Analysis of Three-Dimensional Shapes
(IN2238, TU München, Summer 2015)

Intrinsic metrics
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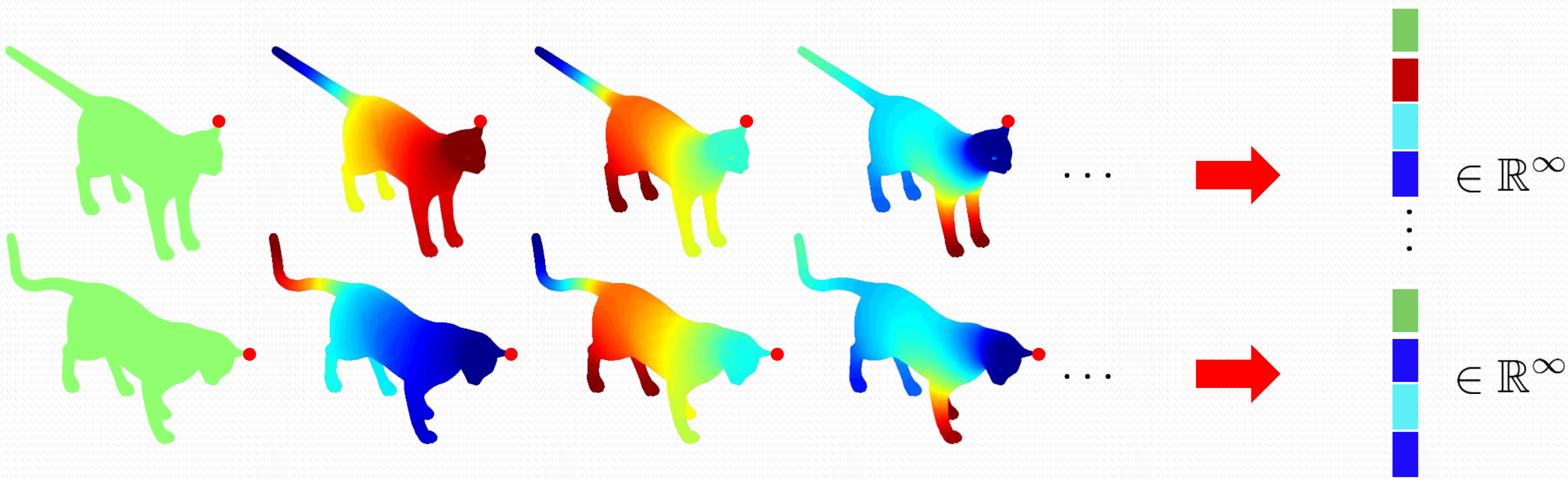
Wrap-up

We introduced the notion of point-based shape descriptor, and provided a few possible definitions such as the GPS, corresponding to the simple mapping:

$$p \mapsto \left(\cancel{\frac{\varphi_0(p)}{\sqrt{\lambda_0}}}, \frac{\varphi_1(p)}{\sqrt{\lambda_1}}, \frac{\varphi_2(p)}{\sqrt{\lambda_2}}, \ldots \right)$$



Minimum distortion correspondence

Typical **minimum-distortion correspondence** problems are defined in terms of **first- and second-order distortion** terms. Given two shapes *X* and *Y*, they consider the following minimization problem over all possible correspondences $C \subset X \times Y$:

$$\min_{C} \mathrm{dis}(C) + \alpha \mathrm{dis}(C \times C)$$

where the distortion terms are defined, for example, as:

$$\mathrm{dis}(C) = \sum_{(x,y)\in C} \|\mathbf{f}_X(x) - \mathbf{f}_Y(y)\|^2$$

descriptor similarity

$$\mathrm{dis}(C \times C) = \sum_{(x,y),(x',y')\in C} (d_X(x,x') - d_Y(y,y'))^2$$

metric similarity

Shapes as metric spaces

As we know, one successful way to model the matching problem is to consider shapes as metric spaces:

$$\underbrace{(M}_{\text{set of points}}, \underbrace{d_M)}_{\text{metric function}}$$

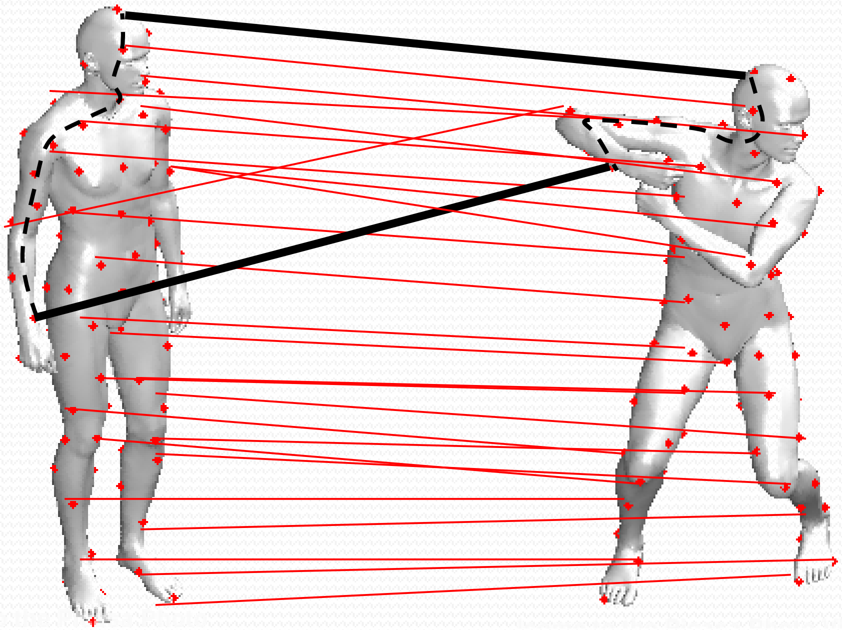
We have seen this simple model arising in several different topics, such as:

- Distance between shapes (Lipschitz, Gromov-Hausdorff, …)
- Multi-dimensional scaling (Euclidean embeddings, canonical forms, …)
- Differential geometry ("natural" distance on regular surfaces)
- Functional maps (distance maps to landmark correspondences)

