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J. Bender, C. Duriez, F. Jaillet, and G. Zachmann (Editors)

Efficient Transfer of Contact-Point Local Deformations: Supplemental Material

M. U. Seiler[1] and J. Spillmann[2] and M. Harders[3]

[1] Computer Vision Lab, ETH Zurich [2] VirtaMed AG [3] Interactive Graphics and Simulation Lab, University of Innsbruck

1. Mathematical Background

The goal of the supplemental material is to provide a brief introduction to the concepts presented in the paper. To this end, we will work with intuitive analogies and omit some of the technicalities that would be required for a mathematically rigorous derivation. That being said, the property of *square-integrability*, *e. g.*, $\int_{-\infty}^{\infty} f(x)^2 dx < \infty$ for a function $f : \mathbb{R} \to \mathbb{R}$, is often a necessary condition that we assume as implicitly given.

As a quick outline, we will be working with instances of *Hilbert spaces*. One can think of them as a vector space equipped with an inner-product that in fact generalizes the well known Euclidean space. Hence, we first repeat some concepts from basic linear algebra and then use analogies to carry over the intuitive understanding of vector bases to the potentially less familiar concept of function bases. In particular, we will have a closer look at theories that circle the orthogonal basis of the Hermite polynomials that is used in the paper.

2. From Vectors to Functions

When we are working with Euclidean vectors, such as $\mathbf{x} \in \mathbb{R}^3$, then we are often working directly with the components written as

$$\mathbf{x} = \begin{bmatrix} 4.2 \\ -7.3 \\ 1.5 \end{bmatrix}. \tag{1}$$

In this notation, we abstract the fact that the vector components are actually understood as coefficients with respect to a basis

$$\mathbf{B} = \begin{bmatrix} \mathbf{e}_x | \mathbf{e}_y | \mathbf{e}_z \end{bmatrix} \tag{2}$$

where $\mathbf{e}_x$, $\mathbf{e}_y$, and $\mathbf{e}_z$ are orthonormal unit vectors in $\mathbb{R}^3$. The coefficients alone are in some sense meaningless until they are anchored by a basis, *i. e.*, $\mathbf{x} = 4.2\mathbf{e}_x - 7.3\mathbf{e}_y + 1.5\mathbf{e}_z$. For a vector $\mathbf{y}$ of arbitrary length $n \in \mathbb{N}$ with the coefficients y_i and basis vectors $\mathbf{e}_i$ for $i \in 1, ..., n$ we can write

$$\mathbf{y} = \sum_{i=1}^{n} y_i \mathbf{e}_i. \tag{3}$$

The same concepts translate to functions. Bases for functions share many properties with bases for vectors, for example they might also have the property of being *orthogonal* with respect to some inner-product analogous to two Euclidean vectors being orthogonal if their respective dot-product - that is the most commonly used inner-product - is zero. Similar to the unit basis vectors $\mathbf{e}_i$, a family of n functions $\phi_i(x) := sin(2\pi i x)$ for $i \in 1, ..., n$ can be used as a basis to represent a particular subset $\mathcal{G}$ of all functions $\mathbb{R} \to \mathbb{R}$ by a linear combination using n coefficients $c_i \in \mathbb{R}$. One specific element $g : \mathbb{R} \to \mathbb{R} \in \mathcal{G}$ takes the form

$$g(x) := \sum_{i=1}^{n} c_i \phi_i(x) = \sum_{i=1}^{n} c_i sin(2\pi i x). \tag{4}$$

In this case, our basis is still a finite set of functions based on doubling frequencies $2\pi i$. We can, however, take all frequencies on the real line into account in order to be able to represent a larger set $\mathcal{H}$ of functions that are linear super positions of sine functions. If one does this, the sum in equation (4) turns into an integral. At the same time, we also replace the coefficients c_i with a function $h_c(t) : \mathbb{R} \to \mathbb{R}$. Then we can write a particular element $h : \mathbb{R} \to \mathbb{R}$ of $\mathcal{H}$ as

$$h(x) = \int_0^{\infty} h_c(t) sin(2\pi t x) dt. \tag{5}$$

Note that the integration starts at 0 because the sine function is symmetric, *i. e.*, $sin(x) = -sin(-x)$. We mention again, that we cannot represent *any* function that maps from $\mathbb{R} \to \mathbb{R}$ but only the ones that are elements of $\mathcal{H}$ which have the limitation of being *odd* functions that pass through the origin, i.e., $h(0) = 0$ since all sine functions are odd and zero at the origin no matter how high it's frequency. More on this can be found in the literature under the topics *sine transform* and *Fourier transform*. The important thing here was really to make a point that functions have bases similar to vectors.

