Geometric Modeling

Summer Semester 2012

Dimensionality Reduction, Intrinsic Geometry and Discrete Differential Operators

UNIVERSITÄT DES SAARLANDES

CLUSTER OF EXCELLENCE

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Dimensionality Reduction

Fitting Affine Subspaces

The following problem can be solved exactly:

- Best fitting line to a set of 2D, 3D points
- Best fitting plane to a set of 3D points
- In general: Affine subspace of $\mathbb{R}^d$, with dimension $d \leq m$ that best approximates a set of data points $\mathbf{x}_i \in \mathbb{R}^m$.

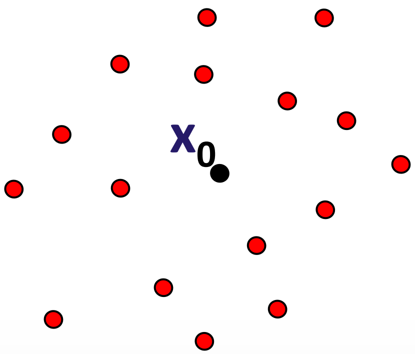
This will lead to the - famous - *principle component analysis (PCA)*.

Start: 0-dim Subspaces

Easy Start: The optimal 0-dimensional affine subspace

- Given a set $\mathbf{X}$ of n data points $\mathbf{x}_i \in \mathbb{R}^m$, what is the point $\mathbf{x}_0$ with minimum least square error to all data points?
- Answer: just the sample mean (average)...:

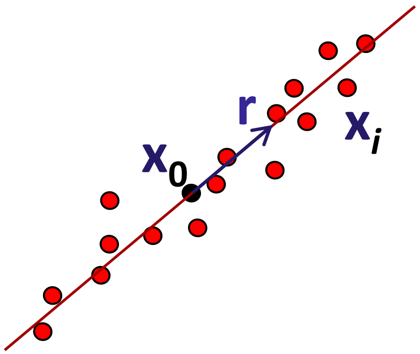
$$\mathbf{x}_0 = \mathrm{m}(\mathbf{X}) \coloneqq \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i$$



One Dimensional Subspaces...

Next:

- What is the optimal line (1D subspace) that approximates a set of data points $\mathbf{X}$?
- Two questions:
  - Optimum origin (point on the line)?
    - This is still the average
  - Optimum direction?
    - We will look at that next...
- Parametric line equation:



$$\mathbf{x}(t) = \mathbf{x}_0 + t.\mathbf{r} \qquad (\mathbf{x}_0 \in \mathbb{R}^m, \mathbf{r} \in \mathbb{R}^m, \|\mathbf{r}\| = 1)$$

Best Fitting Line

Result:

$$\sum_{i=1}^{n} dist(line, \mathbf{x}_i)^2 = -\mathbf{r}^{\mathrm{T}}\mathbf{S}\mathbf{r} + \text{const.}$$

with $\mathbf{S} = \sum_{i=1}^{n}(\mathbf{x}_i - \mathbf{x}_0)(\mathbf{x}_i - \mathbf{x}_0)^{\mathrm{T}}, \ \|\mathbf{r}\| = 1$

Eigenvalue Problem:

- $\mathbf{r}^{\mathrm{T}}\mathbf{S}\mathbf{r}$ **is a Rayleigh quotient**
- **Minimizing the energy: maximum quotient**
- **Solution: eigenvector with *largest* eigenvalue**

General Case

Fitting a d-dimensional affine subspace:

- $d = 1$: **line**
- $d = 2$: **plane**
- $d = 3$: **3D subspace**
- **...**

Simple rule:

- **Use the d eigenvectors with *largest eigenvalues* from the spectrum of S.**
- **Gives the (total) least-squares optimal subspace that approximates the data set $\mathbf{X}$.**

PCA Maximum Variance Formulation

Alternate Formulation:

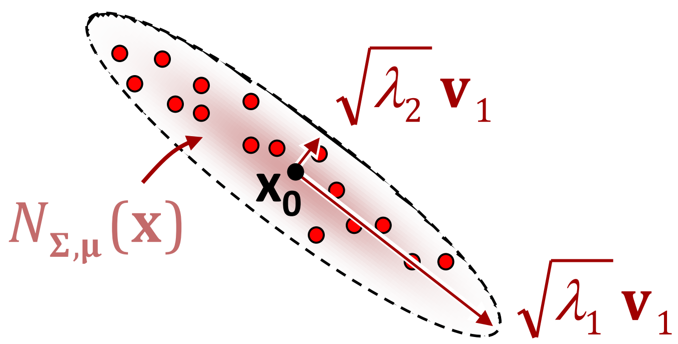
- Let $\mathbf{v} \in \mathbb{R}^m$ be the 1D subspace (with $\mathbf{v}^{\mathrm{T}}\mathbf{v} = 1$), that maximize the variance of data $\mathbf{X} \in \mathbb{R}^m$.
- Each data point $\mathbf{x}_i$ is projected onto a scalar value $\mathbf{v}^{\mathrm{T}}\mathbf{x}_i$.
- The mean of projected data is $\mathbf{v}^{\mathrm{T}}\mathbf{x}_0$.
- The variance of the projected data is given by:
  $\frac{1}{n}\sum_{i=1}^{n}\left(\mathbf{v}^{\mathrm{T}}\mathbf{x}_i - \mathbf{v}^{\mathrm{T}}\mathbf{x}_0\right)^2 = \mathbf{v}^{\mathrm{T}}\mathbf{S}\mathbf{v}$; $\mathbf{S} = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i - \mathbf{x}_0)(\mathbf{x}_i - \mathbf{x}_0)^{\mathrm{T}}$
- The problem now reduces to

$$\mathbf{v}^* = \boldsymbol{arg\ max}\,\{\mathbf{v}^{\mathrm{T}}\mathbf{S}\mathbf{v} + \lambda(1 - \mathbf{v}^{\mathrm{T}}\mathbf{v})\}$$

- Solution:

Eigenvector of **S** with ***largest*** eigenvalue λ_1.

Statistical Interpretation



$$\boldsymbol{\mu} = \mathbf{x}_0 = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i$$

$$\boldsymbol{\Sigma} = \frac{1}{n-1}\mathbf{S} = \frac{1}{n-1}\sum_{i=1}^{n}(\mathbf{x}_i - \mathbf{x}_0)(\mathbf{x}_i - \mathbf{x}_0)^{\mathrm{T}}$$

$$N_{\boldsymbol{\Sigma},\boldsymbol{\mu}}(\mathbf{x}) = \frac{1}{(2\pi)^{\frac{d}{2}}\det(\boldsymbol{\Sigma})^{1/2}}\exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)$$

Observation:

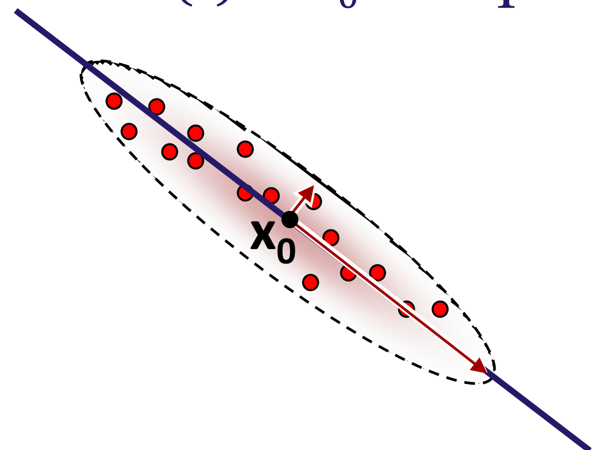
- $\frac{1}{n-1}\mathbf{S}$ is the covariance matrix of the data $\mathbf{X}$.
- PCA can be interpreted as fitting a Gaussian distribution and computing the main axes.

Applications

Fitting a line to a point cloud in $\mathbb{R}^2$:

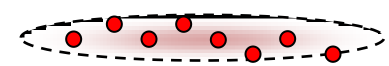
- Sample mean and direction of maximum eigenvalue

$\mathbf{x}(t) = \mathbf{x}_0 + t.\mathbf{v}_1$

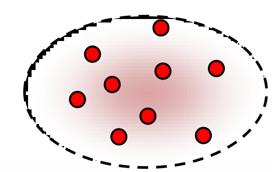


Plane Fitting in $\mathbb{R}^3$:

- Sample mean and the two directions of maximum eigenvalues
- Smallest eigenvalue
  - Eigenvector points in normal direction
  - Aspect ratio (λ_3 / λ_2) is a measure of "flatness" (quality of fit)



(λ_2 / λ_1) small



(λ_2 / λ_1) larger

Applications

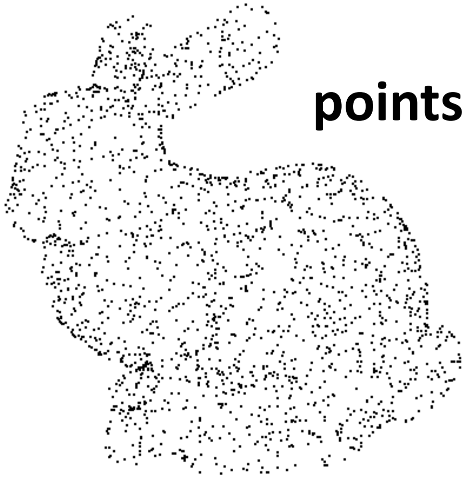
Application: Normal estimation in point clouds

- Given a set of points $\mathbf{X} \in \mathbb{R}^{\mathbf{3}}$ sampled from a smooth surface.
- We want to estimate Surface Normals.

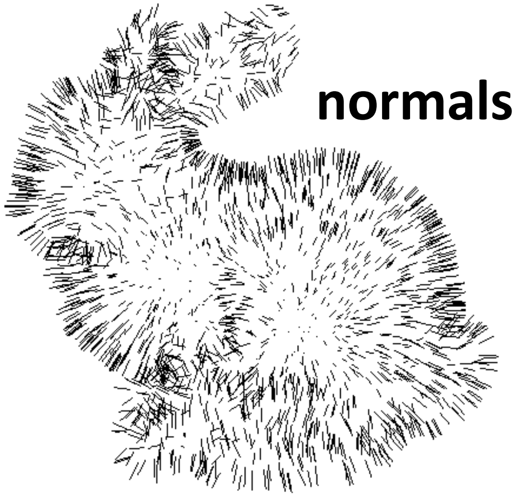
Algorithm:

- For each point, compute the k-nearest neighbors ($k = 20$).
- Compute a PCA (average, main axes) of these points.
- Eigenvector with smallest eigenvalue $\rightarrow$ normal direction.
- The other two eigenvectors $\rightarrow$ tangent vectors.

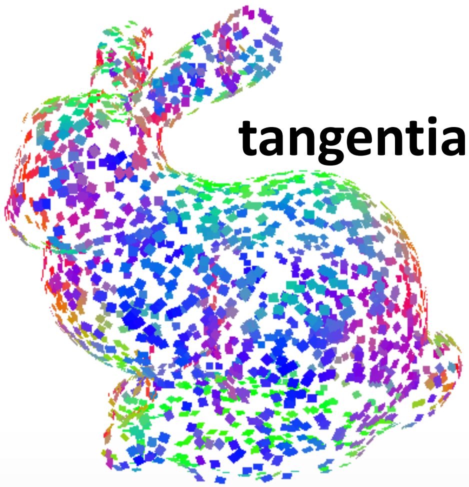
Example



points



normals



tangential frames

Dimensionality Reduction

Notations:

- $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_k, \ldots, \mathbf{x}_n], \quad \mathbf{x}_k \in \mathbb{R}^m$

- $\mathbf{R}$ is a $m \times m$ orthogonal matrix with $\mathbf{R}^{\mathrm{T}}\mathbf{R} = \mathbf{I}_{\boldsymbol{m}}$.

Projection: from $\mathbb{R}^m$ onto $\mathbb{R}^d$ removes $m - d$ rows of $\mathbf{R}^{\mathrm{T}}$ to obtain $\mathbf{Q}^{\mathrm{T}}$

- $\mathbf{Y} = \mathbf{Q}^{\mathrm{T}}\mathbf{X}$ with $\mathbf{Q}^{\mathrm{T}}\mathbf{Q} = \mathbf{I}_{\boldsymbol{d}}$.