Gromov-Hausdorff distance

For example, let’s look again at our discretization of the Gromov-Hausdorff distance between two metric spaces:

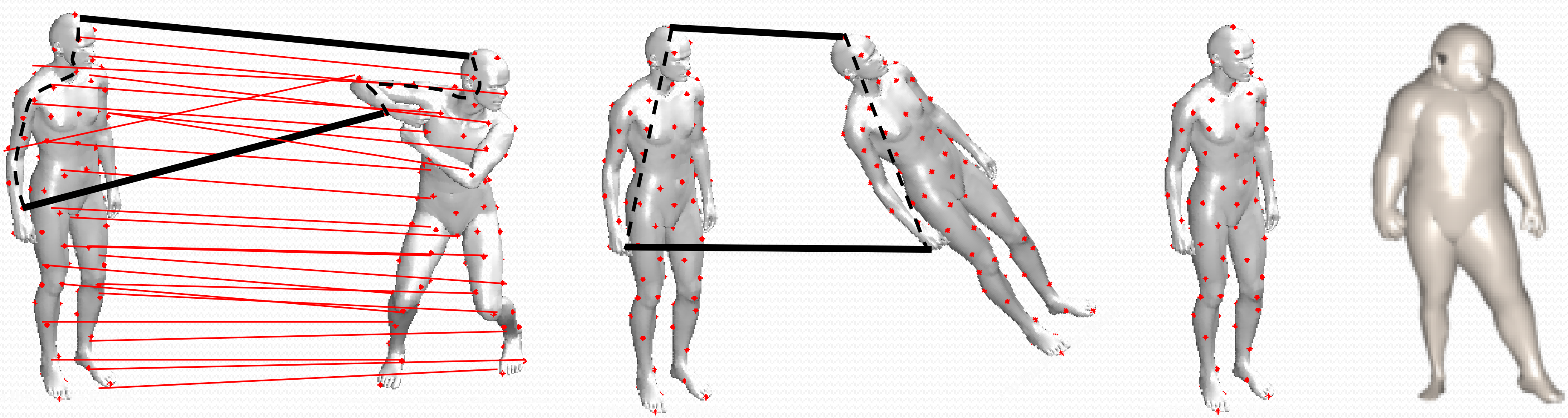
$$d_{\mathcal{GH}}(\mathbf{X},\mathbf{Y}) = \frac{1}{2} \inf_{R \subset \mathbf{X}\times\mathbf{Y}} \sup_{(x,y),(x',y')\in R} \left| d_X(x,x') - d_Y(y,y') \right|$$



Gromov-Hausdorff distance

$$d_{\mathcal{GH}}(\mathbf{X},\mathbf{Y}) = \frac{1}{2} \inf_{R\subset \mathbf{X}\times\mathbf{Y}} \sup_{(x,y),(x',y')\in R} \left| d_X(x,x') - d_Y(y,y') \right|$$

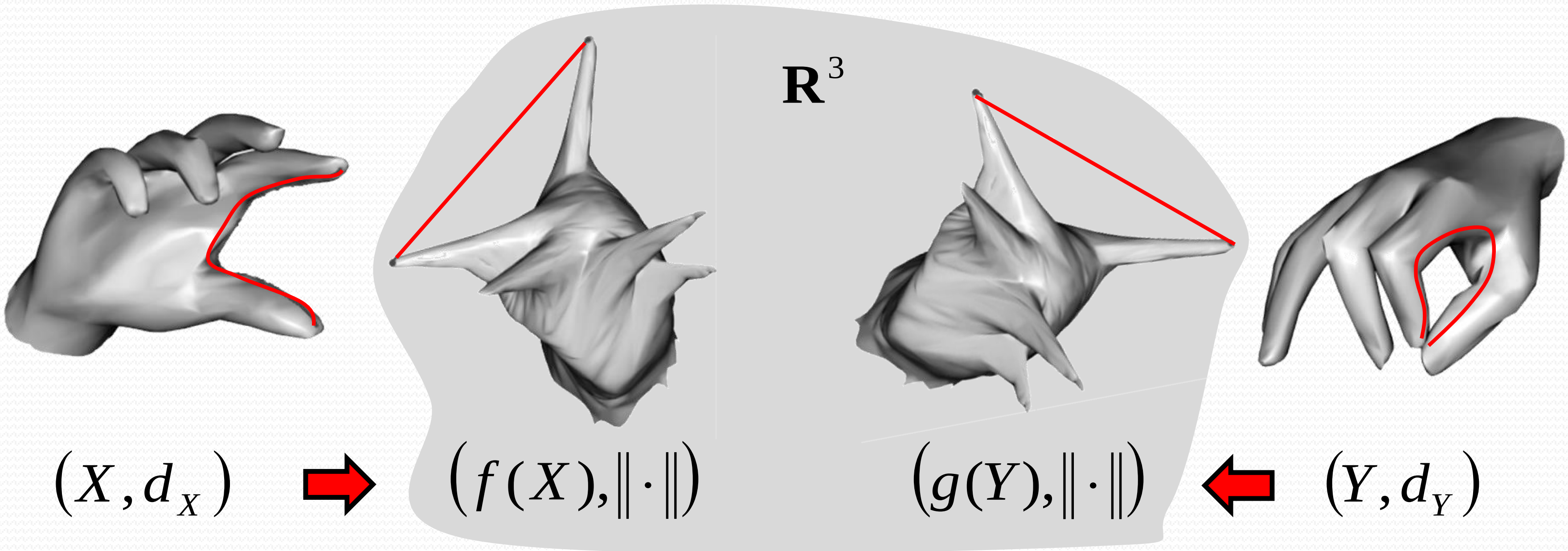
We already know that the correspondence attaining the infimum will be invariant exactly to the kind of transformations to which the metrics d_X, d_Y are invariant.



geodesic metric ⇨ isometries Euclidean metric ⇨ rigid motions ?

