

Fundamentals of Computer Graphics

Heat diffusion

Emanuele Rodolà
rodola@di.uniroma1.it



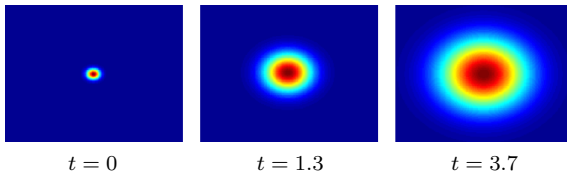
SAPIENZA
UNIVERSITÀ DI ROMA

Heat equation

Heat diffusion is governed by the **heat equation**

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

where function u describes the **heat distribution** at point x after time t



Heat kernel

$$\begin{aligned}\frac{\partial}{\partial t}u(x,t) &= -\Delta u(x,t) \\ u(x,0) &= u_0(x)\end{aligned}$$

A solution is obtained by

$$u(x,t) = \int_{\mathcal{X}} k_t(x,y)u_0(y)dy$$

Heat kernel

$$\begin{aligned}\frac{\partial}{\partial t}u(x, t) &= -\Delta u(x, t) \\ u(x, 0) &= u_0(x)\end{aligned}$$

A solution is obtained by

$$u(x, t) = \int_{\mathcal{X}} k_t(x, y) u_0(y) dy$$

The function $k_t : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is called the **heat kernel** of \mathcal{X}

Heat kernel

$$\begin{aligned}\frac{\partial}{\partial t}u(x, t) &= -\Delta u(x, t) \\ u(x, 0) &= u_0(x)\end{aligned}$$

A solution is obtained by

$$u(x, t) = \int_{\mathcal{X}} k_t(x, y) u_0(y) dy$$

The function $k_t : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is called the **heat kernel** of \mathcal{X}

- $k_t(x, y)$ describes the amount of **heat transferred** from point x to point y in time t

Heat kernel

$$\begin{aligned}\frac{\partial}{\partial t}u(x, t) &= -\Delta u(x, t) \\ u(x, 0) &= u_0(x)\end{aligned}$$

A solution is obtained by

$$u(x, t) = \int_{\mathcal{X}} k_t(x, y) u_0(y) dy$$

The function $k_t : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is called the **heat kernel** of \mathcal{X}

- $k_t(x, y)$ describes the amount of **heat transferred** from point x to point y in time t
- It is a **property of the manifold** \mathcal{X} and does not depend on the initial distribution $u_0(x)$

Dirac initialization

$$u(x, t) = \int_{\mathcal{X}} k_t(x, y) u_0(y) dy$$

Assume the initial distribution is a **Dirac delta** at point $z \in \mathcal{X}$

Dirac initialization

$$u(x, t) = \int_{\mathcal{X}} k_t(x, y) u_0(y) dy$$

Assume the initial distribution is a **Dirac delta** at point $z \in \mathcal{X}$

By definition, the Dirac distribution δ_z satisfies the **sampling property**

$$\int_{\mathcal{X}} f(x) \delta_z(x) dx = f(z)$$

Dirac initialization

$$u(x, t) = \int_{\mathcal{X}} k_t(x, y) u_0(y) dy$$

Assume the initial distribution is a **Dirac delta** at point $z \in \mathcal{X}$

By definition, the Dirac distribution δ_z satisfies the **sampling property**

$$\int_{\mathcal{X}} f(x) \delta_z(x) dx = f(z)$$

With this initialization, the solution to heat equation is simply

$$u(x, t) = \int_{\mathcal{X}} k_t(x, y) \delta_z(y) dy =$$

Dirac initialization

$$u(x, t) = \int_{\mathcal{X}} k_t(x, y) u_0(y) dy$$

Assume the initial distribution is a **Dirac delta** at point $z \in \mathcal{X}$

By definition, the Dirac distribution δ_z satisfies the **sampling property**

$$\int_{\mathcal{X}} f(x) \delta_z(x) dx = f(z)$$

With this initialization, the solution to heat equation is simply

$$u(x, t) = \int_{\mathcal{X}} k_t(x, y) \delta_z(y) dy = k_t(x, z)$$

Note that z is **fixed**, so here $k_t(x, z)$ is a function of x

Heat kernel: Properties

The heat kernel has some useful properties:

- In \mathbb{R}^n it is given by

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

Heat kernel: Properties

The heat kernel has some useful properties:

- In \mathbb{R}^n it is given by

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

- Distance can be recovered by Varadhan's result:

$$d_{\mathcal{X}}^2(x, y) = -\lim_{t \rightarrow 0} 4t \log(k_t(x, y))$$

Heat kernel: Properties

The heat kernel has some useful properties:

- In \mathbb{R}^n it is given by

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

- Distance can be recovered by Varadhan's result:

$$d_{\mathcal{X}}^2(x, y) = -\lim_{t \rightarrow 0} 4t \log(k_t(x, y))$$

- If $T : \mathcal{X} \rightarrow \mathcal{Y}$ is an isometry, then

$$k_t^{\mathcal{X}}(x, y) = k_t^{\mathcal{Y}}(T(x), T(y))$$

Heat kernel: Spectral decomposition

$$\frac{\partial}{\partial t} u(x, t) = -\Delta u(x, t)$$

Heat kernel: Spectral decomposition

$$\frac{\partial}{\partial t}u(x,t) = -\Delta u(x,t)$$

Any solution $u(x,t)$ can be written in the Laplacian eigenbasis $\{\phi_i\}$ as:

$$u(x,t) \approx \sum_{i=0}^k c_i(t)\phi_i(x)$$

Heat kernel: Spectral decomposition

$$\frac{\partial}{\partial t} u(x, t) = -\Delta u(x, t)$$

Any solution $u(x, t)$ can be written in the Laplacian eigenbasis $\{\phi_i\}$ as:

$$u(x, t) \approx \sum_{i=0}^k c_i(t) \phi_i(x)$$

Thus, the right-hand side becomes

$$\Delta u(x, t) =$$

Heat kernel: Spectral decomposition

$$\frac{\partial}{\partial t} u(x, t) = -\Delta u(x, t)$$

Any solution $u(x, t)$ can be written in the Laplacian eigenbasis $\{\phi_i\}$ as:

$$u(x, t) \approx \sum_{i=0}^k c_i(t) \phi_i(x)$$

Thus, the right-hand side becomes

$$\Delta u(x, t) = \sum_{i=0}^k c_i(t) \Delta \phi_i(x) =$$

Heat kernel: Spectral decomposition

$$\frac{\partial}{\partial t} u(x, t) = -\Delta u(x, t)$$

Any solution $u(x, t)$ can be written in the Laplacian eigenbasis $\{\phi_i\}$ as:

$$u(x, t) \approx \sum_{i=0}^k c_i(t) \phi_i(x)$$

Thus, the right-hand side becomes

$$\Delta u(x, t) = \sum_{i=0}^k c_i(t) \Delta \phi_i(x) = \sum_{i=0}^k c_i(t) \lambda_i \phi_i(x)$$

Heat kernel: Spectral decomposition

$$\frac{\partial}{\partial t}u(x,t) = -\Delta u(x,t)$$

Any solution $u(x,t)$ can be written in the Laplacian eigenbasis $\{\phi_i\}$ as:

$$u(x,t) \approx \sum_{i=0}^k c_i(t)\phi_i(x)$$

Thus we can write:

$$\frac{\partial}{\partial t}u(x,t) = -\sum_{i=0}^k c_i(t)\lambda_i\phi_i(x)$$

Heat kernel: Spectral decomposition

$$\frac{\partial}{\partial t} u(x, t) = -\Delta u(x, t)$$

Any solution $u(x, t)$ can be written in the Laplacian eigenbasis $\{\phi_i\}$ as:

$$u(x, t) \approx \sum_{i=0}^k c_i(t) \phi_i(x)$$

Thus we can write:

$$\sum_{i=0}^k \frac{\partial}{\partial t} c_i(t) \phi_i(x) = - \sum_{i=0}^k c_i(t) \lambda_i \phi_i(x)$$