Reconstruction: of $\mathbb{R}^m$ from $\mathbb{R}^d$ removes $m - d$ columns of $\mathbf{R}$ to obtain $\mathbf{Q}$

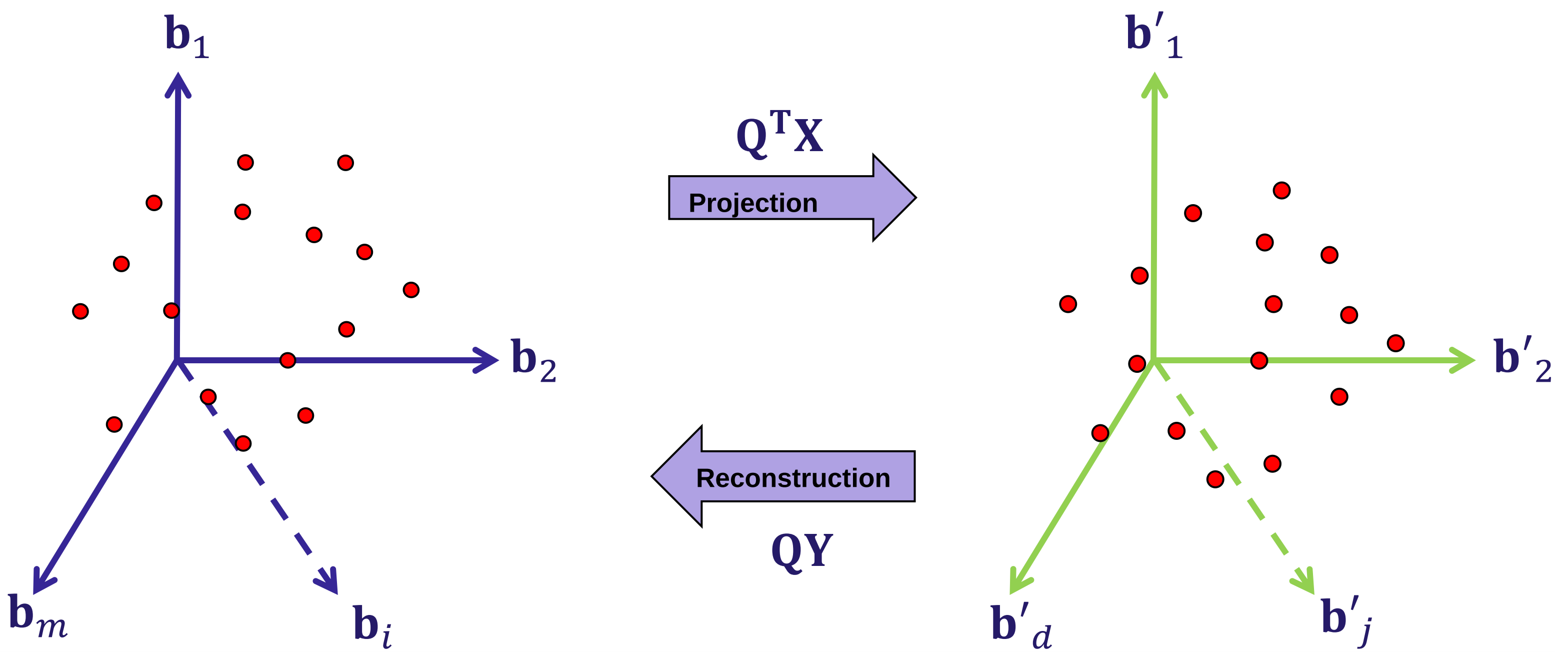
- $\mathbf{X} = \mathbf{Q}\mathbf{Y}$ with $\mathbf{Q}^{\mathrm{T}}\mathbf{Q} = \mathbf{I}_{\boldsymbol{d}}$.

$\det(\mathbf{R}) = +1$ implies a *Rotation* matrix.

Dimensionality Reduction

Idea: Projection of higher dimensional data to a lower dimensional subspace.

- $\mathbf{X} \in \mathbb{R}^m \rightarrow \mathbf{Y} \in \mathbb{R}^d$ **where** $\boxed{d \ll m}$ ***Information is LOST**



- ***Linear*** **Dimensionality Reduction using PCA computes** $\mathbf{Q} = \mathbf{VI}_d$.

Metric Multi Dimensional Scaling

PCA uses Covariance matrix

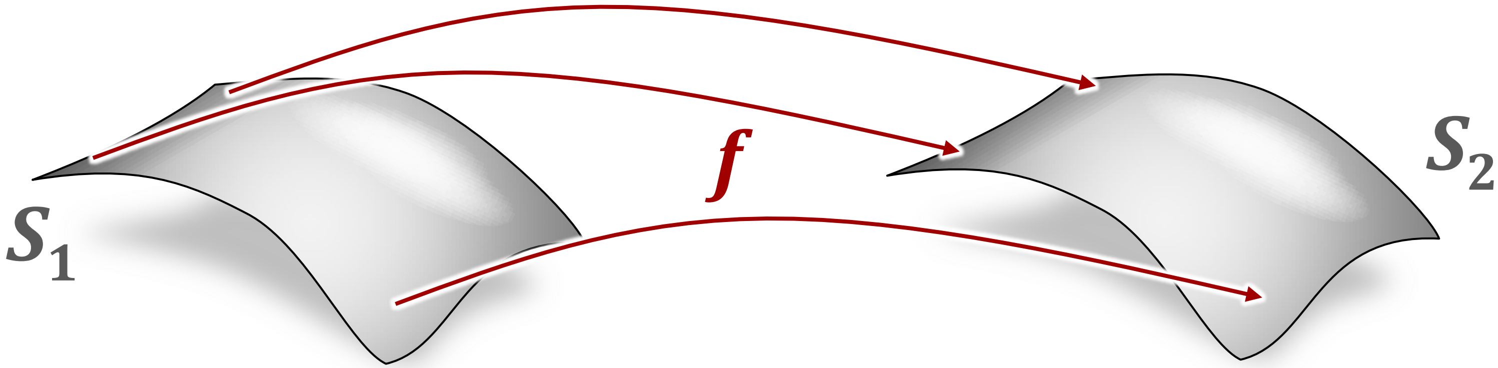
- $\mathbf{S} = \frac{1}{n}\mathbf{X}\mathbf{X}^{\mathrm{T}}$ assuming *centered* data (*i.e.* zero mean).
- The data points are represented in a vector space.
- Dimension of $\mathbf{S}$ is $m \times m$.

MDS uses Gram Matrix (*dot products*)

- $\mathbf{G} = \mathbf{X}^{\mathrm{T}}\mathbf{X}$ captures (dis)similarity of data points.
- The data points are *not explicitly required*.
- Dimension of $\mathbf{G}$ is $n \times n$.
- Goal is to *embed* the data in d-dimensional space such that some metric is preserved.

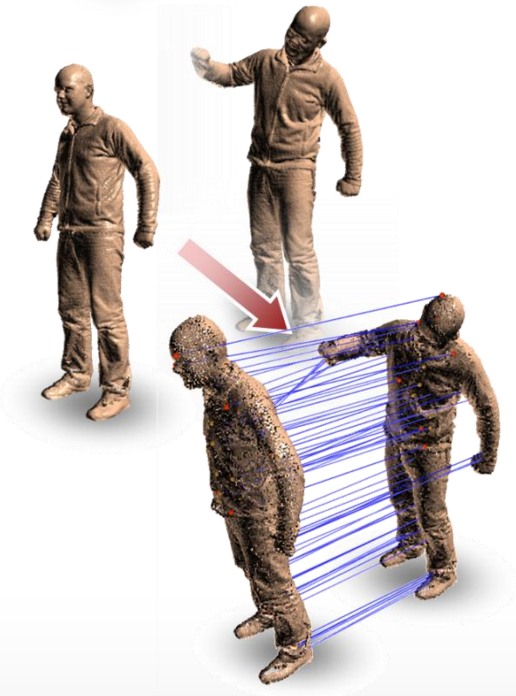
Part III: Intrinsic Geometry and Intrinsic Mappings

Scenario



Mapping between Surfaces

- Intrinsic view – only metric tensor
- Ignore isometric deformations
- Applications:
  - Deformable shape matching
  - Texture mapping (flat $\rightarrow$ 3D) "parametrization"



Differential Geometry Revisited

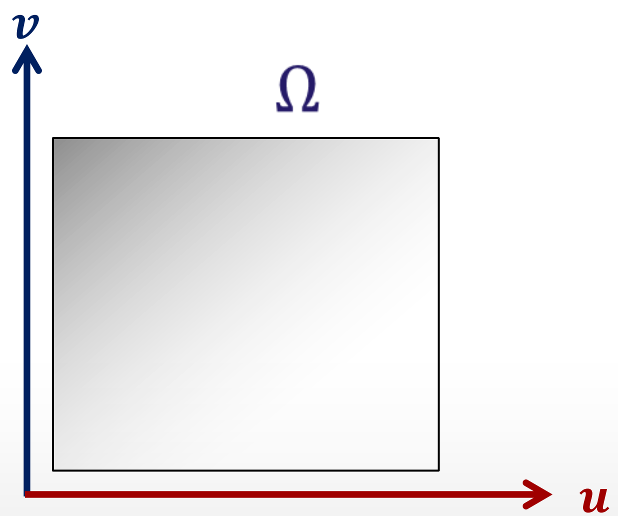
Parametric Patches

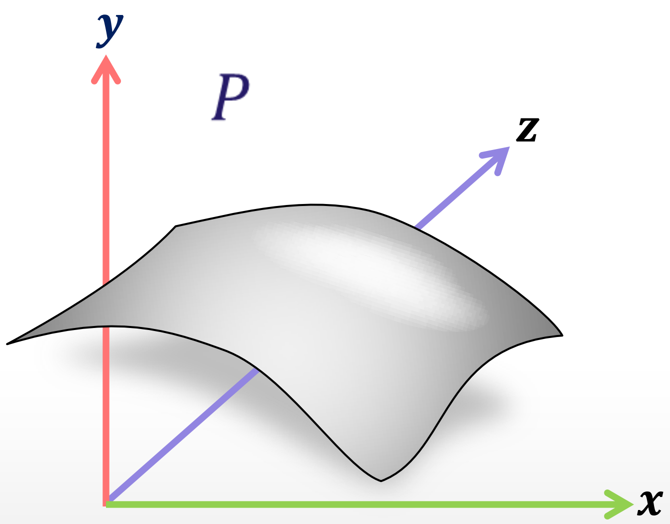
Parametric Surface Patches:

A smoothly differentiable function

$$f : \mathbb{R}^2 \supseteq \Omega \to \mathbb{R}^3 \text{ describes } P = f(\Omega), P \subseteq \mathbb{R}^3.$$

$$f(u,v) = \big(x(u,v), y(u,v), z(u,v)\big)$$

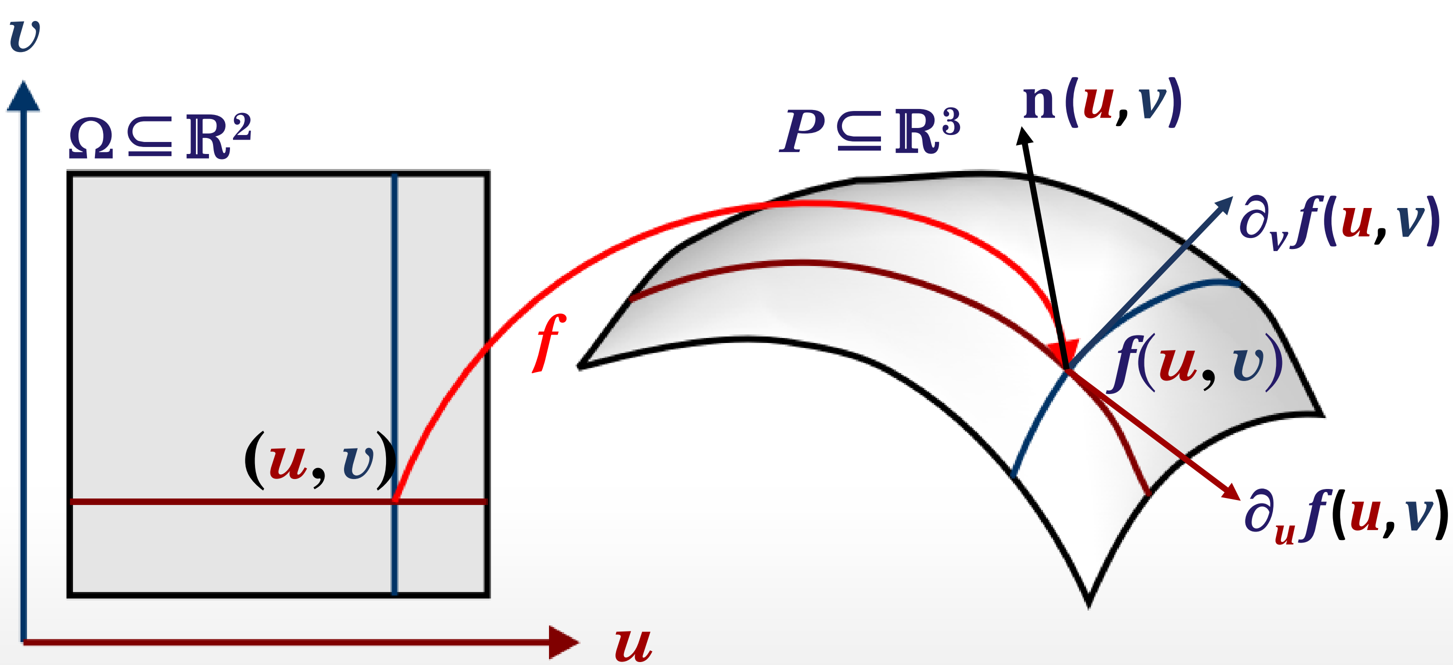




Parametric Patches

Function $f(u,v) \to \mathbb{R}^3$

- Canonical tangents: $\partial_u f(u,v),\ \partial_v f(u,v)$
- Normal: $\mathbf{n}(u,v) = \frac{\partial_u f(u,v) \times \partial_v f(u,v)}{\|\partial_u f(u,v) \times \partial_v f(u,v)\|}$

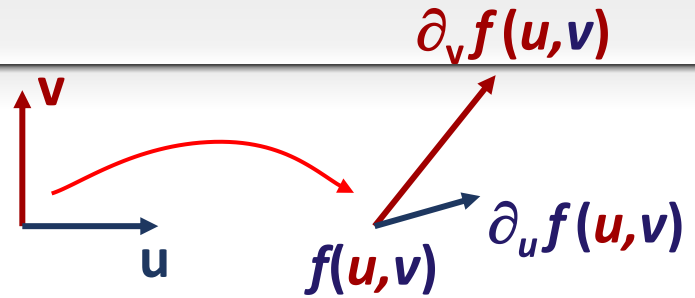


Fundamental Forms

Fundamental Forms:

- Describe the local parameterized surface.
- Measure...
  - ...distortion of length (first fundamental form)
  - ...surface curvature (second fundamental form)

First Fundamental Form



First Fundamental Form

- Also known as ***metric tensor***.
- It can be written as a 2×2 symmetric matrix:

$$\mathbf{I} = \begin{pmatrix} \partial_u f \partial_u f & \partial_u f \partial_v f \\ \partial_u f \partial_v f & \partial_v f \partial_v f \end{pmatrix} =: \begin{pmatrix} E & F \\ F & G \end{pmatrix}$$

- The matrix is symmetric and positive definite (regular parametrization, semi-definite otherwise)
- Defines a *generalized scalar product* that measures lengths and angles *on the surface*.