Multi-dimensional scaling

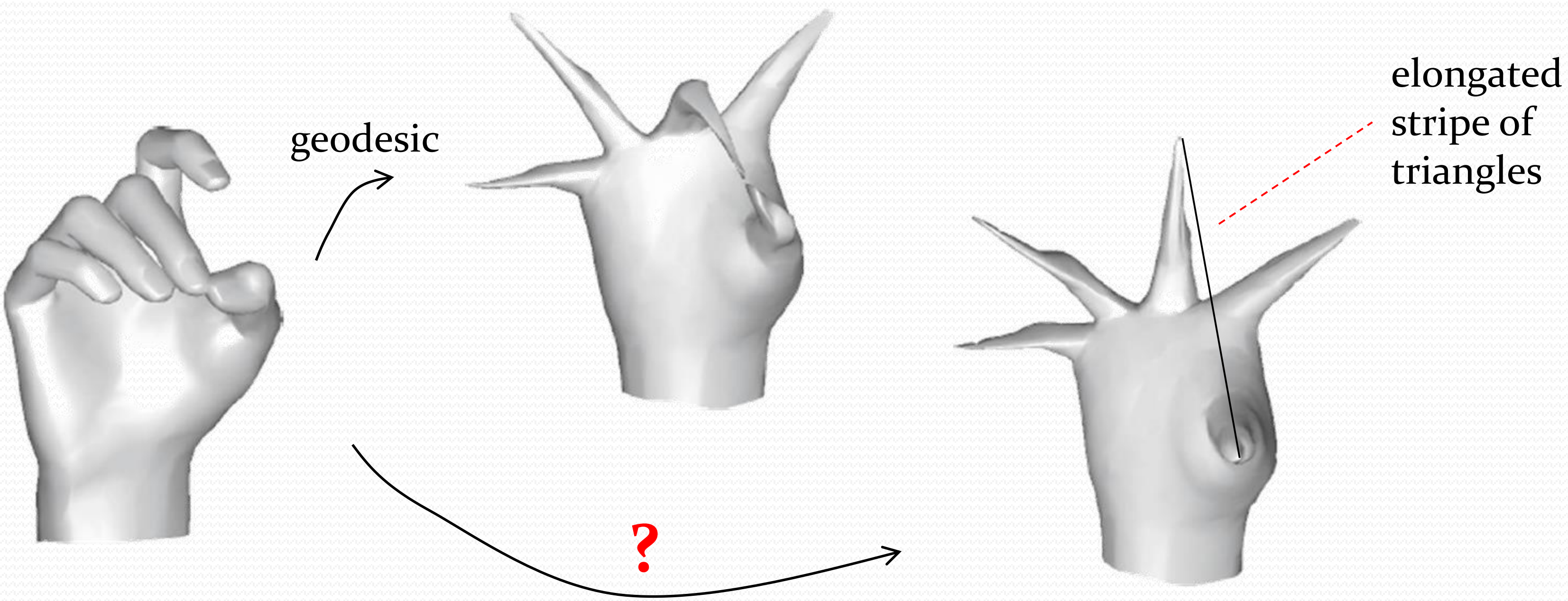
$$f = \underset{f: X \to \mathbf{R}^m}{\arg\min} \sum_{i>j} \left| d_X(x_i, x_j) - d_{\mathbf{R}^m}(f(x_i), f(x_j)) \right|^2$$



Multi-dimensional scaling

$$f = \underset{f:X \to \mathbf{R}^m}{\arg\min} \sum_{i>j} \left| d_X(x_i, x_j) - d_{\mathbf{R}^m}(f(x_i), f(x_j)) \right|^2$$

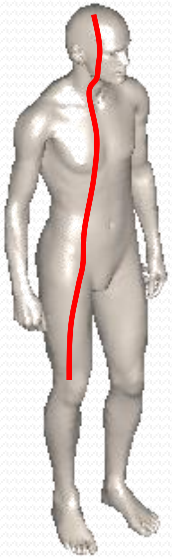
Topological noise can significantly alter distances.



Geodesic distance

We have seen that the first fundamental form on regular surfaces allows us to measure lengths of curves lying on the surface.

We defined the distance $d(p,q)$ between two points of S as



$$d(p,q) = \inf_{\alpha:[0,1]\to S} \int_0^1 \|\alpha'(t)\| dt$$

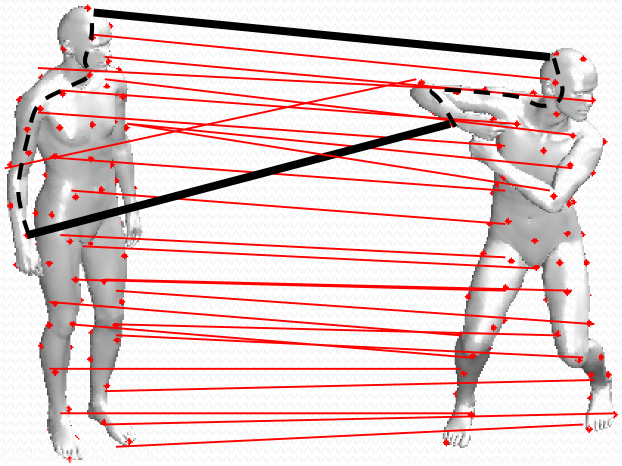
where $\alpha(0) = p$, $\alpha(1) = q$.

This “natural” intrinsic distance on the surface is commonly referred to as **geodesic distance** in the shape analysis literature.

Geodesic distance

$$d(p,q) = \inf_{\alpha:[0,1]\to S} \int_0^1 \|\alpha'(t)\| dt = \inf_{\alpha:[0,1]\to S} \int_0^1 \sqrt{I(\alpha'(t))} dt$$

Since isometries preserve the first fundamental form, the *geodesic distance is preserved under isometries*.