Heat kernel: Spectral decomposition

$$\frac{\partial}{\partial t}u(x,t) = -\Delta u(x,t)$$

Any solution $u(x,t)$ can be written in the Laplacian eigenbasis $\{\phi_i\}$ as:

$$u(x,t) \approx \sum_{i=0}^k c_i(t)\phi_i(x)$$

Thus we can write:

$$\frac{\partial}{\partial t}c_i(t) = -c_i(t)\lambda_i$$

Heat kernel: Spectral decomposition

$$\frac{\partial}{\partial t}u(x,t) = -\Delta u(x,t)$$

Any solution $u(x,t)$ can be written in the Laplacian eigenbasis $\{\phi_i\}$ as:

$$u(x,t) \approx \sum_{i=0}^k c_i(t)\phi_i(x)$$

Thus we can write:

$$c_i(t) = d_i e^{-\lambda_i t}$$

Heat kernel: Spectral decomposition

$$\frac{\partial}{\partial t}u(x,t) = -\Delta u(x,t)$$

Any solution $u(x,t)$ can be written in the Laplacian eigenbasis $\{\phi_i\}$ as:

$$u(x,t) \approx \sum_{i=0}^k c_i(t)\phi_i(x)$$

Thus we can write:

$$c_i(t) = d_i e^{-\lambda_i t}$$

We arrive at

$$u(x,t) \approx \sum_{i=0}^k d_i e^{-\lambda_i t} \phi_i(x)$$

Heat kernel: Spectral decomposition

$$\frac{\partial}{\partial t}u(x,t) = -\Delta u(x,t)$$

Any solution $u(x,t)$ can be written in the Laplacian eigenbasis $\{\phi_i\}$ as:

$$u(x,t) \approx \sum_{i=0}^k c_i(t)\phi_i(x)$$

Thus we can write:

$$c_i(t) = d_i e^{-\lambda_i t}$$

We arrive at

$$u(x,t) \approx \sum_{i=0}^k d_i e^{-\lambda_i t} \phi_i(x)$$

Almost there: we need to find an expression for the coefficients d_i

Heat kernel: Spectral decomposition

$$u(x, t) \approx \sum_{i=0}^k d_i e^{-\lambda_i t} \phi_i(x)$$

We use the given **initial condition** to solve for d_i

Heat kernel: Spectral decomposition

$$u(x, t) \approx \sum_{i=0}^k d_i e^{-\lambda_i t} \phi_i(x)$$

We use the given **initial condition** to solve for d_i

For $t = 0$, it must be:

$$u(x, 0) \approx \sum_{i=0}^k d_i e^{-\lambda_i 0} \phi_i(x)$$

Heat kernel: Spectral decomposition

$$u(x, t) \approx \sum_{i=0}^k d_i e^{-\lambda_i t} \phi_i(x)$$

We use the given **initial condition** to solve for d_i

For $t = 0$, it must be:

$$u(x, 0) \approx \sum_{i=0}^k d_i \phi_i(x)$$

Heat kernel: Spectral decomposition

$$u(x, t) \approx \sum_{i=0}^k d_i e^{-\lambda_i t} \phi_i(x)$$

We use the given **initial condition** to solve for d_i

For $t = 0$, it must be:

$$u_0(x) \approx \sum_{i=0}^k d_i \phi_i(x)$$

Heat kernel: Spectral decomposition

$$u(x, t) \approx \sum_{i=0}^k d_i e^{-\lambda_i t} \phi_i(x)$$

We use the given **initial condition** to solve for d_i

For $t = 0$, it must be:

$$u_0(x) \approx \sum_{i=0}^k d_i \phi_i(x)$$

For example, for $u_0(x) = \delta_y(x)$ we get

$$\delta_y(x) \approx \sum_{i=0}^k d_i \phi_i(x)$$

Heat kernel: Spectral decomposition

$$u(x, t) \approx \sum_{i=0}^k d_i e^{-\lambda_i t} \phi_i(x)$$

We use the given **initial condition** to solve for d_i

For $t = 0$, it must be:

$$u_0(x) \approx \sum_{i=0}^k d_i \phi_i(x)$$

For example, for $u_0(x) = \delta_y(x)$ we get

$$\delta_y(x) \approx \sum_{i=0}^k d_i \phi_i(x) \implies d_i = \langle \phi_i, \delta_y \rangle_{\mathcal{X}}$$