Second Fundamental Form

Second Fundamental Form

- Also known as *shape operator* or *curvature tensor*.
- It can be written as a 2×2 symmetric matrix:

$$\mathbf{II} = \begin{pmatrix} \partial_{uu} f . \mathbf{n} & \partial_{uv} f . \mathbf{n} \\ \partial_{uv} f . \mathbf{n} & \partial_{vv} f . \mathbf{n} \end{pmatrix} =: \begin{pmatrix} e & f \\ f & g \end{pmatrix}$$

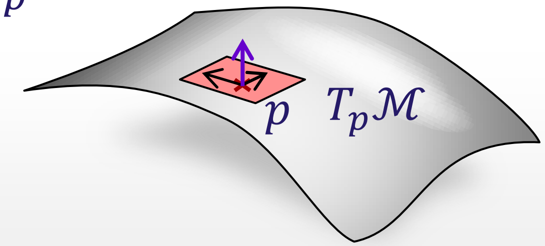
Eigen-analysis:

- Eigenvalues of *second fundamental form* for an *orthonormal tangent* basis are called *principal curvatures* κ_1, κ_2.
- Corresponding orthogonal eigenvectors are called *principal directions of curvature*.

How to build a metric

Tangent Space

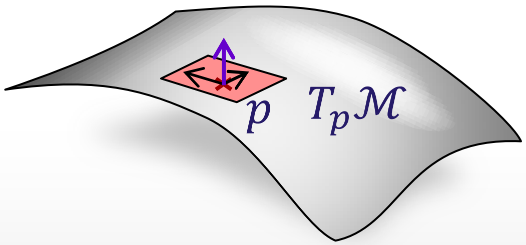
- For a d-dimensional manifold $\mathcal{M}$, at each point $p \in \mathcal{M}$ there exist a vector space $T_p\mathcal{M}$, called "*Tangent Space*".
- It consist of all tangent vectors to manifold at point p.
- A metric at point p is a function $g_p: T_p\mathcal{M} \times T_p\mathcal{M} \to \mathbb{R}$ such that:
  - g_p is Bilinear : $g_p(a\boldsymbol{\alpha}_p + b\boldsymbol{\beta}_p, \boldsymbol{\gamma}_p) = a g_p(\boldsymbol{\alpha}_p, \boldsymbol{\gamma}_p) + b g_p(\boldsymbol{\beta}_p, \boldsymbol{\gamma}_p)$ and $g_p(\boldsymbol{\gamma}_p, a\boldsymbol{\alpha}_p + b\boldsymbol{\beta}_p) = a g_p(\boldsymbol{\gamma}_p, \boldsymbol{\alpha}_p) + b g_p(\boldsymbol{\gamma}_p, \boldsymbol{\beta}_p)$
  - g_p is Symmetric: $g_p(\boldsymbol{\alpha}_p, \boldsymbol{\beta}_p) = g_p(\boldsymbol{\beta}_p, \boldsymbol{\alpha}_p)$
  - g_p is Non-degenerated: $\boldsymbol{\beta}_p \mapsto g_p(\boldsymbol{\alpha}_p, \boldsymbol{\beta}_p), \ \forall \boldsymbol{\alpha}_p \neq \mathbf{0}$



How to build a metric

Inner Product Metric

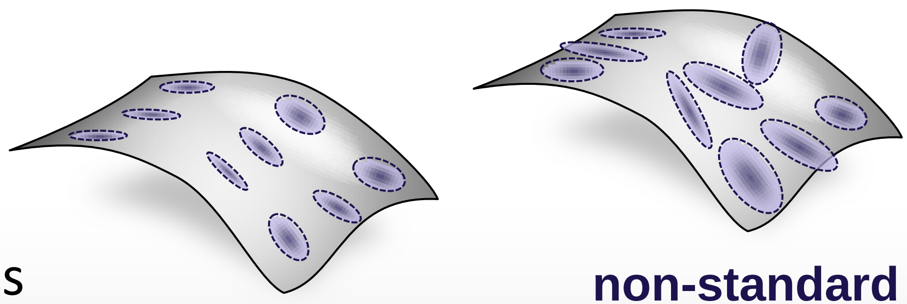
- Two tangent vector at point p can be defined as:
  - $\boldsymbol{\alpha_p} = \alpha_1 \partial_u f + \alpha_2 \partial_{\boldsymbol{v}} f$ and $\boldsymbol{\beta_p} = \beta_1 \partial_u f + \beta_2 \partial_{\boldsymbol{v}} f$
- The Inner product is defined as:
  - $g_p(\boldsymbol{\alpha_p}, \boldsymbol{\beta_p}) = \langle \boldsymbol{\alpha_p}, \boldsymbol{\beta_p} \rangle = [\alpha_1 \quad \alpha_2] \begin{bmatrix} E & F \\ F & G \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix}$
  - It inherently uses the first fundamental form.
- $g_p(\boldsymbol{\alpha_p}, \boldsymbol{\beta_p})$ is *symmetric*, *bilinear* and *non-degenerated* and hence a metric.



Riemannian Manifolds

Riemannian Manifold

- Manifold topology, d-dimensional
  - We mostly focus on 2-manifolds, embedded in $\mathbb{R}^3$
- Real differentiable manifold.
- Local parametrization: tangent space
- Intrinsic metric (metric tensor everywhere)
  - Allows to define various geometric notions on manifold:
    - Angles
    - Lengths of curves
    - Areas (or volumes)
    - Curvature
    - Gradients of functions
    - Divergence of vector fields



standard metric

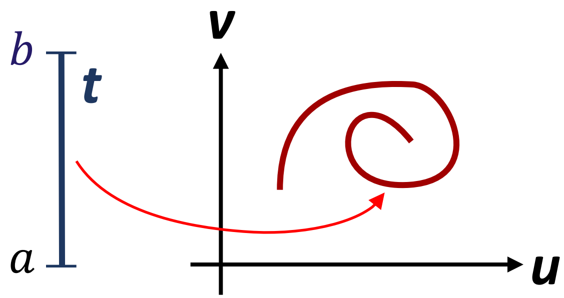
non-standard (pos-def.)

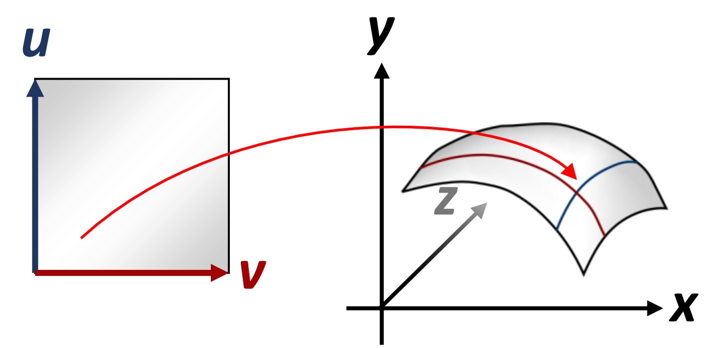
Riemannian Manifolds

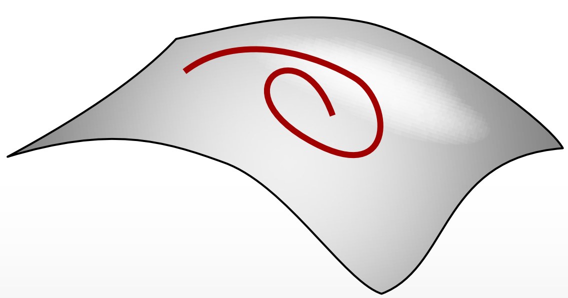
Arclength:

- Let $g(t) = (u, v)$, in an interval $[a, b]$.
- $f\big(u(t), v(t)\big)$ will trace out a parametric curve in P.

Arclength of parametric curve in interval $[a, b]$:







Riemannian Manifolds

Arclength:

- Let $g(t) = (u, v)$, in an interval $[a, b]$.
- $f\big(u(t), v(t)\big)$ will trace out a parametric curve in P.

Arclength of parametric curve in interval $[a, b]$:

$$
\begin{aligned}
s &= \int_a^b \left\| \frac{d}{dt} f\big(u(t), v(t)\big) \right\| dt \\
&= \int_a^b \| du\, \partial_u f + dv\, \partial_v f \| dt \\
&= \int_a^b \sqrt{du^2 \partial_u f . \partial_u f + 2du\, dv\, \partial_u f . \partial_v f + dv^2 \partial_v f . \partial_v f}\; dt \\
&= \int_a^b \sqrt{du^2 E \; + 2du\, dv\, F + dv^2 G}\; dt \\
&= \int_a^b \sqrt{\begin{bmatrix} du & dv \end{bmatrix} \begin{bmatrix} E & F \\ F & G \end{bmatrix} \begin{bmatrix} du \\ dv \end{bmatrix}}\; dt
\end{aligned}
$$

Riemannian Manifolds

Surface Area:

- Apply integral transformation theorem:

$$\text{area}(P) = \iint_{\Omega} \|\partial_u f \times \partial_v f\| \, du \, dv$$

- Using Langrange's identity:

$$\text{area}(P) = \iint_{\Omega} \sqrt{(\partial_u f . \partial_u f)(\partial_v f . \partial_v f) - (\partial_u f . \partial_v f)^{2}} \, du \, dv$$

$$= \iint_{\Omega} \sqrt{EG - F^{2}} \, du \, dv$$

$$= \iint_{\Omega} \sqrt{\det \begin{bmatrix} E & F \\ F & G \end{bmatrix}} \, du \, dv$$

Riemannian Manifolds

Curvature:

- **Principle Curvature :** Eigenvalues of *second fundamental form* for an *orthonormal tangent* basis.

  κ_1, κ_2

- **Normal Curvature :** *norm of the projection of the derivative* $\frac{d\boldsymbol{T}}{ds}$ *on normal plane* $\mathbf{n}$.

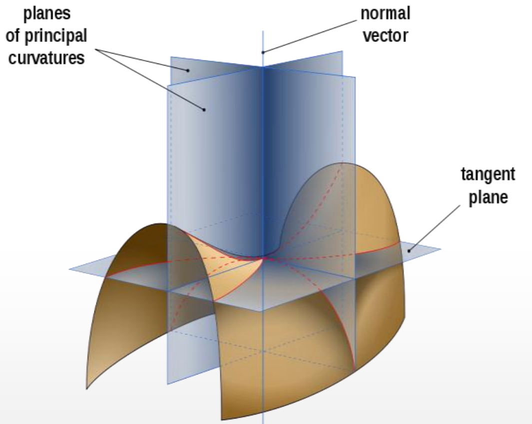
  $\kappa_N = \kappa(\mathbf{n}) = \mathbf{n}^T \begin{pmatrix} e & f \\ f & g \end{pmatrix} \mathbf{n}$ with $max(\kappa(\mathbf{n})) = \kappa_1$ and $min(\kappa(\mathbf{n})) = \kappa_2$

- **Mean Curvature :**

  $$H = \frac{1}{2}(\kappa_1 + \kappa_2) = \det\begin{pmatrix} e & f \\ f & g \end{pmatrix}$$

- **Gaussian Curvature :**

  $$K = \kappa_1 \kappa_2 = \frac{1}{2}\mathrm{tr}\begin{pmatrix} e & f \\ f & g \end{pmatrix}$$



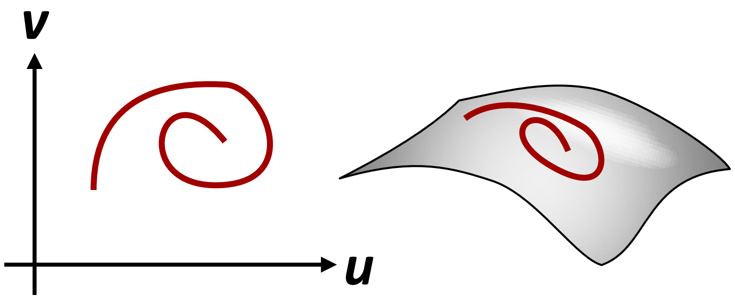
Source: Wikipedia

Riemannian Manifolds

Curvature:

- **Geodesic Curvature :** norm of the projection of the derivative $\frac{dT}{ds}$ on the tangent plane.
  - **It allows to distinguish inherent curvature of the curve in the *(u,v)* space from the curvature induced by mapping f in $\mathcal{M}$.**
- **Total Curvature :**

$$\kappa_T = \sqrt{\kappa_N^2 + \kappa_g^2}$$



- **For circles :** $\kappa_N = 1.$
- **For *Great* circles :** $\kappa_T = \kappa_N = 1$, $\kappa_g = 0$ *i.e. locally Flat e.g.* Earth
- **For *Small* circles of radius** r **:** $\kappa_g = \sqrt{1 - r^2/r}$

Riemannian Manifolds

Geodesics:

- Curves on a surface which minimize length between the end points are called *Geodesics.*

$$s = \int_a^b \sqrt{\begin{bmatrix} du & dv \end{bmatrix} \begin{bmatrix} E & F \\ F & G \end{bmatrix} \begin{bmatrix} du \\ dv \end{bmatrix}}\, dt$$

$$energy = \int_a^b \begin{bmatrix} du & dv \end{bmatrix} \begin{bmatrix} E & F \\ F & G \end{bmatrix} \begin{bmatrix} du \\ dv \end{bmatrix} dt$$

- A path minimizing *energy* is just a geodesic parameterized by *arc length*.
- A curve on a surface with zero *geodesic curvature* is a geodesic.