Heat diffusion

We have seen how **heat diffusion** on regular surfaces allows to capture their intrinsic geometry. In particular, we studied the following model:

$$\frac{\partial u(x,t;u_0)}{\partial t} = \Delta u(x,t;u_0)$$
$$u(x,0) = u_0(x)$$

A solution to the heat equation is given by:

$$u(x,t;u_0) = \int_S k_t(x,y)u_0(y)dy$$

The function $k_t : S \times S \to \mathbb{R}$, called **heat kernel**, describes how much heat is transferred from one point to the other in time *t*.

Heat kernel

We provided an explicit expression for the heat kernel in $\mathbb{R}^n$:

$$k_t^{\mathbb{R}^n}(x,y) = \frac{1}{(\sqrt{4\pi t})^n} \exp(-\frac{\|x-y\|^2}{4t})$$

as well as in the case of regular surfaces *S*:

$$k_t^S(x,y) = \sum_k e^{-\lambda_k t} \phi_k(x) \phi_k(y)$$

We didn't give any formal proof, but we stated that one can recover the *geodesic distance* on a surface directly from the heat kernel:

$$d_S^2(x,y) = \lim_{t \to 0} 4t \log(k_t^S(x,y))$$

A distance based on heat diffusion

Based on these observations, we ask the following question:

Can we define a *new* notion of distance based on the ideas of heat diffusion?

A natural candidate for such a distance is the heat kernel $k_t^S(x,y)$ itself.

However, it is not difficult to see that such a function does *not* satisfy all the metric axioms. In particular, if we look again at the spectral decomposition

$$k_t^S(x,y) = \sum_k e^{-\lambda_k t} \phi_k(x) \phi_k(y)$$

we immediately realize that $k_t^S(x,y) = 0 \not\Leftrightarrow x = y$

Diffusion kernel

The heat kernel $k_t(x, y)$ satisfies the properties of a **diffusion kernel**:

$k_t(x, y) \geq 0$ (non-negativity)

$k_t(x, y) = k_t(y, x)$ (symmetry)

Exercise

$\int\int k_t^2(x, y)dxdy < \infty$ (square integrability)

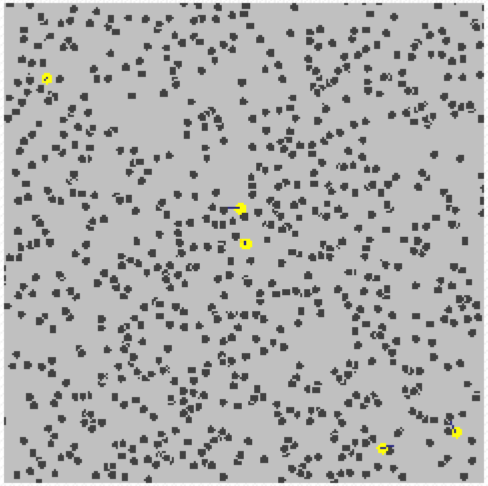
$\int\int k_t(x, y)f(x)f(y)dxdy \geq 0$ (positive semi-definiteness)

$\int k_t(x, y)dy = 1$ (conservation) ⇦ in matrix notation, this corresponds to a stochastic matrix

Random walks

A **random walk** is a path modeled as a succession of random steps.

For example, the path traced by a molecule in a liquid, or the path walked by a drunken sailor from the bar to a lamp post.



Brownian motion is the random motion of particles suspended in a fluid. The randomness is the result of the particles colliding with the fluid molecules (or atoms in the case of a gas).

Brownian motion

The physical phenomenon of Brownian motion was modeled mathematically by Einstein in 1905.

In particular, he showed that if $u(x,t)$ is the **density** of Brownian particles (number of particles per unit volume) at point *x* and time *t*, then *u* satisfies the diffusion equation:

$$\frac{\partial u}{\partial t} = D\Delta u$$

where *D* is the *mass diffusivity* or *diffusion coefficient*, in general a non-linear function which depends on physical properties such as temperature and viscosity

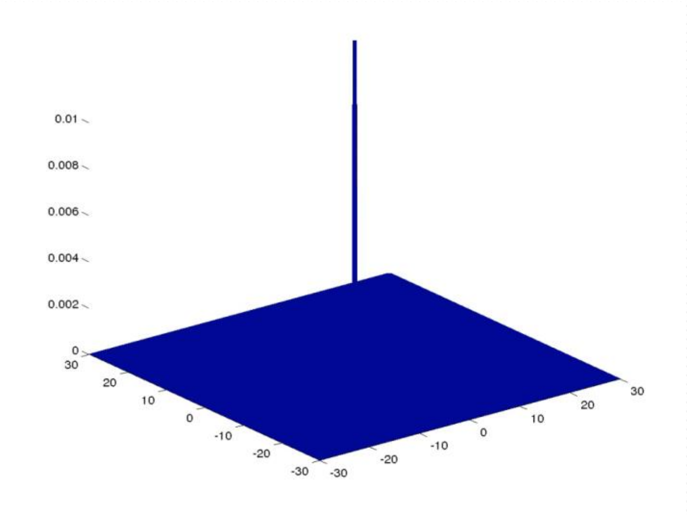
We already know that a solution to this diffusion equation (with $D = 1$) is given by:

$$u(x,t;u_0) = \int_S k_t(x,y)u_0(y)dy$$

Brownian particles

For example, assuming that N particles start from the origin, in Euclidean space the diffusion equation has the solution:

$$u(x,t) = \frac{N}{(\sqrt{4\pi D t})^n} \exp(-\frac{\|x\|^2}{4Dt})$$



In this view, we can regard heat diffusion as Brownian particles running away from their initial distribution.

In the case of a manifold, we can imagine these tiny particles moving chaotically over the surface and away from the initial position.

Probability density function

Now recall that we have the conservation property:

$$\int_S u(x,t)dx = 1$$

In other words, the particle density function $u(x,t)$ can be seen as a **probability density function** associated to the position of a particle undergoing a Brownian motion.