Heat kernel: Spectral decomposition

$$u(x, t) \approx \sum_{i=0}^k d_i e^{-\lambda_i t} \phi_i(x)$$

We use the given **initial condition** to solve for d_i

For $t = 0$, it must be:

$$u_0(x) \approx \sum_{i=0}^k d_i \phi_i(x)$$

For example, for $u_0(x) = \delta_y(x)$ we get

$$\delta_y(x) \approx \sum_{i=0}^k d_i \phi_i(x) \implies d_i = \phi_i(y)$$

Heat kernel: Spectral decomposition

Therefore, if $u_0(x) = \delta_y(x)$, we have the solution:

$$u(x, t) \approx \sum_{i=0}^k e^{-\lambda_i t} \phi_i(x) \phi_i(y)$$

Heat kernel: Spectral decomposition

Therefore, if $u_0(x) = \delta_y(x)$, we have the solution:

$$k_t(x, y) \approx \sum_{i=0}^k e^{-\lambda_i t} \phi_i(x) \phi_i(y)$$

Recall (see “Dirac initialization” slide) that this also defines the **heat kernel** between x and y

Heat kernel: Spectral decomposition

Therefore, if $u_0(x) = \delta_y(x)$, we have the solution:

$$k_t(x, y) \approx \sum_{i=0}^k e^{-\lambda_i t} \phi_i(x) \phi_i(y)$$

Recall (see “Dirac initialization” slide) that this also defines the **heat kernel** between x and y

In **matrix notation**, the heat kernel can be written as a $n \times n$ matrix

$$\mathbf{K}_t = \mathbf{\Phi} \text{diag}(e^{-\lambda_i t}) \mathbf{\Phi}^\top$$

Heat kernel: Spectral decomposition

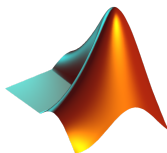
Therefore, if $u_0(x) = \delta_y(x)$, we have the solution:

$$k_t(x, y) \approx \sum_{i=0}^k e^{-\lambda_i t} \phi_i(x) \phi_i(y)$$

Recall (see “Dirac initialization” slide) that this also defines the **heat kernel** between x and y

In **matrix notation**, the heat kernel can be written as a $n \times n$ matrix

$$\mathbf{K}_t = \mathbf{\Phi} \text{diag}(e^{-\lambda_i t}) \mathbf{\Phi}^\top$$



Heat kernel signature

We stated that:

If $T : \mathcal{X} \rightarrow \mathcal{Y}$ is an **isometry**, then

$$k_t^{\mathcal{X}}(x, y) = k_t^{\mathcal{Y}}(T(x), T(y))$$

and the vice-versa also holds.

Heat kernel signature

We stated that:

If $T : \mathcal{X} \rightarrow \mathcal{Y}$ is an **isometry**, then

$$k_t^{\mathcal{X}}(x, y) = k_t^{\mathcal{Y}}(T(x), T(y))$$

and the vice-versa also holds.

We use this property to define a **local descriptor** based on the heat kernel;

Consider the diagonal of the heat kernel:

$$k_t(x, x) = \sum_{i=0}^k e^{-\lambda_i t} \phi_i(x)^2$$

Heat kernel signature

We stated that:

If $T : \mathcal{X} \rightarrow \mathcal{Y}$ is an **isometry**, then

$$k_t^{\mathcal{X}}(x, y) = k_t^{\mathcal{Y}}(T(x), T(y))$$

and the vice-versa also holds.