Types of Mappings

Given: Riemannian Manifolds $\mathcal{M}_1, \mathcal{M}_2$

Consider: Functions $\psi: \mathcal{M}_1 \to \mathcal{M}_2$

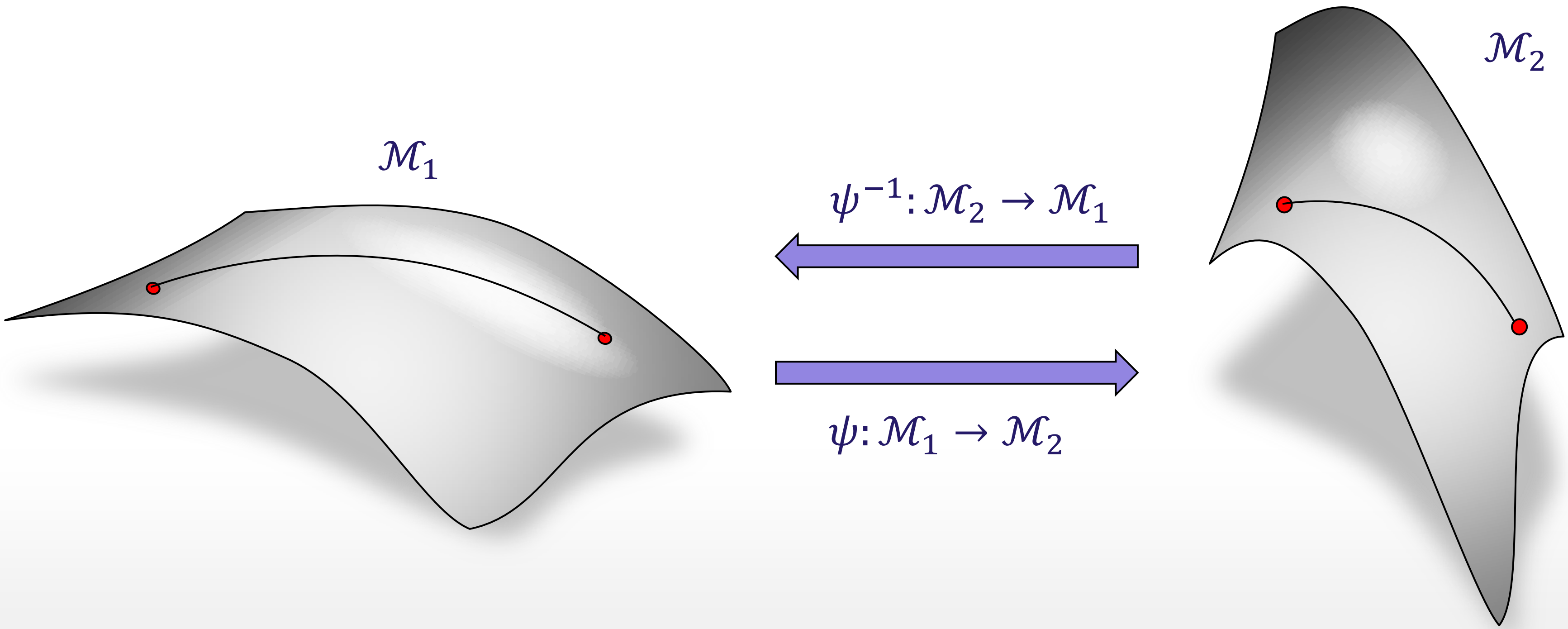
Important types of mappings:

- *Isometric*: preserves distances, angles and area
- *Conformal*: preserves (only) angles
- *Equi-areal (incompressible)*: preserves area

Isometric Mapping

Definition

- An mapping ψ between two surface patch $\mathcal{M}_1$ and $\mathcal{M}_2$ is an isometric mapping if it preserves distance on them.
- An isometric mapping is **symmetric** *i.e.* ψ^{-1} is also an isometry.

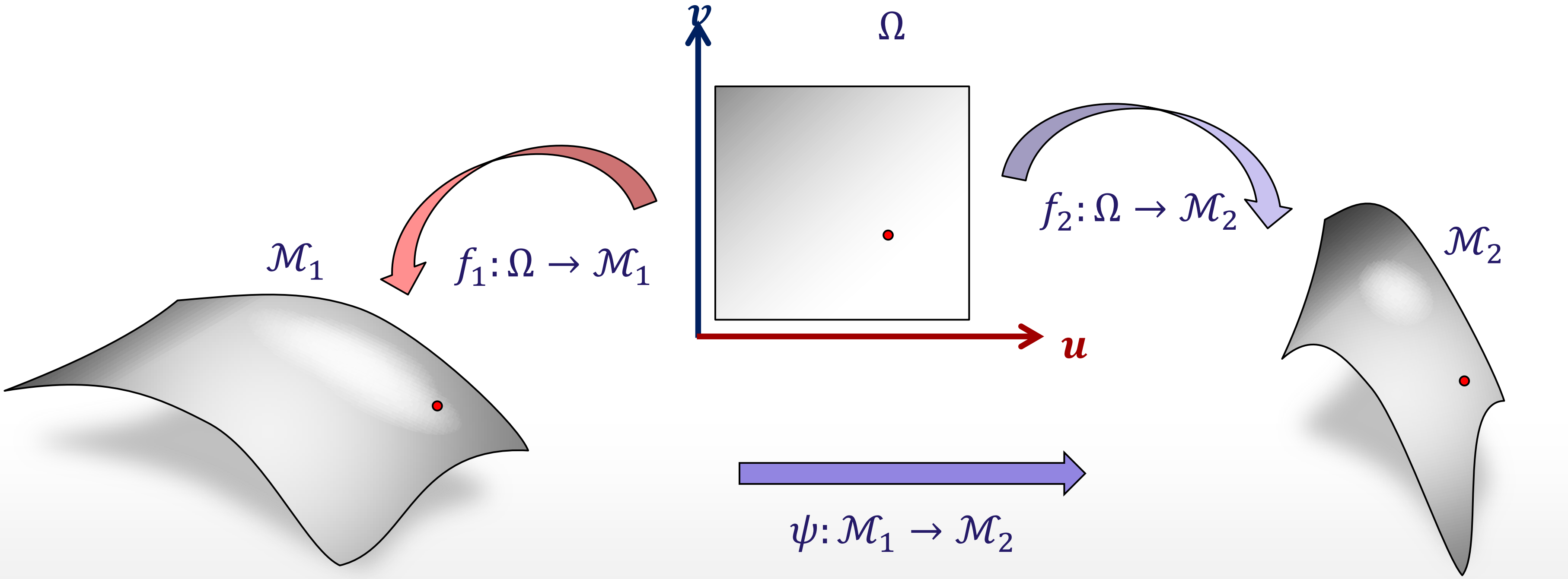


Isometric Mapping

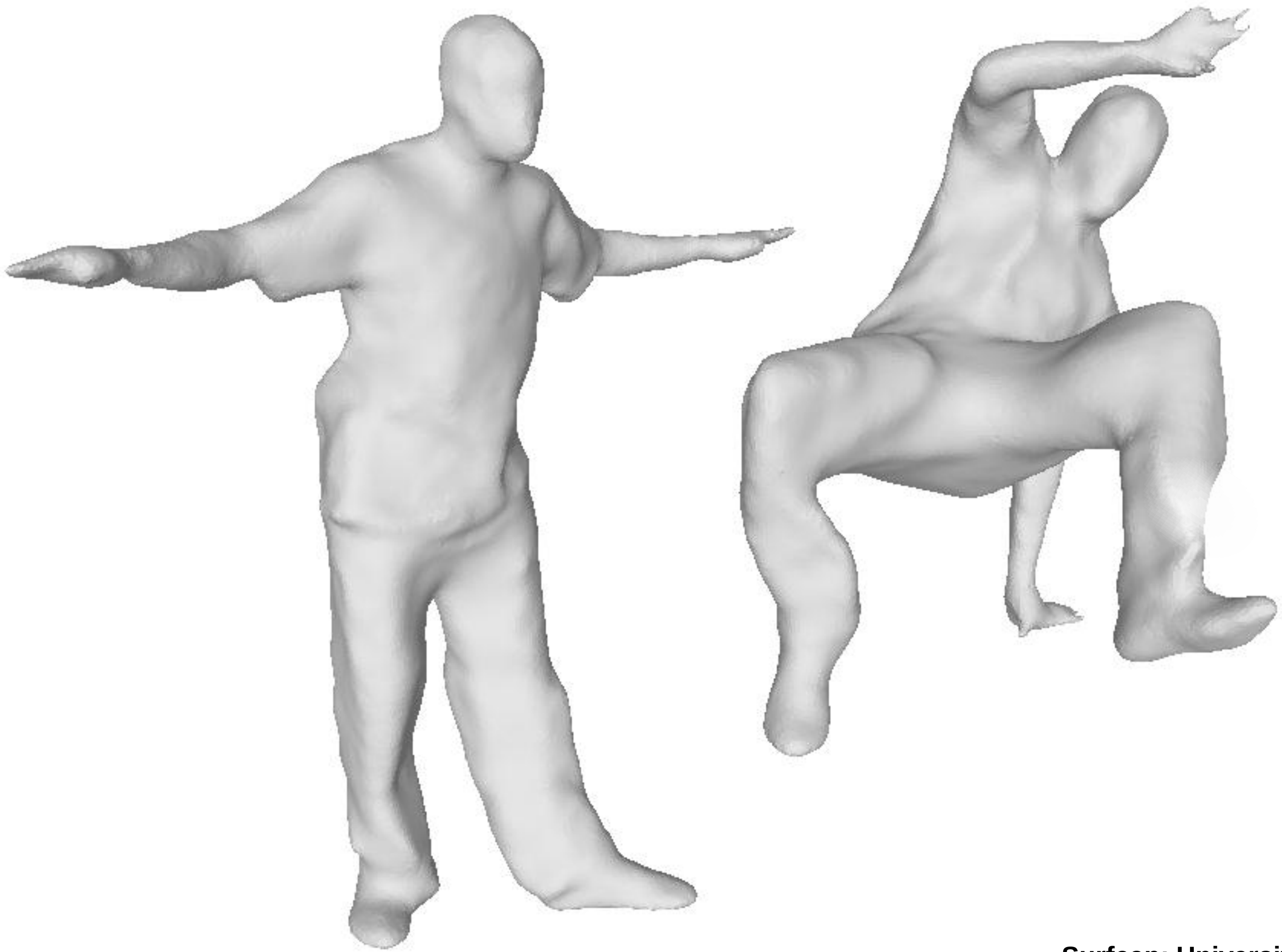
Isometric surfaces have same parametric domain

- If $\psi: \mathcal{M}_1 \to \mathcal{M}_2$ is an isometric mapping then both surfaces have same intrinsic parameterization. *i.e.*