Thus, the heat diffusion equation provides a model of the **time evolution** of the probability density function $u(x,t)$.

$$\frac{\partial u}{\partial t} = D\Delta u$$

Brownian motion and heat kernel

$$\int_S u(x,t)dx = 1$$

Yesterday we have seen that, if we start from a δ_z distribution centered around $z \in S$, we get:

$$u(x,t;\delta_z) = \int_S k_t(x,y)\delta_z(y)dy = k_t(x,z)$$

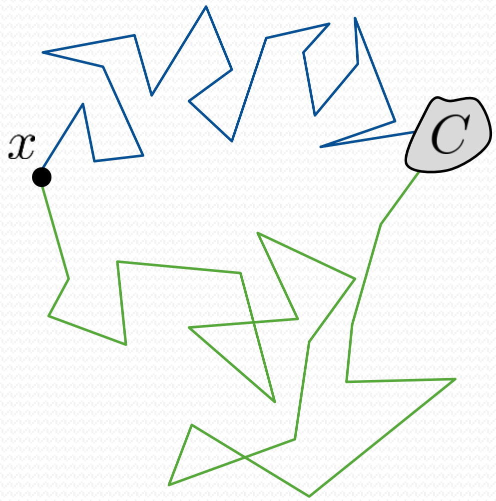
Thus, the probability that a particle is in a small region *C* around point *x* after time *t*, is given by

$$\int_{C\subset S} u(x,t;\delta_z)dx = \int_{C\subset S} k_t(x,z)dx$$

A probabilistic interpretation

This tells us that $k_t(x,y)$ is the **probability density function** of **transition** from *x* to *y* by a **random walk** of length *t*.

$$u(x,t;u_0) = \int_S k_t(x,y)u_0(y)dy$$



Brownian motion starting at point *x*, reaching *C* in time *t*, with probability given by:

$$\int_C k_t(x,y)dy$$

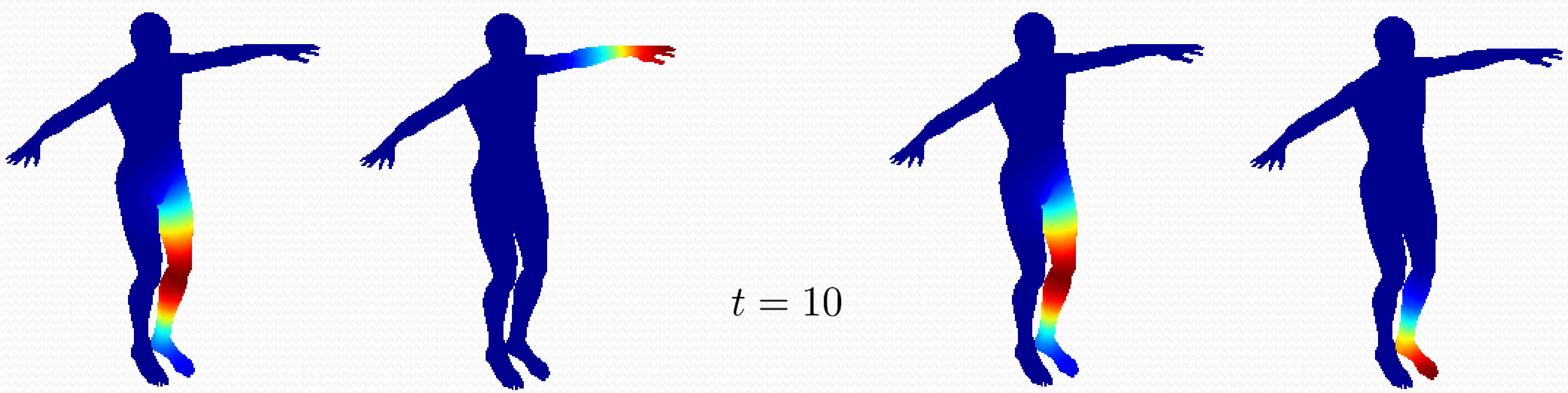
To emphasize this relationship, some authors denote the heat kernel by $p_t(x,y)$

Diffusion distance

A family of **diffusion distances** $\{d_t\}_{t\in\mathbb{R}_+}$ can be defined by

$$d_t^2(x,y) = \|k_t(x,\cdot) - k_t(y,\cdot)\|^2 = \int_S (k_t(x,z) - k_t(y,z))^2 dz$$

which is nothing but a L_2 distance between two probability density functions. <u>Note that the expression above is defining d_t^2, not d_t</u>.



$t = 10$

$d_t^2(x,t) = 3.6340$ $\qquad$ $d_t^2(x,t) = 0.5479$

Properties

$$d_t^2(x,y) = \|k_t(x,\cdot) - k_t(y,\cdot)\|^2 = \int_S (k_t(x,z) - k_t(y,z))^2 dz$$

- It is a metric.

- Diffusion time *t* plays the role of a scale parameter.

- It reflects the connectivity of the data at a given scale (denoted by *t*). If two points *x* and *y* are close (in the diffusion sense), there is a large probability of transition from *x* to *y* and vice versa.

- The definition involves summing over **all paths** of length $2t$ connecting *x* to *y*. As a consequence, this number is very robust to noise perturbation, unlike the geodesic distance (this path-length argument will be evident in two slides).

«Lengths of paths»

One useful property of the heat kernel (which we hinted at in the last bullet point of the previous slide) is the following:

$$k_{2T}(x,y) = \int_S k_T(x,z)k_T(z,y)dz$$

To prove this property, we start with a particular initial heat distribution:

$$u_0(x) = u(x,0) = k_T(x,y) \qquad \text{for some } y$$

Then, applying the heat diffusion model, it must be:

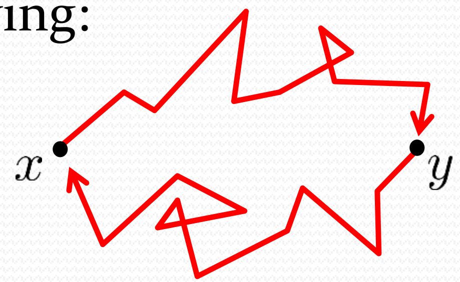
$$\left.\begin{aligned} u(x,t) &= k_{t+T}(x,y) \\ \frac{\partial u(x,t;u_0)}{\partial t} &= \Delta u(x,t;u_0) \end{aligned}\right\} u(x,t) = \int_S k_t(x,z)u_0(z)dz = \int_S k_t(x,z)k_T(z,y)dz$$

Setting $t = T$ and equating the two expressions for $u(x,t)$, we obtain the desired result.

