**1.00**	0.33	0.33
	800	**1.00**	**0.67**	0.33
	1600	**1.00**	0.58	0.67
	3200	**1.00**	**1.00**	0.67

Table 5.4. Average Maps of each criterion (Average estimated dimensionalities in parentheses).

Dataset	# of nodes	DNML	AIC	BIC
E-8	400	**1.000**(8.0)	0.625(14.0)	0.625(5.0)
	800	0.750(12.0)	0.556(14.7	**0.833**(6.7)
	1600	**0.871**(9.3)	0.583(14.7)	0.486(3.7)
	3200	**1.000**(8.0)	**1.000**(8.0)	0.670(4.0)
H-8	400	**0.333**(2.0)	**0.333**(3.2)	**0.333**(2.0)
	800	0.333(3.5)	**0.513**(4.3)	0.333(2.0)
	1600	0.431(4.0)	**0.958**(8.7)	0.333(2.0)
	3200	**0.833**(6.7)	0.375(17.3)	0.333(3.8)
S-8	400	0.304(15.5)	**0.333**(3.5)	**0.333**(2.0)
	800	**0.424**(13.3)	**0.444**(3.83)	0.333(2.0)
	1600	0.544(14.3)	**0.625**(5.3)	0.333(2.5)
	3200	**0.708**(16.7)	**0.736**(7.3)	0.333(3.3)

Table 5.2. Results of average estimated curvature for latent variable models with the true curvatures.

# of nodes	−1.25	−1.00	−0.75	0.10	0.20	0.30
400	−0.22	−0.21	−0.20	0.21	0.31	0.36
800	−0.18	−0.16	−0.16	0.18	0.27	0.30
1600	−0.12	−0.11	−0.10	0.13	0.20	0.21
3200	−0.09	−0.08	−0.07	0.10	0.12	0.12

→Accurate estimation of curvature is still challenging!

2. Experiment with Real-World Networks

DNML performs high conciseness with sufficient amount of nodes.

Table 5.6. Selected dimensionality and curvature of each method.

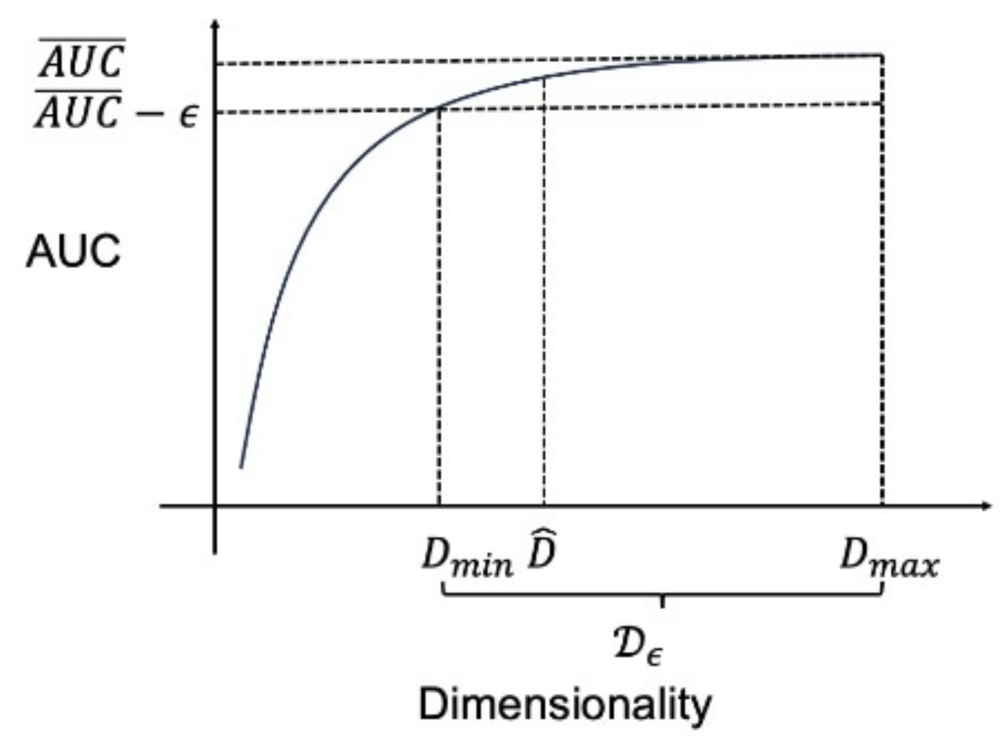
Network	DNML	AIC	BIC
AstroPh	$\mathbb{H}^{12}_{-0.25}$	$\mathbb{H}^{15}_{-0.25}$	$\mathbb{H}^{8}_{-0.27}$
HepPh	$\mathbb{E}^{16}$	$\mathbb{H}^{14}_{-0.32}$	$\mathbb{H}^{6}_{-0.36}$
Airport	$\mathbb{E}^{7}$	$\mathbb{E}^{7}$	$\mathbb{H}^{3}_{-0.73}$
WN-mammal	$\mathbb{H}^{4}_{-0.69}$	$\mathbb{H}^{4}_{-0.71}$	$\mathbb{H}^{3}_{-0.72}$
WN-solid	$\mathbb{H}^{4}_{-0.69}$	$\mathbb{H}^{5}_{-0.70}$	$\mathbb{H}^{3}_{-0.71}$

Table 5.5. Statistics of real-world datsets.

Network	# Nodes	# Edges
AstroPh	18, 772	198, 080
ca-HepPh	12, 008	118, 505
Airport	3, 188	18, 630
WN-mammal	1, 180	6, 540
WN-solid	1, 232	5, 696

Table 5.7. Average conciseness of each method.

Network	$\epsilon_{\max}$	DNML	AIC	BIC
AstroPh	0.05	**0.484**	**0.467**	0.362
	0.10	**0.532**	0.484	**0.540**
HepPh	0.05	**0.496**	0.398	0.351
	0.10	0.518	0.436	**0.544**
Airport	0.05	**0.390**	**0.405**	0.000
	0.10	**0.549**	**0.550**	0.425
WN-mammal	0.05	0.000	0.000	0.000
	0.10	**0.416**	0.385	0.341
WN-solid	0.05	0.398	**0.549**	0.080
	0.10	0.637	**0.676**	0.521



$$\text{conciseness}(\hat{D}, \epsilon_{\max}) := \frac{1}{\epsilon_{\max} P} \sum_{i=0,1,\ldots,P} c\left(\hat{D}, \frac{i}{P}\epsilon_{\max}\right),$$

$$c(\hat{D}, \epsilon) := \begin{cases} 1 - \frac{\log_2 \hat{D} - \log_2 D_{\min}}{\log_2 D_{\max} - \log_2 D_{\min}} & (\hat{D} \in \mathcal{D}_\epsilon), \\ 0 & (\hat{D} \notin \mathcal{D}_\epsilon), \end{cases}$$

Summary

Research question

- How can we determine the dimensionality and curvature of graph embedding?

Solution

- Latent variable models for graph embedding.
  - Universal latent variable models over all curvature using wrapped normal distributions.
- Apply decomposed normalized maximum likelihood (DNML) code-length to the model.

Contribution

- Derivation of the explicit formula of DNML code-length.
- Empirical validation of our proposed method.

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