$$f_1^{-1}(\mathcal{M}_1) = f_2^{-1}(\mathcal{M}_2) = \Omega(u, v)$$



Isometric Mapping

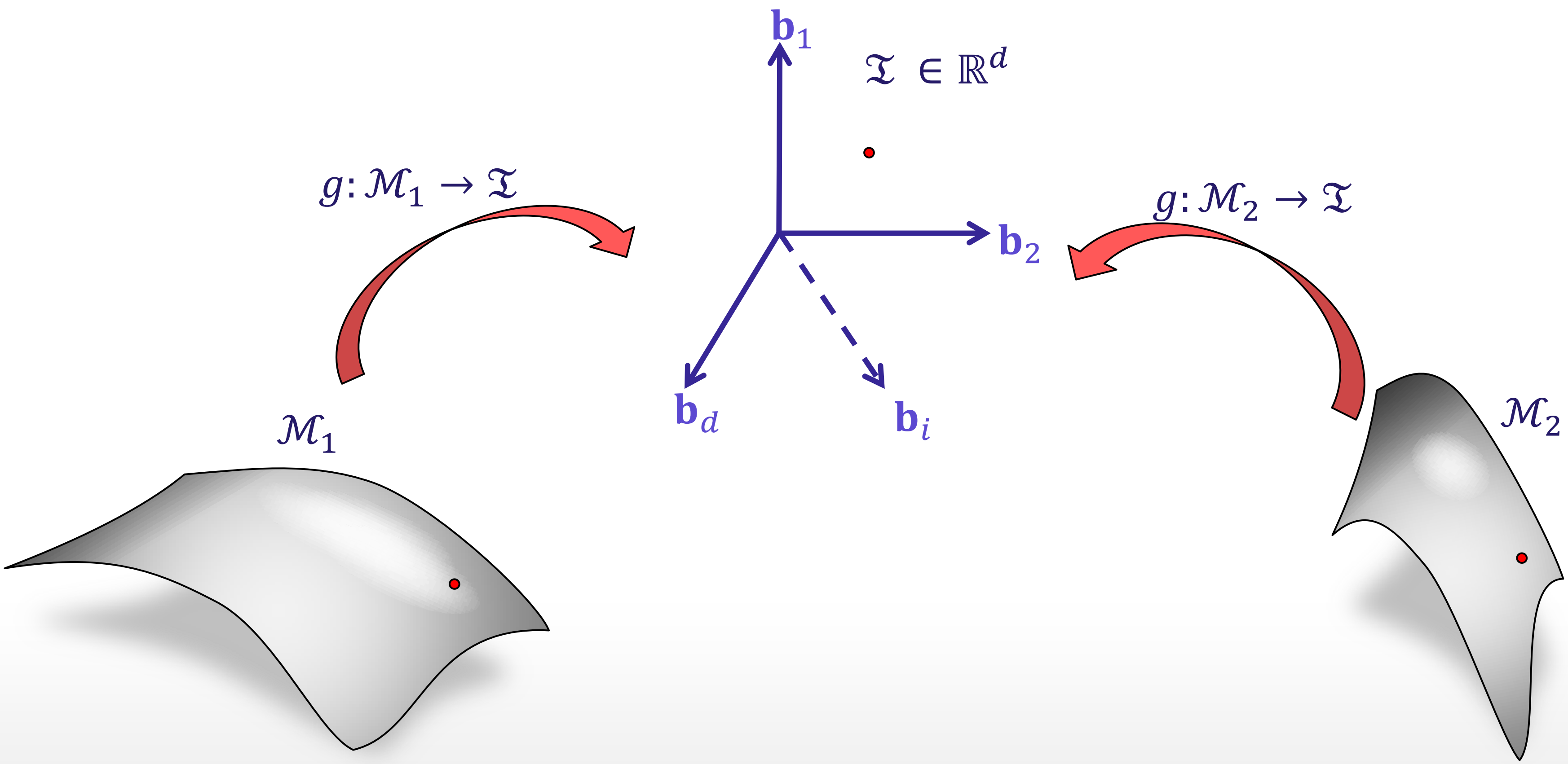


Surfcap: University of Surry

Isometric Mapping

To solve Isometry

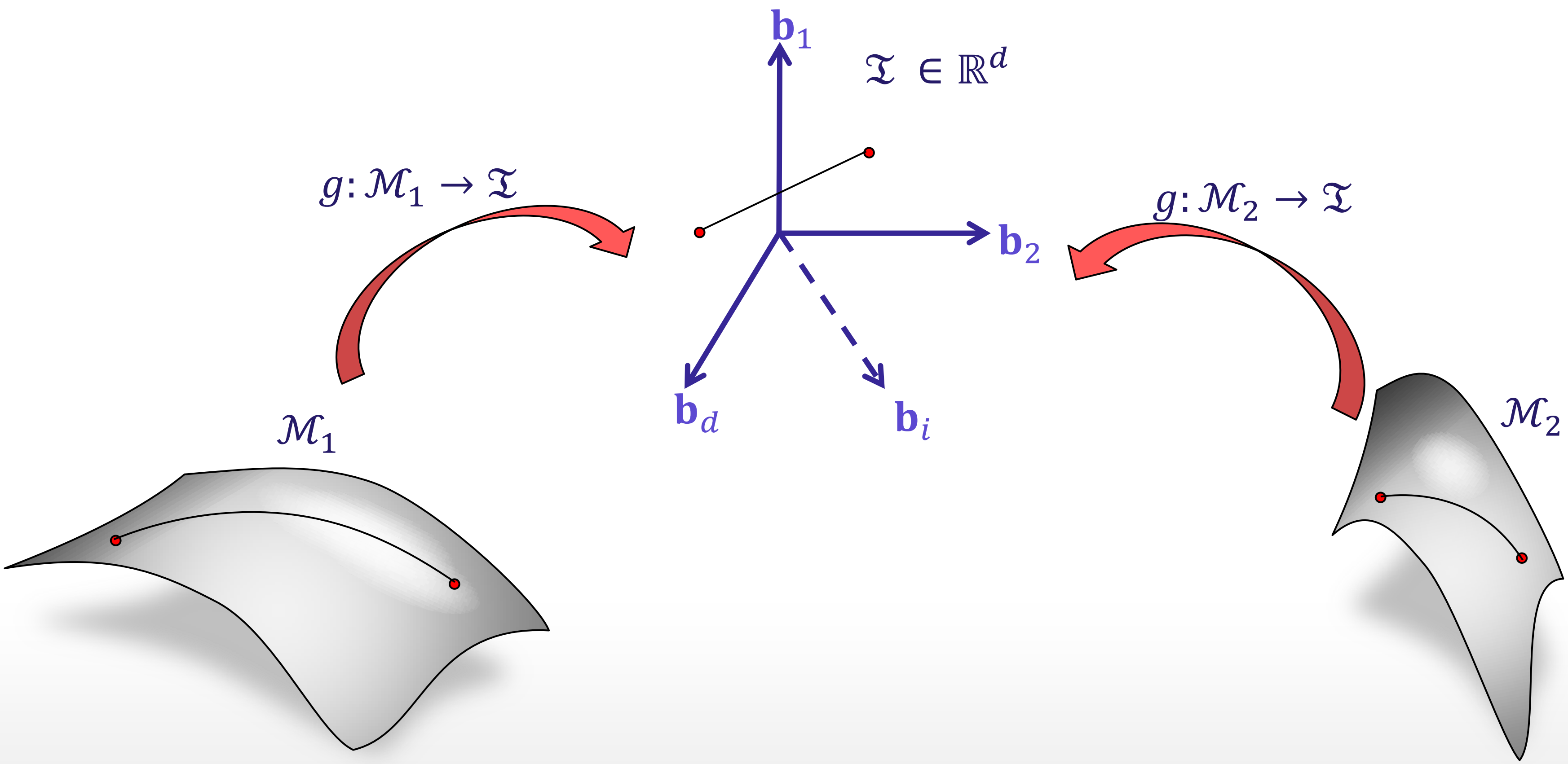
- **Either** find the explicit parameterization f_1 and f_2 to recover the implicit domain.
- **OR** find an intrinsic mapping g of $\mathcal{M}_1$ and $\mathcal{M}_2$ to an isometry invariant space $\mathfrak{T}$.



Isometric Mapping

Property of Isometry Invariant Space

- **Geodesic** distance between any pair of points in $\mathcal{M}_1$ and their images in $\mathcal{M}_2$ should be equivalent to **Euclidean** distance between their images in $\mathfrak{T}$.

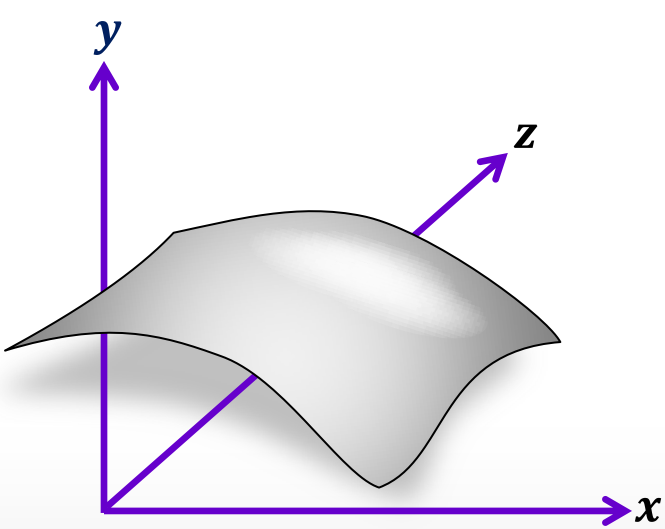


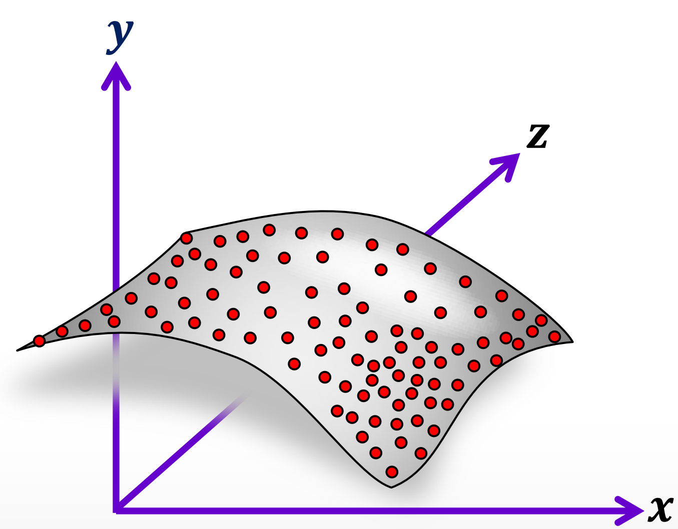
Spectral Graph Methods for 3D Shape Analysis

Discrete Manifold Representation

Surface Patches in Practice

- Most existing shape acquisition methods often yield noisy point clouds instead of a nice parametric surface representation.
- Finding a parameterization of complex real world object is practically infeasible.

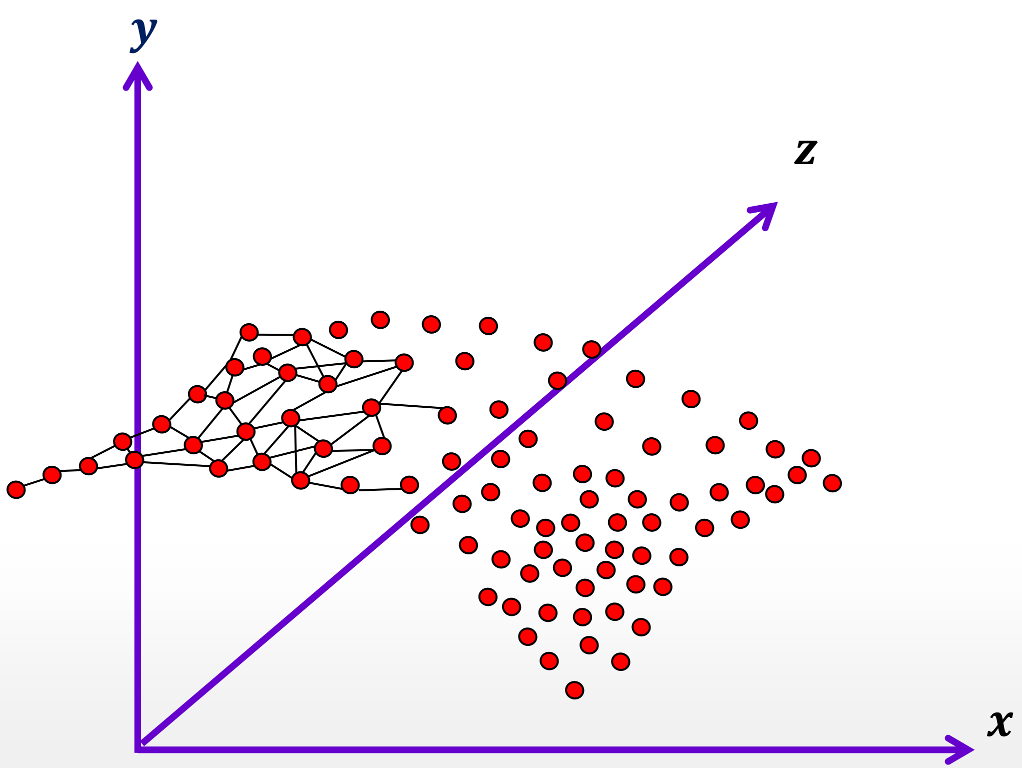




Graph Based Representation

Represent surface patch with an underlying locally connected graph structure

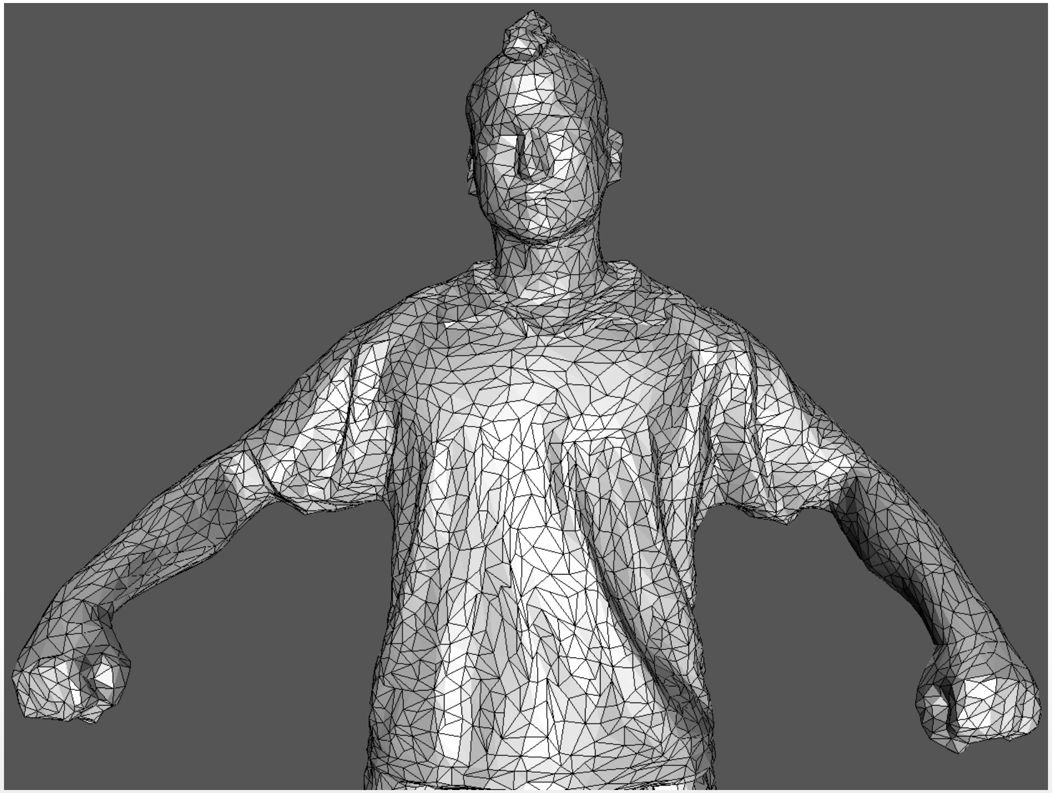
- Distances are assumed to be locally Euclidean.
- In practice we assume that Isometric transforms keep the **topology** (*i.e.* the *connectivity*) of underlying graph intact.



Graph Based Representation

Popular Representation

- **Mesh** representation of 3D object is traditionally popular.
- It enables a direct application of Graph based tools for shape analysis tasks.



Spectral Graph Theory (SGT)

Spectral Graph Theory analyze properties of graphs via eigenvalues and eigenvectors of various graph matrices.

- Builds on well studied algebraic properties of graph matrices.
- Provides a natural link between **differential operators** on continuous and discrete manifold representation.
- Allows to ***Embed*** a discrete manifold (graph) into an isometry invariant space.
- Provide intrinsic ***Spectral metric*** for isometry invariant distance computation.