Alternative definition

One special case of the previous property is the following:

$$\int_S k_t^2(x,y)dy = \int_S k_t(x,y)k_t(y,x)dy = k_{2t}(x,x)$$



Therefore, we can write:

$$\begin{aligned} d_t^2(x,y) &= \int_S (k_t(x,z) - k_t(y,z))^2 dz \\ &= \int_S (k_t^2(x,z) + k_t^2(y,z) - 2k_t(x,z)k_t(y,z))dz \\ &\boxed{= k_{2t}(x,x) + k_{2t}(y,y) - 2k_{2t}(x,y)} \end{aligned}$$

Indeed, this is the original definition given by Coifman et al. (see suggested reading).

Diffusion distance in the LB basis

$$d_t^2(x,y) = \|k_t(x,\cdot) - k_t(y,\cdot)\|^2 = \|\sum_i e^{-\lambda_i t}\phi_i(x)\phi_i(\cdot) - \sum_i e^{-\lambda_i t}\phi_i(y)\phi_i(\cdot)\|^2$$

$$= \|\sum_i e^{-\lambda_i t}\phi_i(\cdot)(\phi_i(x) - \phi_i(y))\|^2 = \int_S \left(\sum_i e^{-\lambda_i t}\phi_i(z)(\phi_i(x) - \phi_i(y))\right)^2 dz$$

$$= \int_S \left(\sum_i e^{-\lambda_i t}\phi_i(z)(\phi_i(x) - \phi_i(y))\right)\left(\sum_j e^{-\lambda_j t}\phi_j(z)(\phi_j(x) - \phi_j(y))\right) dz$$

$$= \int_S \sum_{i,j} e^{-\lambda_i t} e^{-\lambda_j t}(\phi_i(x) - \phi_i(y))(\phi_j(x) - \phi_j(y))\phi_i(z)\phi_j(z)dz$$

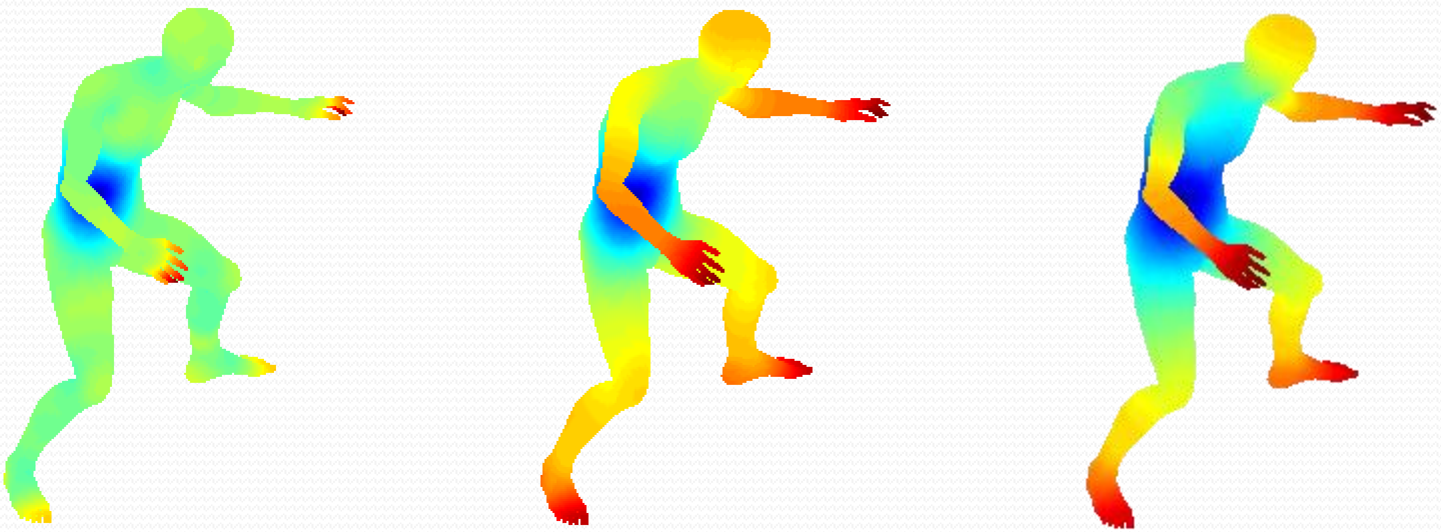
$$= \sum_{i,j} e^{-\lambda_i t} e^{-\lambda_j t}(\phi_i(x) - \phi_i(y))(\phi_j(x) - \phi_j(y))\langle\phi_i, \phi_j\rangle$$

$$\boxed{\begin{array}{ll} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{array}}$$

$$= \sum_i e^{-2\lambda_i t}(\phi_i(x) - \phi_i(y))^2\langle\phi_i, \phi_i\rangle = \sum_i e^{-2\lambda_i t}(\phi_i(x) - \phi_i(y))^2$$