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3. The Unit Basis for Functions

Next we look at a very interesting basis function: *Dirac's delta function* denoted by δ. In a way it serves as the standard basis for functions. It is, however, omitted in daily use similar to the unit basis vectors for Euclidean vectors mentioned earlier. It can be defined purely axiomatically by stating $\forall x \in \mathbb{R} : x \neq 0 \rightarrow (\delta(x) = 0)$, *i. e.*, it is 0 everywhere except at the origin and its integral $\int_{-\infty}^{\infty} \delta(x)dx = 1$ sums up to 1. There are several ways to explicitly define such a function. However, a definition based on the Gaussian bell curve,

$$\delta(x) := \lim_{\sigma \to 0} \frac{1}{\sqrt{\pi}\sigma} \exp\left(-\frac{x^2}{\sigma^2},\right), \tag{6}$$

simplifies many calculations. It is localized to a single unique point in space, but, when transformed into the Fourier basis evenly covers all frequencies. In this sense, δ can be seen as the opposite of a harmonic function that spreads evenly in space but has a single frequency, *i. e.*, it is a peak at a single point in frequency space. The Dirac delta functions is a basis that simply amounts to specifying the value of $f : \mathbb{R} \rightarrow \mathbb{R}$ at any point using the coefficient function $f_c : \mathbb{R} \rightarrow \mathbb{R}$ since

$$f(x) = \int_{\mathbb{R}} \delta(t-x)\, f_c(t)\, dt = f_c(x) \tag{7}$$

and it is thus seemingly of little use by itself. It can, however, be used to formally define discrete samples of functions by using a "comb" of Dirac functions.

The definition based on the Gaussian bell curve has a single parameter σ with which we can control the locality to define a new function $\tilde{f} : \mathbb{R} \rightarrow \mathbb{R}$ that is low-pass filtered

$$\tilde{f}(x) := \int_{\mathbb{R}} \frac{1}{\sqrt{\pi}\sigma} \exp\left(-\frac{(t-x)^2}{\sigma^2}\right) f_c(t)\, dt\,. \tag{8}$$

Since σ can be modified continuously, it allows us in a way to select how we would like to represent information. In the limit $\sigma \rightarrow 0$ all the information is compressed to a single point, by setting it to some finite value $\sigma > 0$ we extend the influence from a single point to a local region around x.

What makes the formulation very interesting is its versatility in the context of linear operators, such as differentiation, integration, or transforms to some frequency space, *e. g.*, to the Fourier space. As an example, we investigate the first derivative of $\tilde{f}$ with respect to x:

$$\begin{aligned} \frac{\partial}{\partial x}\tilde{f}(x) &= \int_{\mathbb{R}} \frac{1}{\sqrt{\pi}\sigma} \frac{\partial}{\partial x} \exp\left(-\frac{(t-x)^2}{\sigma^2}\right) f_c(t)\, dt \qquad (9) \\ &= \int_{\mathbb{R}} -\frac{1}{\sqrt{\pi}\sigma} \exp\left(-\frac{(t-x)^2}{\sigma^2}\right) \frac{2(t-x)}{\sigma^2} f_c(t)\, dt \qquad (10) \end{aligned}$$

The differential operator commutes with the integral and thus we take the derivative of the exponential function with respect to x. Similar mathematical concepts are, for example, used in SPH-based fluid simulation.

4. Decomposing a Function

Similar to decomposing a vector into a linear combination of its basis vectors we can decompose a function into a sum of basis functions. We start again with the vector analogy.