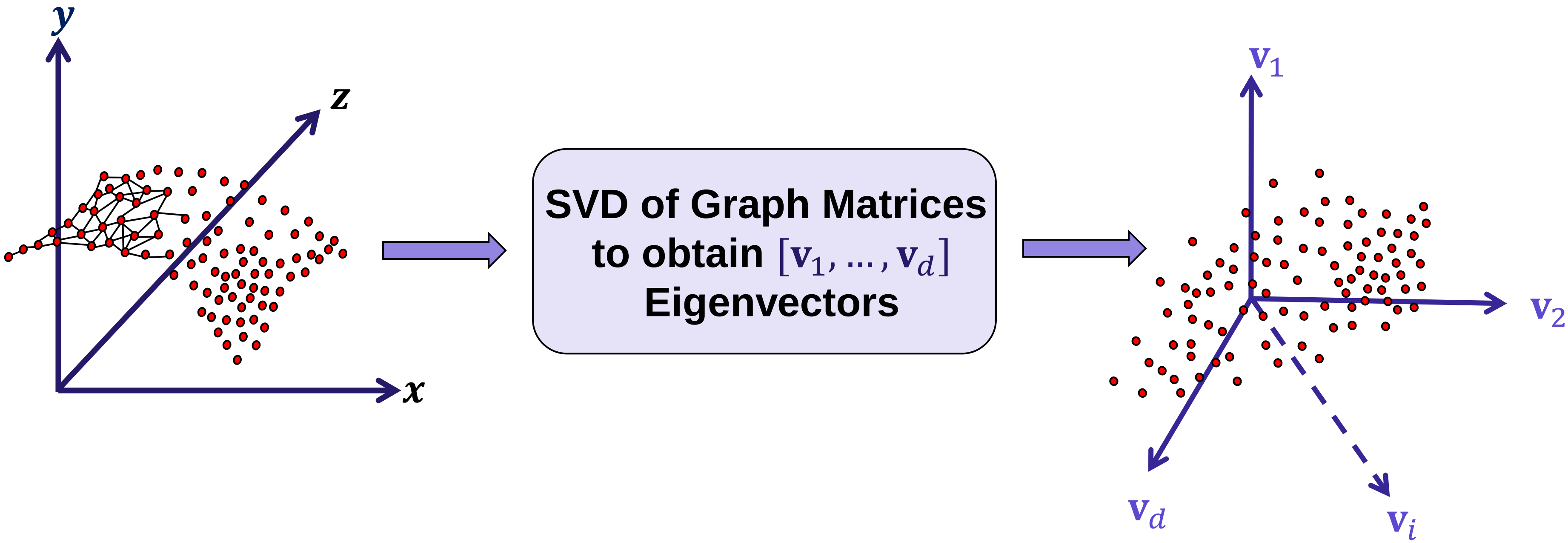
References:

- F. R. K. Chung. Spectral Graph Theory. 1997.
- M. Belkin and P. Niyogi. Laplacian Eigenmaps for Dimensionality Reduction and Data Representation. Neural Computation, 15, 1373{1396 (2003).
- U. von Luxburg. A Tutorial on Spectral Clustering. Statistics and Computing, 17(4), 395{416 (2007).*
- Software: http://open-specmatch.gforge.inria.fr/index.php.

Spectral Graph Theory (SGT)

Isometry Invariant Space

Spectral Embedding



Input $\mathbb{R}^3$ space

Output $\mathbb{R}^d$ space

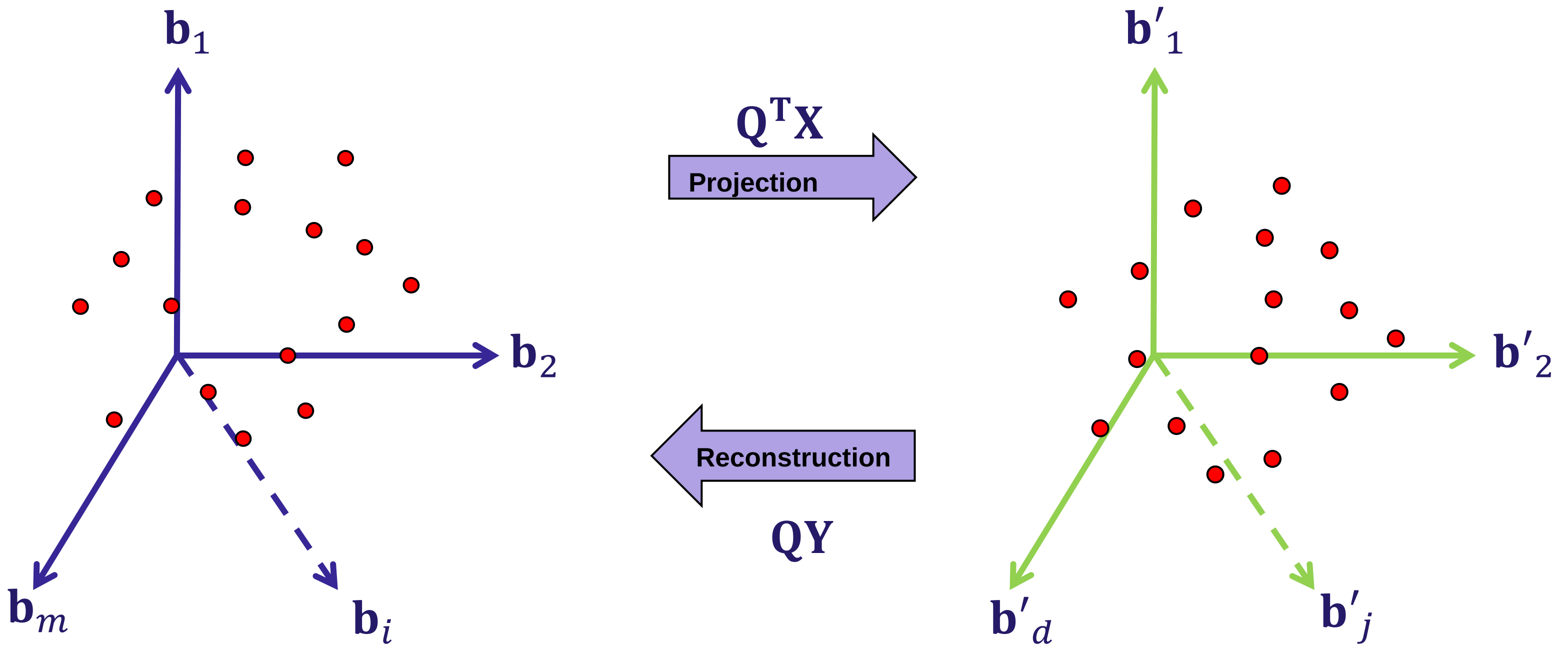
Geodesic distances in the input space $\mathbb{R}^3$ can be approximated by Euclidean distances in the new space $\mathbb{R}^d$ spanned by eigenvectors of certain Graph matrices.

* Typically $d \gg 3$, *i.e. we can now embed the surface in a higher dimensional space.*

Recall Dimensionality Reduction (DR)

Idea: Projection of higher dimensional data to a lower dimensional subspace.

- $\mathbf{X} \in \mathbb{R}^m \rightarrow \mathbf{Y} \in \mathbb{R}^d$ **where** $\boxed{d \ll m}$ ***Information is LOST**



- ***Linear*** **Dimensionality Reduction using PCA computes** $\mathbf{Q} = \mathbf{VI}_d$.

Difference between SGT and DR

In Dimensionality Reduction

- In linear DR (PCA) we consider eigendecomposition of Scatter/Covariance matrix of size ($m \times m$), where m is the original dimension of input data.
- Matrices here are typically **full** with all entries as non-zero.
- We find a least square fitting of the data.

In Spectral Graph Theory

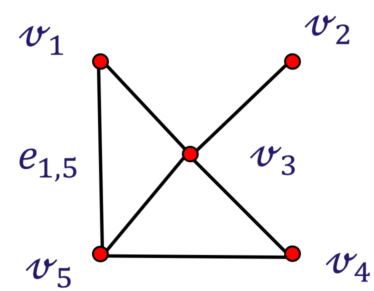
- We consider eigen-decomposition of various Graph matrices of size ($n \times n$) where n is the number of data points.
- Matrices here are typically **sparse** with very few entries as non-zero.
- We minimize a different criteria that preserve geodesic distances on the surface patch.

Graph Matrices

Basic Graph Notations

- Consider a simple graph with no loops and multiple edges $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$:
  - $\mathcal{V} = \{v_1, \dots, v_n\}$ as vertex set with its cardinality *i.e.* (number of vertices) $|\mathcal{V}| = n$.
  - $\mathcal{E} = \{e_{i,j}\}$ as edge set with each element $e_{i,j}$ representing an edge between two adjacent vertex $v_j \backsim v_i$.

Adjacency and Degree Matrix



A graph with 5 vertices and 6 edges.

- Adjacency matrix of graph $\mathcal{G}$ is a *symmetric* matrix :
  - $\mathbf{A} = [a_{i,j}]_{n\times n}$ with $a_{i,j} = \begin{cases} \omega_{i,j} & \text{if } e_{i,j} \in \mathcal{E} \\ 0 & \text{if } e_{i,j} \notin \mathcal{E} \\ 0 & \text{if } i = j \end{cases}$
  - $\omega_{i,j}$ is a weight assigned to each edge and in case of unweighted graph $\omega_{i,j} = 1$.

- Degree matrix of graph $\mathcal{G}$ is :
  - $\mathbf{D} = [diag(d_i)]_{n\times n}$ where $d_i = \sum_{\forall v_j \sim v_i} \omega_{i,j}$.
  - A graph $\mathcal{G}$ is ***connected*** if $d_i > 0, \forall i \in \{1{:}n\}$
  - A graph $\mathcal{G}$ is ***regular*** if $d_i = d_j, \forall i\, \forall j \in \{1{:}n\}$

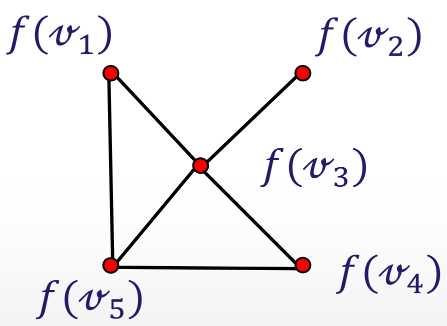
$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \end{bmatrix}, \mathbf{D} = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 3 \end{bmatrix}$$

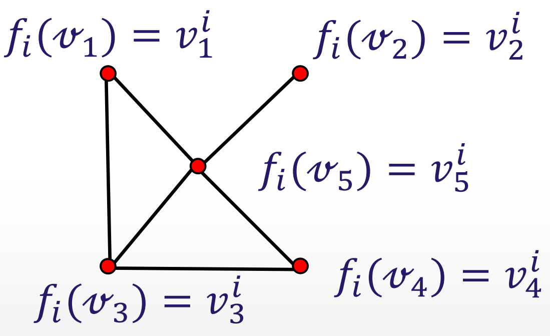
Discrete Functions on Graph

Definition

- Let f be a smooth real valued function on graph $\mathcal{G}$ such that $f\colon \mathcal{V} \to \mathbb{R}$.
  - It assign a real number to each node of the graph.
  - A discrete **vector** representation of a continuous function f is written as $\boldsymbol{f} \in \mathbb{R}^n$ where $\boldsymbol{f} = (f(v_1), \dots, f(v_n))^{\boldsymbol{T}}$.

- Eigen-decomposition of Adjacency matrix $\mathbf{A}$ yields n smooth eigenvectors that can be seen as discrete functions defined on graph vertices.
  - $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$ with $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_n]$ as matrix of eigenvectors.
  - Hence $\mathbf{v}_i = (f_i(v_1), \dots, f_i(v_n))^{\boldsymbol{T}} = (v_1^i, \dots, v_n^i)^{\boldsymbol{T}}$



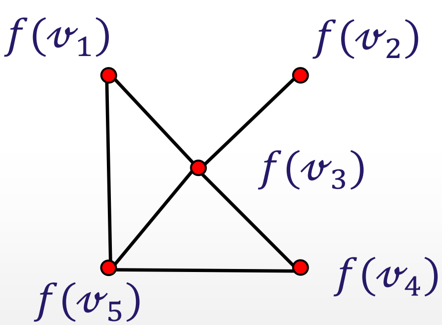


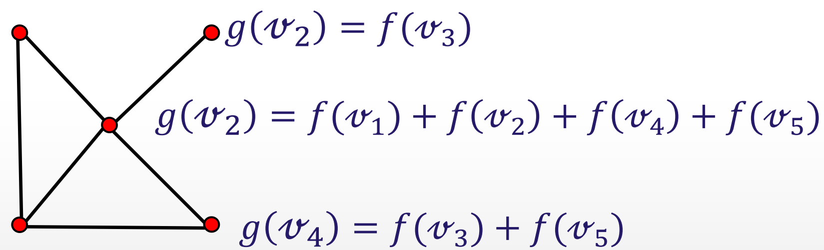
Graph Matrix as Discrete Operator

Adjacency Matrix as an Operator

- Adjacency matrix $\mathbf{A}$ can be viewed as an operator.
  - $\boldsymbol{g} = \mathbf{A}\boldsymbol{f}$ where $\boldsymbol{g}(v_i) = \sum_{\forall v_j \sim v_i} f(v_j)$
- In quadratic form we can write.
  - $\boldsymbol{f}^T\mathbf{A}\boldsymbol{f} = \sum_{e_{i,j}} f(v_i)f(v_j)$

$$\begin{bmatrix} g(v_1) \\ g(v_2) \\ g(v_3) \\ g(v_4) \\ g(v_5) \end{bmatrix} = \boldsymbol{g} = \mathbf{A}\boldsymbol{f} = \begin{bmatrix} 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} f(v_1) \\ f(v_2) \\ f(v_3) \\ f(v_4) \\ f(v_5) \end{bmatrix} = \begin{bmatrix} f(v_3) + f(v_5) \\ f(v_3) \\ f(v_1) + f(v_2) + f(v_4) + f(v_5) \\ f(v_3) + f(v_5) \\ f(v_1) + f(v_3) + f(v_4) \end{bmatrix}$$