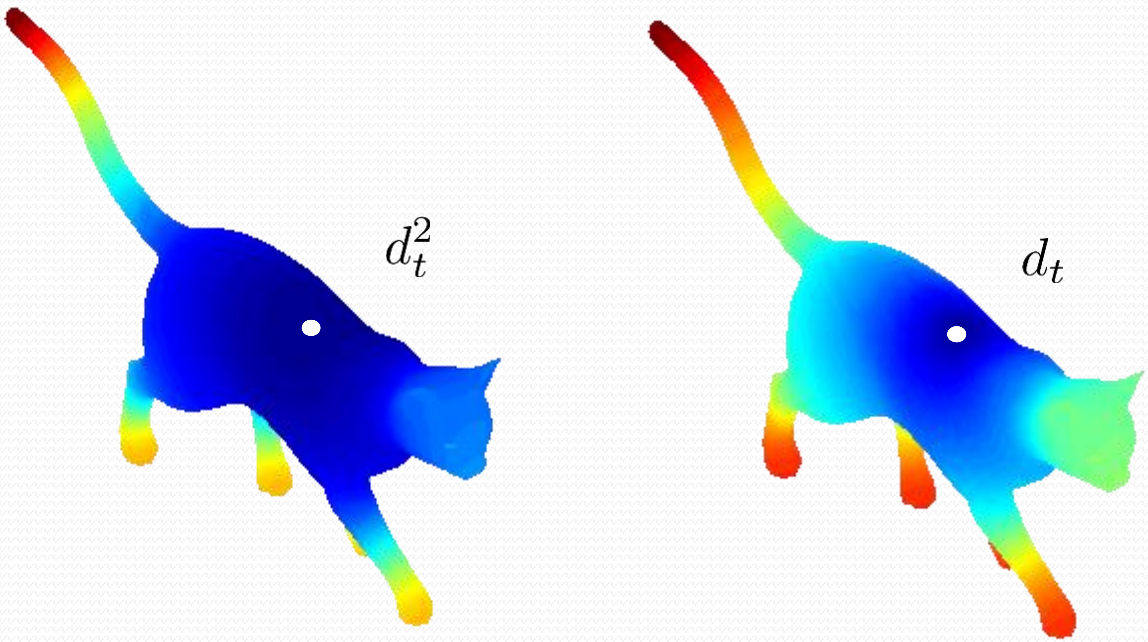
Example: Diffusion distance

$$d_t^2(x,y) = \sum_i e^{-2\lambda_i t}(\phi_i(x) - \phi_i(y))^2$$



$t = 1$ $t = 5$ $t = 10$

Pitfall



Diffusion map

$$d_t^2(x,y) = \sum_i e^{-2\lambda_i t}(\phi_i(x) - \phi_i(y))^2$$

The definition we gave for the diffusion distance suggests the following Euclidean embedding, called **diffusion map**:

$$p \mapsto \left(e^{-\lambda_1 t}\phi_1(p), e^{-\lambda_2 t}\phi_2(p), e^{-\lambda_3 t}\phi_3(p) \ldots\right) \quad \text{for a fixed } t \in \mathbb{R}_+$$

The diffusion distance is the Euclidean distance among diffusion maps.

We have already seen another similar embedding, which we called GPS:

$$p \mapsto \left(\frac{\phi_1(p)}{\sqrt{\lambda_1}}, \frac{\phi_2(p)}{\sqrt{\lambda_2}}, \frac{\phi_3(p)}{\sqrt{\lambda_3}}, \ldots\right)$$

Scale-invariant intrinsic metric

$$p \mapsto \left(e^{-\lambda_1 t}\phi_1(p), e^{-\lambda_2 t}\phi_2(p), e^{-\lambda_3 t}\phi_3(p) \ldots\right)$$

It is not difficult to see (check it!) that the diffusion map is **not** scale invariant.

However, by analogy between GPS and diffusion map, the previous slides raise the question on whether the following definition is a valid intrinsic metric function:

$$d^2(x,y) = \sum_i \frac{1}{\lambda_i}(\phi_i(x) - \phi_i(y))^2$$

That is, the L_2 distance between two global point signatures at points *x* and *y*.

Commute-time distance

$$d^2(x,y) = \sum_i \frac{1}{\lambda_i}(\phi_i(x) - \phi_i(y))^2$$

Indeed, it can be proved that this is in fact a metric function! Since we already proved that the GPS embedding is scale-invariant, it is not difficult to see that this metric is also scale-invariant.

The resulting metric is called **commute-time distance**.

Similarly to the diffusion distance, this distance can be rewritten in "kernel notation" as:

$$d^2(x,y) = g(x,x) + g(y,y) - 2g(x,y)$$

where $g(x,y) = \sum_k \frac{1}{\lambda_k}\phi_k(x)\phi_k(y)$ is the **commute-time kernel**.

Commute-time kernel

At this point, it is interesting to notice the following fact:

$$\int_0^\infty k_t(x,y)dt = \int_0^\infty \sum_k e^{-\lambda_k t}\phi_k(x)\phi_k(y)dt$$

(integrate over all possible times)