We use this property to define a **local descriptor** based on the heat kernel;

Consider the diagonal of the heat kernel:

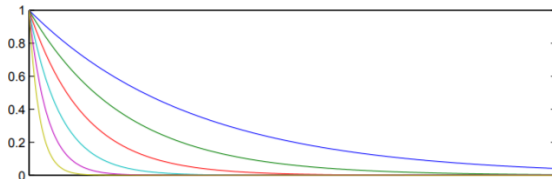
$$k_t(x, x) = \sum_{i=0}^k e^{-\lambda_i t} \phi_i(x)^2$$

The **heat kernel signature** is then defined as:

$$\text{hks}(x) = (k_{t_1}(x, x), \dots, k_{t_T}(x, x)) \in \mathbb{R}^T$$

Heat kernel signature

$$\text{hks}(x) = (k_{t_1}(x, x), \dots, k_{t_T}(x, x)) \in \mathbb{R}^T$$



If \mathcal{X} and \mathcal{Y} are isometric, corresponding points $(x, y) \in \mathcal{X} \times \mathcal{Y}$ are expected to have similar signatures

Diffusion distance

Does the heat kernel define a **distance** function?

$$k_t(x, y) \approx \sum_{i=0}^k e^{-\lambda_i t} \phi_i(x) \phi_i(y)$$

Diffusion distance

Does the heat kernel define a **distance** function? No.

$$k_t(x, y) \approx \sum_{i=0}^k e^{-\lambda_i t} \phi_i(x) \phi_i(y)$$

Diffusion distance

Does the heat kernel define a **distance** function? No.

$$k_t(x, y) \approx \sum_{i=0}^k e^{-\lambda_i t} \phi_i(x) \phi_i(y)$$

A family of **diffusion distances** can be defined by:

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

Diffusion distance

Does the heat kernel define a **distance** function? No.

$$k_t(x, y) \approx \sum_{i=0}^k e^{-\lambda_i t} \phi_i(x) \phi_i(y)$$

A family of **diffusion distances** can be defined by:

$$d_t^2(x, y) = \|k_t(x, \cdot) - k_t(\cdot, y)\|^2 = \int_{\mathcal{X}} (k_t(x, z) - k_t(z, y))^2 dz$$

Diffusion distance

Does the heat kernel define a **distance** function? No.

$$k_t(x, y) \approx \sum_{i=0}^k e^{-\lambda_i t} \phi_i(x) \phi_i(y)$$

A family of **diffusion distances** can be defined by:

$$d_t^2(x, y) = \|k_t(x, \cdot) - k_t(\cdot, y)\|^2 = \int_{\mathcal{X}} (k_t(x, z) - k_t(z, y))^2 dz$$

- The definition above satisfies all properties of a **metric**

Diffusion distance

Does the heat kernel define a **distance** function? No.

$$k_t(x, y) \approx \sum_{i=0}^k e^{-\lambda_i t} \phi_i(x) \phi_i(y)$$

A family of **diffusion distances** can be defined by:

$$d_t^2(x, y) = \|k_t(x, \cdot) - k_t(\cdot, y)\|^2 = \int_{\mathcal{X}} (k_t(x, z) - k_t(z, y))^2 dz$$

- The definition above satisfies all properties of a **metric**
- Diffusion time $t \geq 0$ plays the role of a **scale** parameter

Diffusion distance

Does the heat kernel define a **distance** function? No.

$$k_t(x, y) \approx \sum_{i=0}^k e^{-\lambda_i t} \phi_i(x) \phi_i(y)$$

A family of **diffusion distances** can be defined by:

$$d_t^2(x, y) = \|k_t(x, \cdot) - k_t(\cdot, y)\|^2 = \int_{\mathcal{X}} (k_t(x, z) - k_t(z, y))^2 dz$$

- The definition above satisfies all properties of a **metric**
- Diffusion time $t \geq 0$ plays the role of a **scale** parameter
- Interpretation: If two points x and y are close, there is a large **probability of transition** from x to y and vice-versa

Diffusion distance

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

Diffusion distance

$$\begin{aligned}d_t^2(x, y) &= \|k_t(x, \cdot) - k_t(\cdot, y)\|^2 \\&= \int_{\mathcal{X}} (k_t(x, z) - k_t(z, y))^2 dz\end{aligned}$$