Discrete Laplace Operator

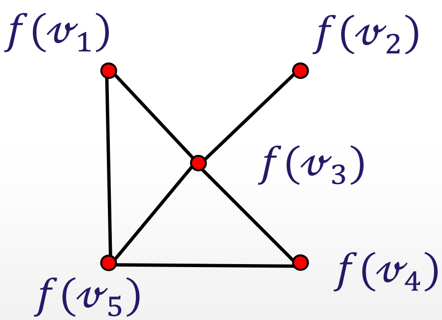
Laplacian Matrix

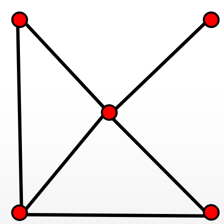
- Laplacian matrix $\mathbf{L}$ of graph $\mathcal{G}$ is a $n \times n$ *symmetric* matrix :

$$\mathbf{L} = \mathbf{D} - \mathbf{A}$$

- This matrix can also be viewed as an operator :
  - $\boldsymbol{g} = \mathbf{L}\boldsymbol{f}$ where $\boldsymbol{g}(v_i) = \sum_{\forall v_j \sim v_i} \big(f(v_i) - f(v_j)\big)$

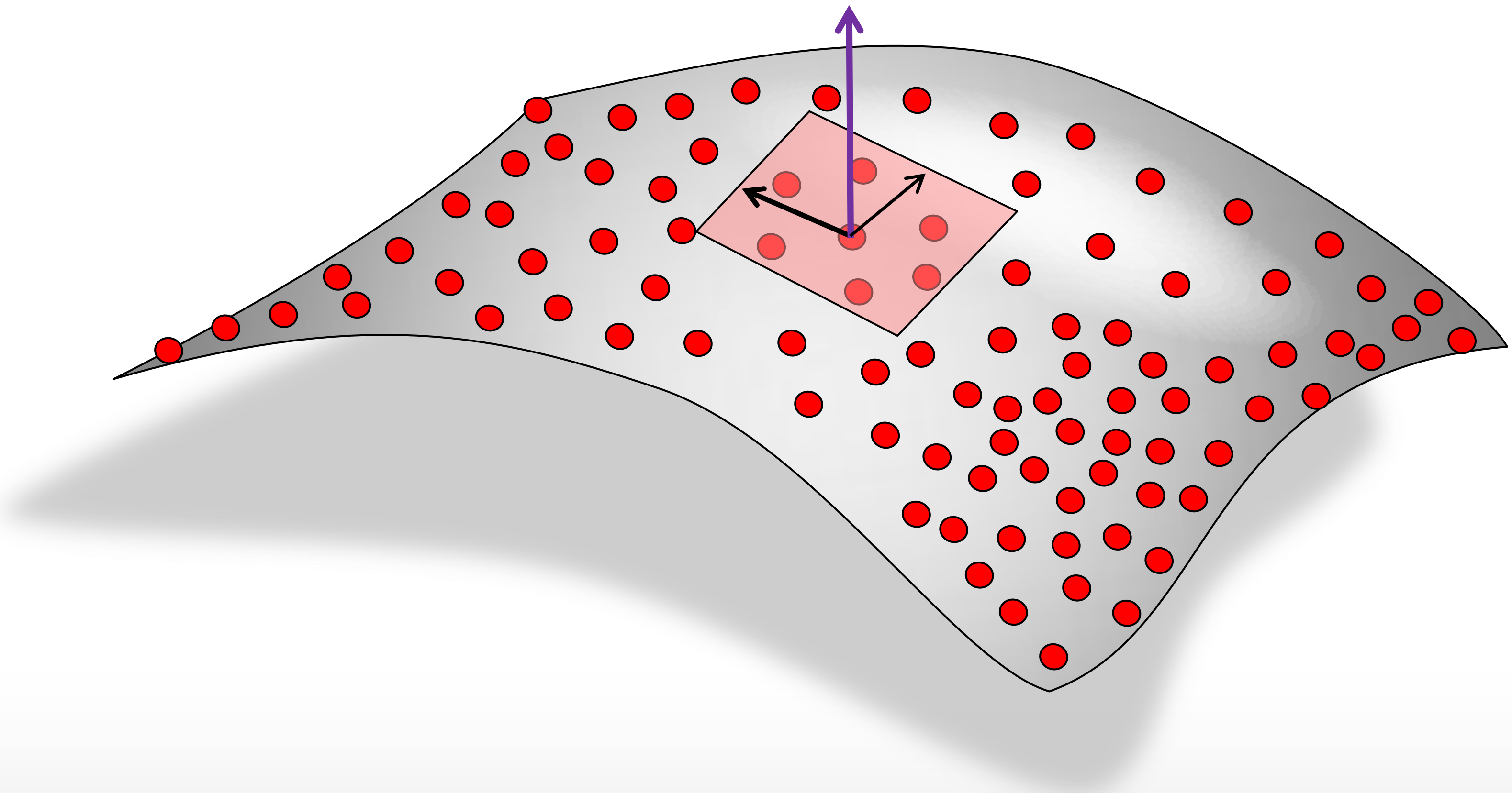
- In quadratic form we can write:
  - $\boldsymbol{f}^T \mathbf{L} \boldsymbol{f} = \sum_{\forall v_j \sim v_i} \big(f(v_i) - f(v_j)\big)^2$



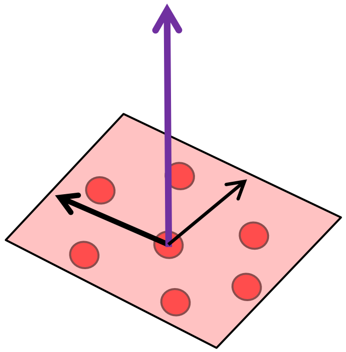


$g(v_2) = f(v_3) + f(v_5) - 2f(v_2)$

Continuous V/s Discrete Laplace



Local Parametrization



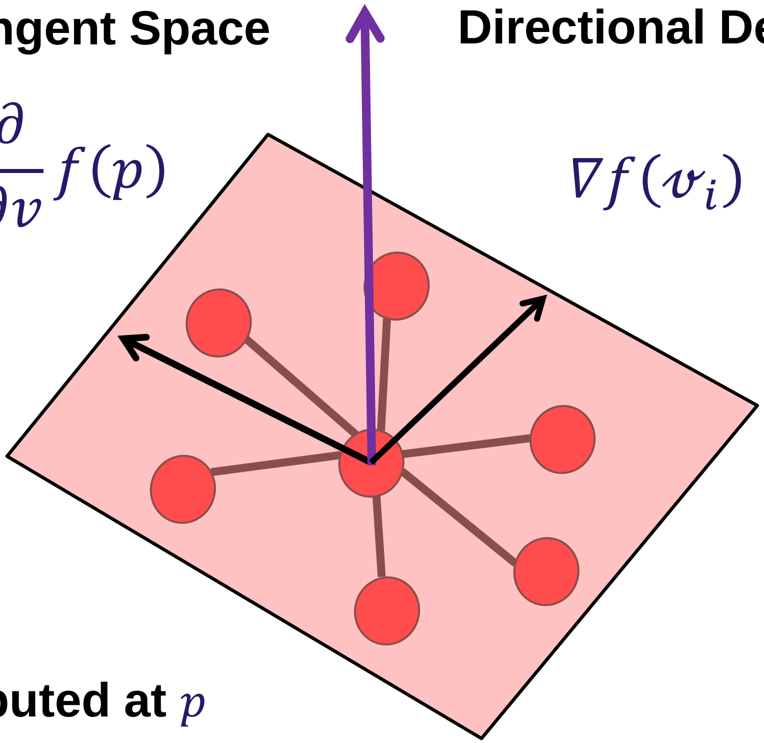
Continuous V/s Discrete Laplace

Derivative vector in Tangent Space

$$\nabla f(p) = \frac{\partial}{\partial u} f(p) + \frac{\partial}{\partial v} f(p)$$

Directional Derivative w.r.t. edge $e_{i,j}$

$$\nabla f(v_i) = f(v_i) - f(v_j)$$



Laplace operator computed at p

$$\Delta f(p) = \operatorname{div} \nabla f(p) = \nabla . \nabla f(p)$$

$$\Delta f(p) = \frac{\partial^2}{\partial u^2} f(p) + \frac{\partial^2}{\partial v^2} f(p)$$

Laplace operator computed at v_i

$$\Delta f(v_i) = \operatorname{div} \nabla f(v_i) = \nabla^T \nabla f(v_i)$$

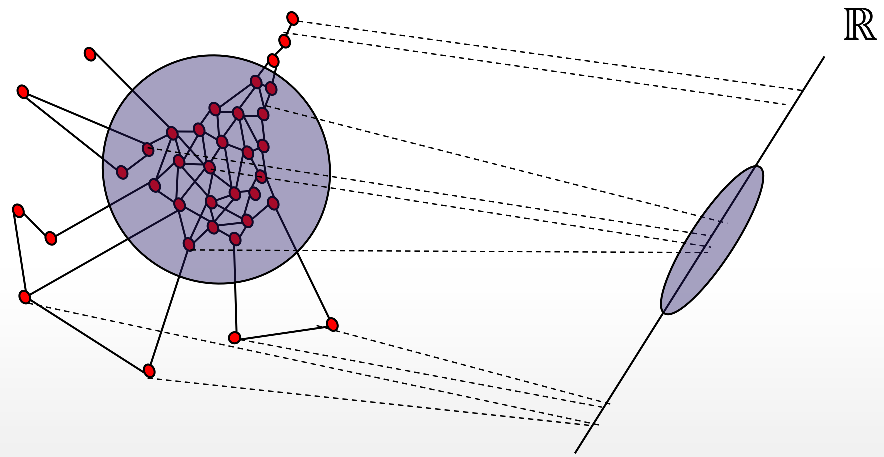
$$\mathbf{L} f(v_i) = \sum_{\forall j \sim i} f(v_i) - f(v_j)$$

Discrete Laplace Operator

Laplacian Operator

- Minimization of quadratic form $\boldsymbol{f}^T \mathbf{L} \boldsymbol{f} == \sum_{\forall v_j \sim v_i} \left(f(v_i) - f(v_j)\right)^2$ over $\boldsymbol{f}$ yield a smooth function that maps neighboring vertices of $\mathcal{G}$ together.
  - Hence it is desired that $f(v_i)$ and $f(v_j)$ are mapped closer on the real line.

- One important consequence of this is that if a graph is *not* ***regular*** (i.e. *not uniformly connected*) then a set of ***stongly*** connected vertices will be mapped closer as compare to set of ***weakly*** connected vertices.



Laplacian Eigenvectors

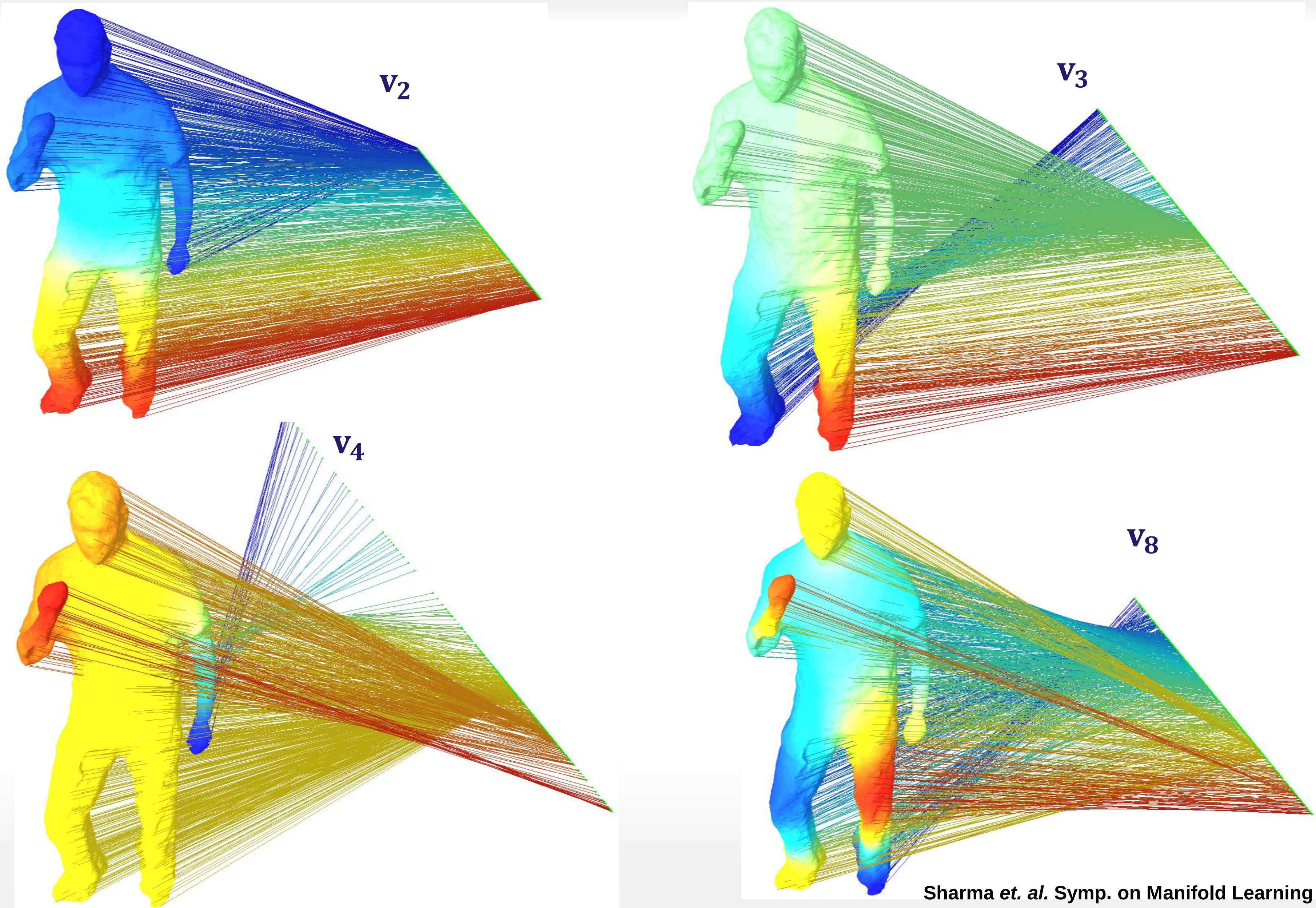
Laplacian Eigenvectors

- Minimization of quadratic form $\boldsymbol{f}^T \mathbf{L} \boldsymbol{f}$ over $\boldsymbol{f}$ can be written as **Rayleigh quotient** :

$$\min_{\boldsymbol{f}} \frac{\boldsymbol{f}^T \mathbf{L} \boldsymbol{f}}{\boldsymbol{f}^T \boldsymbol{f}}$$

- The solution of minimization is a family of smooth orthonormal functions *i.e.* eigen-functions of $\mathbf{L}$ matrix corresponding to increasing eigenvalues.
- $\mathbf{LV} = \mathbf{\Lambda V}$ with $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_n]$ and $\mathbf{\Lambda} = \mathbf{diag}(\lambda_1, \dots, \lambda_n)$ such that $0 = \lambda_1 < \lambda_2 \leq \lambda_3 \dots \leq \lambda_n$.
- $\mathbf{L1} = \mathbf{0}$, $\lambda_1 = 0$ (If graph is connected). Trivial solution as *constant vector.*
- $\mathbf{Lv}_2 = \lambda_2 \mathbf{v}_2$ is called the Fiedler vector.
- $\forall i \in \{2{:}\,n\}$, $\mathbf{v}_i^{\mathrm{T}} \mathbf{1} = \mathbf{0}$ by orthonormal property of eigenvectors.
- Hence, $\sum_{j=1:n} \mathbf{v}_i(j) = 0$.