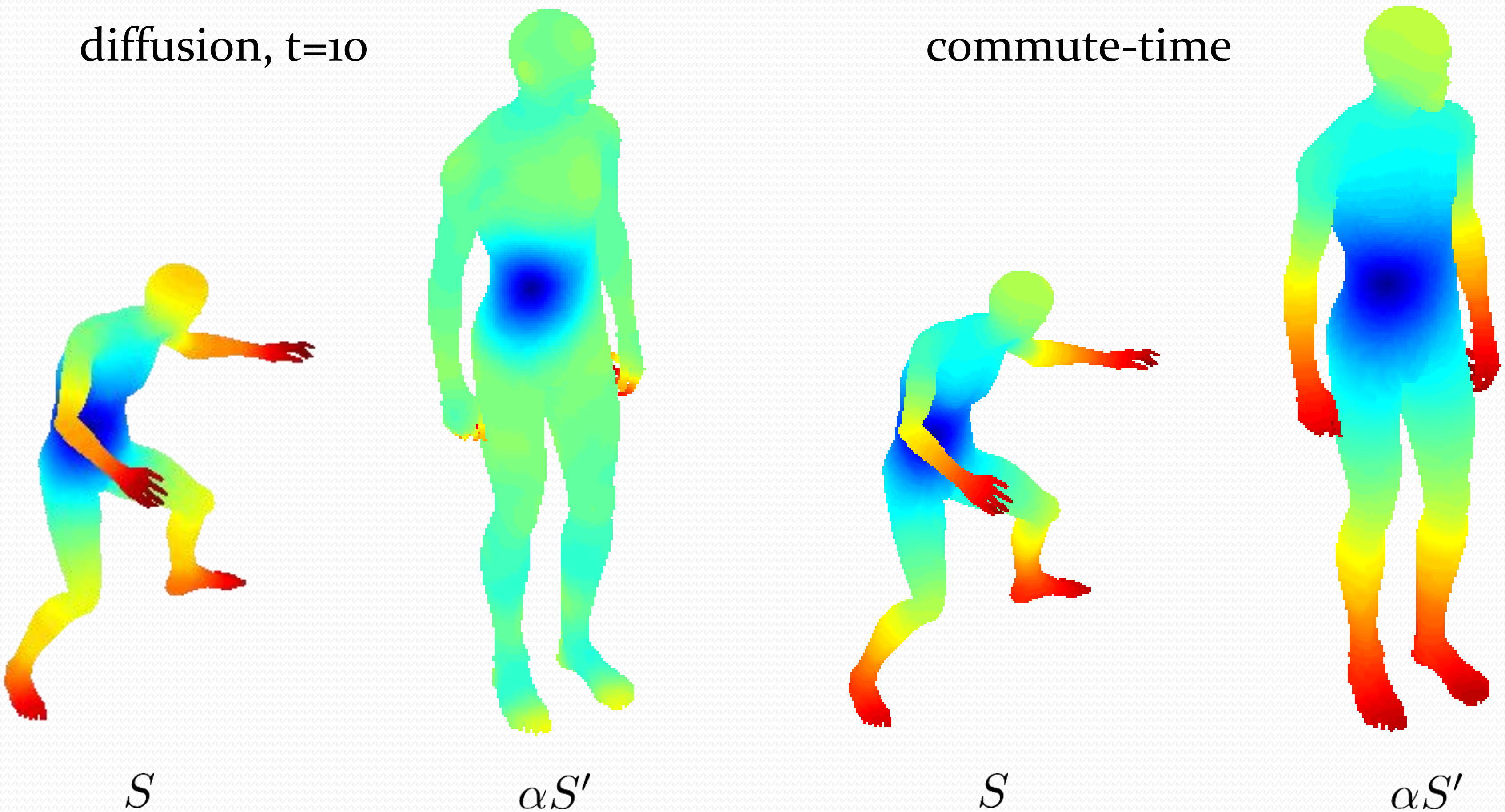
$$= \sum_k \phi_k(x)\phi_k(y) \int_0^\infty e^{-\lambda_k t}dt$$

$$= \sum_k \phi_k(x)\phi_k(y) \frac{1}{-\lambda_k} e^{-\lambda_k t}|_0^\infty$$

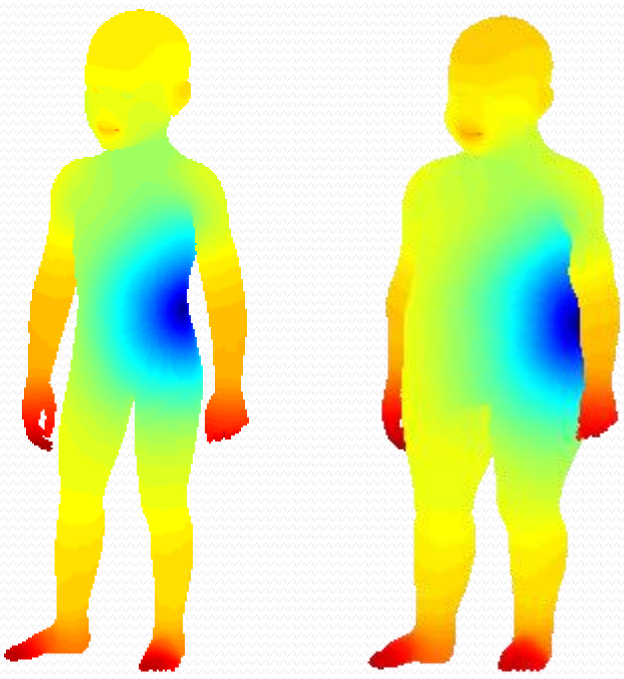
$$= \sum_k \frac{1}{\lambda_k}\phi_k(x)\phi_k(y) = g(x,y)$$

In other words, the commute-time kernel corresponds to the probability density function of transition from point *x* to *y* by a **random walk of any length**.

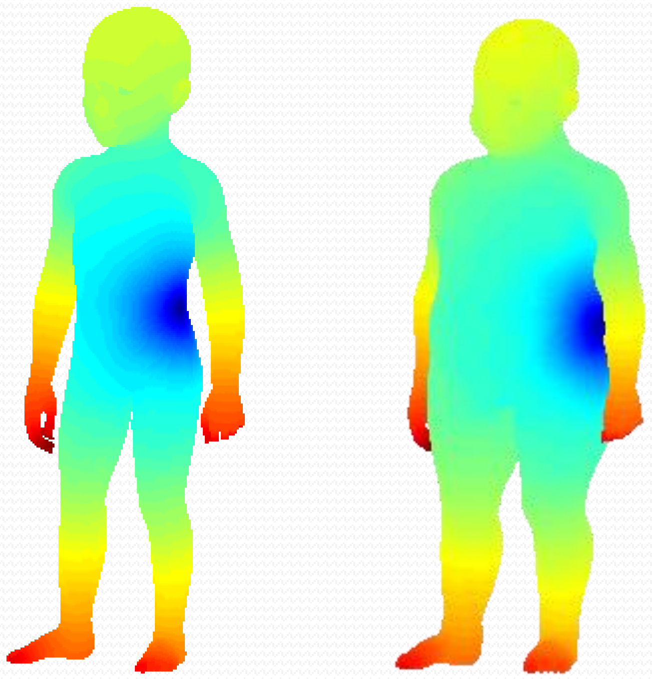
Example: Commute-time distance



Example: Non-isometries



diffusion, t=5



commute-time

Suggested reading

- *Geometric diffusions as a tool for harmonic analysis and structure definition of data: Diffusion maps.* Coifman et al. PNAS 2005.
- *Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen*. Einstein. Annalen der Physik 2005.
- *Discrete minimum distortion correspondence problems for non-rigid shape matching*. Wang et al. Proc. SSVM 2011.