Diffusion distance

$$\begin{aligned}d_t^2(x, y) &= \|k_t(x, \cdot) - k_t(\cdot, y)\|^2 \\&= \int_{\mathcal{X}} (k_t(x, z) - k_t(z, y))^2 dz \\&= \int_{\mathcal{X}} k_t(x, z)^2 + k_t(z, y)^2 - 2k_t(x, z)k_t(z, y) dz\end{aligned}$$

Diffusion distance

$$\begin{aligned}d_t^2(x, y) &= \|k_t(x, \cdot) - k_t(\cdot, y)\|^2 \\&= \int_{\mathcal{X}} (k_t(x, z) - k_t(z, y))^2 dz \\&= \int_{\mathcal{X}} k_t(x, z)^2 + k_t(z, y)^2 - 2k_t(x, z)k_t(z, y) dz \\&= \int_{\mathcal{X}} k_t(x, z)k_t(z, x) + k_t(y, z)k_t(z, y) - 2k_t(x, z)k_t(z, y) dz\end{aligned}$$

Diffusion distance

$$\begin{aligned}d_t^2(x, y) &= \|k_t(x, \cdot) - k_t(\cdot, y)\|^2 \\&= \int_{\mathcal{X}} (k_t(x, z) - k_t(z, y))^2 dz \\&= \int_{\mathcal{X}} k_t(x, z)^2 + k_t(z, y)^2 - 2k_t(x, z)k_t(z, y) dz \\&= \int_{\mathcal{X}} k_t(x, z)k_t(z, x) + k_t(y, z)k_t(z, y) - 2k_t(x, z)k_t(z, y) dz \\&= k_{2t}(x, x) + k_{2t}(y, y) - 2k_{2t}(x, y)\end{aligned}$$

Diffusion distance

$$\begin{aligned}d_t^2(x, y) &= \|k_t(x, \cdot) - k_t(\cdot, y)\|^2 \\&= \int_{\mathcal{X}} (k_t(x, z) - k_t(z, y))^2 dz \\&= \int_{\mathcal{X}} k_t(x, z)^2 + k_t(z, y)^2 - 2k_t(x, z)k_t(z, y) dz \\&= \int_{\mathcal{X}} k_t(x, z)k_t(z, x) + k_t(y, z)k_t(z, y) - 2k_t(x, z)k_t(z, y) dz \\&= k_{2t}(x, x) + k_{2t}(y, y) - 2k_{2t}(x, y)\end{aligned}$$

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

Diffusion distance

$$\begin{aligned}d_t^2(x, y) &= \|k_t(x, \cdot) - k_t(\cdot, y)\|^2 \\&= \int_{\mathcal{X}} (k_t(x, z) - k_t(z, y))^2 dz \\&= \int_{\mathcal{X}} k_t(x, z)^2 + k_t(z, y)^2 - 2k_t(x, z)k_t(z, y) dz \\&= \int_{\mathcal{X}} k_t(x, z)k_t(z, x) + k_t(y, z)k_t(z, y) - 2k_t(x, z)k_t(z, y) dz \\&= k_{2t}(x, x) + k_{2t}(y, y) - 2k_{2t}(x, y)\end{aligned}$$

$$\begin{aligned}d_t^2(x, y) &= \|k_t(x, \cdot) - k_t(\cdot, y)\|^2 \\&= \dots \\&= \sum_{i=0}^k e^{-2\lambda_i t} (\phi_i(x) - \phi_i(y))^2\end{aligned}$$

Exercise: Functional maps and HKS

Solve for a functional map between two deformable shapes by using HKS as corresponding functions.

Specifically:

- Use shapes $\mathcal{X} = \text{tr_reg_001}$ and $\mathcal{Y} = \text{tr_reg_002}$
- Compute 100-dimensional heat kernel signatures for all vertices of \mathcal{X} and \mathcal{Y} (choose your own diffusion times)
- Express the two descriptor fields as $k \times 100$ spectral coefficient matrices \mathbf{A} and \mathbf{B} , where k is the eigenbasis dimension for both \mathcal{X} and \mathcal{Y}
- Solve for the $k \times k$ functional map matrix \mathbf{C} in a least squares sense
- Use \mathbf{C} to transfer delta functions from \mathcal{X} to \mathcal{Y} , and visually evaluate the quality of the estimated functional map