Laplacian Eigenvectors



Sharma *et. al.* Symp. on Manifold Learning 2009

Types of Laplace Discretization

$$\boldsymbol{g} = \mathbf{L}\boldsymbol{f} \text{ where } \boldsymbol{g}(v_i) = \sum_{\forall v_j \sim v_i} \omega_{ij}\big(f(v_i) - f(v_j)\big)$$

Binary Weighting (*Non Geometric*)

- Weights of adjacency matrix are set to 0 or 1, *i.e.* all edges are equally weighted. Also known as ***Umbrella*** operator.

Gaussian Weighting

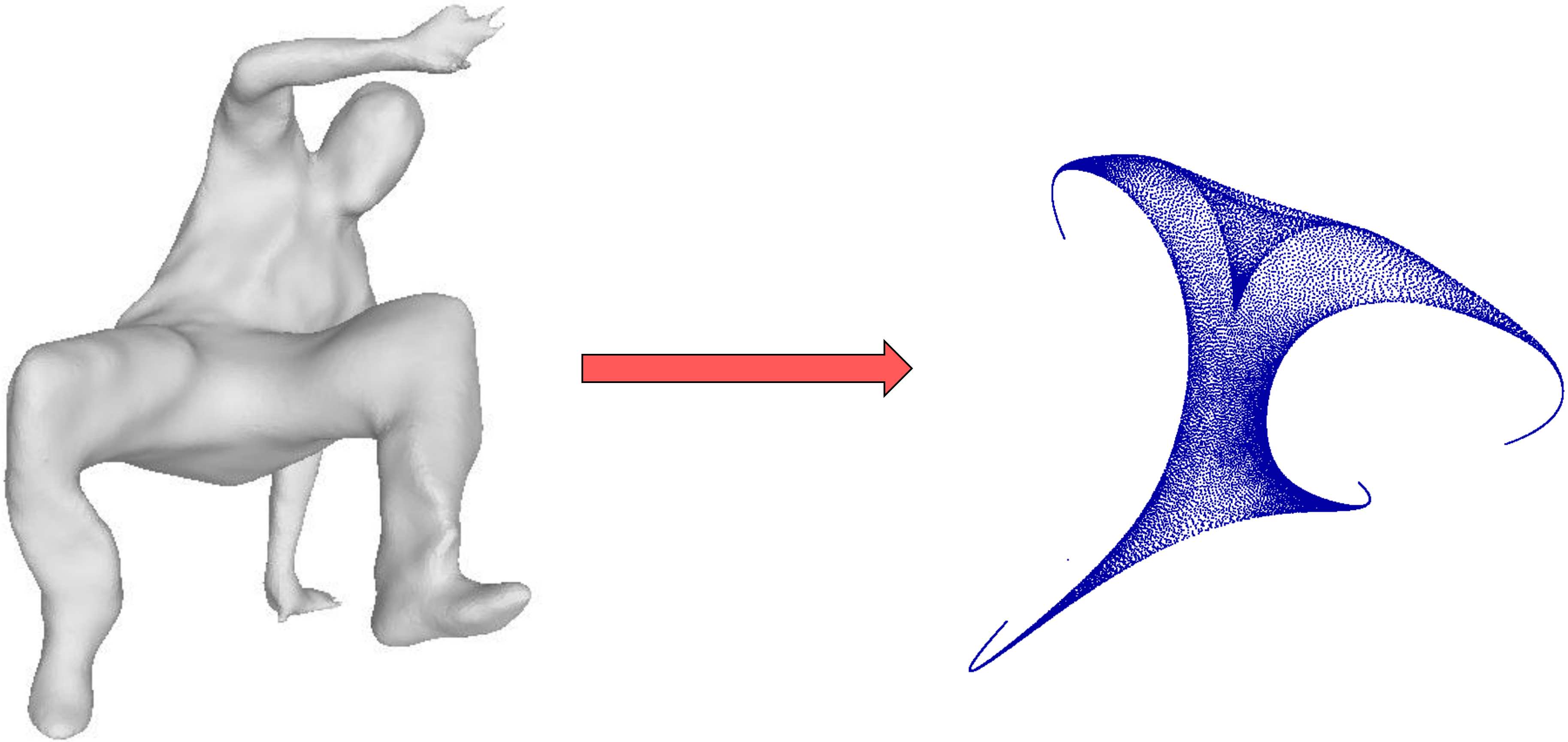
- Weights of adjacency matrix are set to $\mathcal{N}_{\mu,\sigma}\left(-\mathrm{Euclid}(v_i, v_j)\right)$, *i.e.* edges with small length are weighted more than the larger once.

Cotangent Weighting

- Weights of adjacency matrix are computed in terms of cotangent of angles of triangle in the triangulated mesh, *i.e.* areas with higher curvature are weighted *more*.

Discrete Laplace operators: No free lunch, M. Wardetzky, S. Mathur, F. Kälberer and E. Grinspun, In SGP 2007

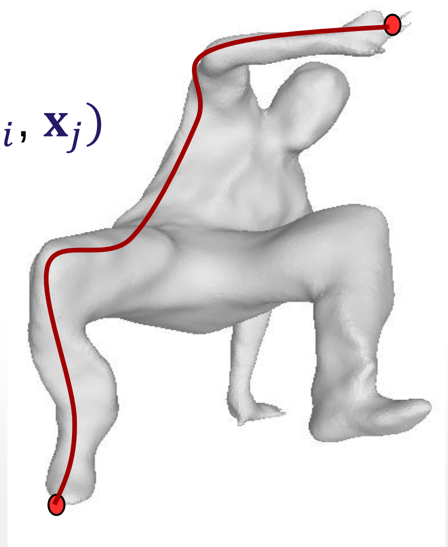
Laplacian Embedding

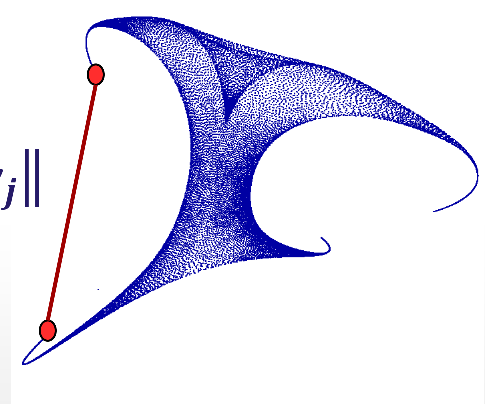


Spectral Metric

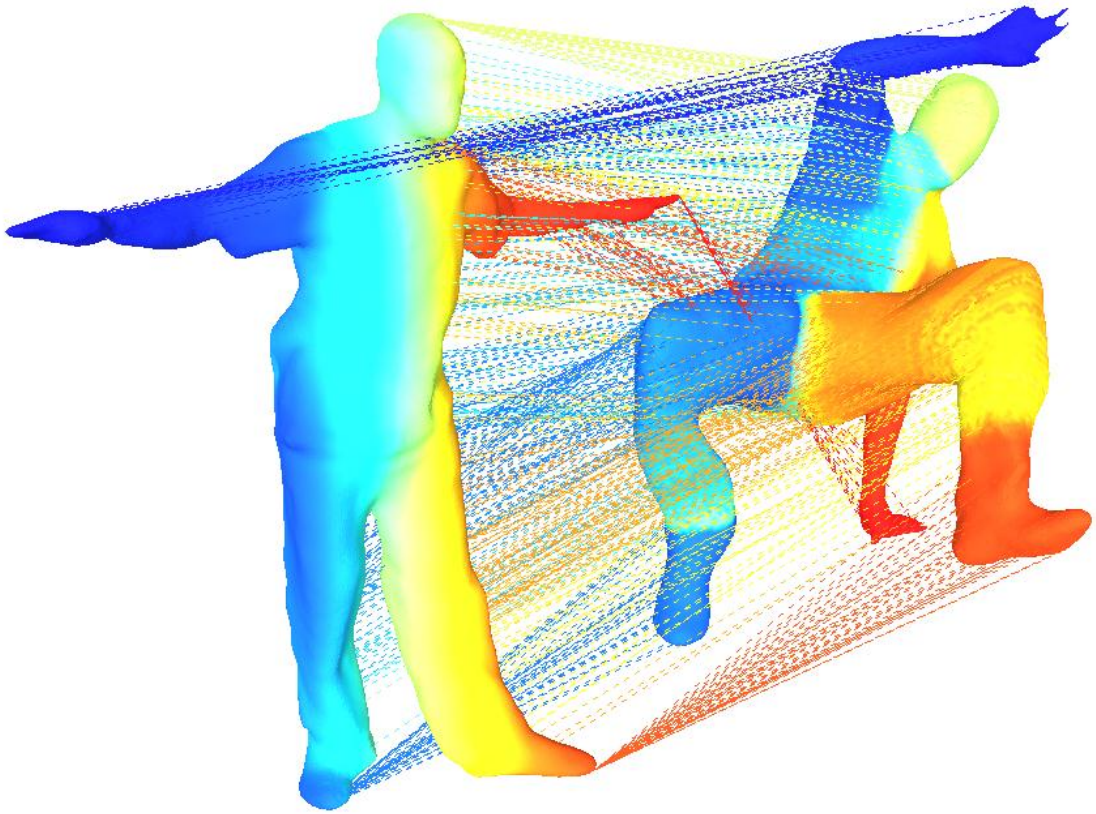
Distance computation on surface

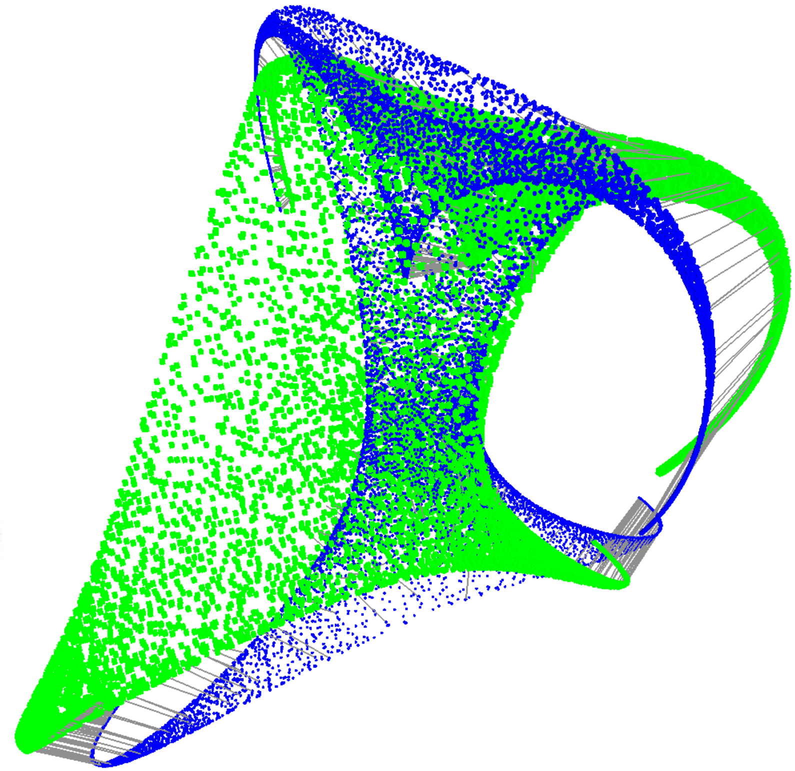
- Given a 3D shape represented as $\mathbf{X} \in \mathbb{R}^3$ and its d-dimensional embedding as $\mathbf{Y} = [\mathbf{v}_2, \dots, \mathbf{v}_{d+1}]^{\mathrm{T}}$.
- Each point $\mathbf{x}_i \in \mathbf{X}$ is represented as $\boldsymbol{y}_i = (\mathbf{v}_2(i), \dots, \mathbf{v}_{d+2}(i))^{\mathrm{T}}$.
- Geodesic$(\mathbf{x}_i, \mathbf{x}_j) \approx \|\boldsymbol{y}_i - \boldsymbol{y}_j\| = \sqrt{\sum_{k=2}^{d+1}(\mathbf{v}_k(i) - \mathbf{v}_k(j))^2}$.





Spectral Matching





Mateus *et. al.* CVPR 2008

Questions?