As stated earlier, the vector $\mathbf{x} \in \mathbb{R}^3$ can be written as a sum of orthonormal basis vectors $\mathbf{x} = c_1\,\mathbf{e}_1 + c_2\,\mathbf{e}_2 + c_3\,\mathbf{e}_3$. The question is now how can one compute c_1 given $\mathbf{x}$ and $\mathbf{e}_1$? The solution is well known and is a basic application of the inner product for $\mathbf{a}, \mathbf{b} \in \mathbb{R}^3$ as $\langle \mathbf{a}, \mathbf{b} \rangle = \sum_{i=1}^{3} a_i \phi_i$. With a simple calculation it can be shown that $c_1 = \langle \mathbf{x}, \mathbf{e}_1 \rangle = \langle c_1\,\mathbf{e}_1 + c_2\,\mathbf{e}_2 + c_3\,\mathbf{e}_3, \mathbf{e}_1 \rangle = \langle c_1\mathbf{e}_1, \mathbf{e}_1 \rangle + \langle c_2\mathbf{e}_2, \mathbf{e}_1 \rangle + \langle c_3\mathbf{e}_3, \mathbf{e}_1 \rangle = \langle c_1\mathbf{e}_1, \mathbf{e}_1 \rangle = c_1 \langle \mathbf{e}_1, \mathbf{e}_1 \rangle = c_1$. Note that, this only holds for normalized bases, *i. e.*, $\langle \mathbf{e}_1, \mathbf{e}_1 \rangle = 1$.

Analogously, one can define an inner product for a function space and use it to *project* a function onto its basis functions. We reuse the same symbol (as it is clear from the context which inner product is meant) and define it as

$$\langle f, g \rangle := \int_{-\infty}^{\infty} f(t)\, g(t)\, dt \tag{11}$$

for two real-valued (square-integrable) functions f and g. We reuse our family of n basis functions $\phi_i : \mathbb{R} \rightarrow \mathbb{R}$ to demonstrate how to compute the corresponding coefficients

$$c_i = \langle f, \phi_i \rangle = \int_{-\infty}^{\infty} f(t)\, \phi_i(t)\, dt \text{ and thus } g(x) = \sum_{i=1}^{n} \langle g, \phi_i \rangle\, \phi_i(x). \tag{12}$$

Which leads to our next topic: numerical integration.

5. Monte Carlo Fitting of Hermite Polynomials

In this section we briefly derive our Monte Carlo integration scheme that we use to evaluate Hermitian moments. Note that, we redefine some entities, such as f, g, and ϕ , but their conceptual usage is consistent. To start, consider the problem

$$I_\Omega \in \mathbb{R} := \int_\Omega f(\mathbf{x}) dV \tag{13}$$

of computing the definite integral I_Ω over a finite domain $\Omega \subset \mathbb{R}^3$ of a function $f : \Omega \rightarrow \mathbb{R}$.

By using Monte Carlo integration, I_Ω can be approximated by a finite sum S_n as

$$I_\Omega \approx S_n := \frac{V}{n} \sum_{i=1}^{n} f(\mathbf{x}_i) \tag{14}$$

of n evaluations of the integrand f at sample points $\mathbf{x}_i \in \Omega$ that are drawn uniformly from Ω. Additionally, the result is scaled with the volume per sample point $\frac{V}{n}$ where $V = \int_\Omega 1 dV$ is the volume of Ω and n is the number of sample points.

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However, one might be interested in solving an indefinite integral, like

$$\tilde{I}_{\mathbb{R}^3} := \int_{\mathbb{R}^3} g(\mathbf{x})\phi(\mathbf{x})dV \approx \tilde{S}_n = \frac{V}{n}\sum_{i=1}^{n} g(\mathbf{x}_i)\phi(\mathbf{x}_i), \quad (15)$$

that is the integral of a product of two functions $g : \mathbb{R}^3 \to \mathbb{R}$ and $\phi : \mathbb{R}^3 \to \mathbb{R}$. This leads to problems, since now the volume V of the integration domain is not finite anymore.

In a next step we require that ϕ is a normalized kernel, *i. e.*, the indefinite integral of ϕ sums up to 1:

$$\int_{\mathbb{R}^3} \phi(\mathbf{x})dV = 1 \approx \frac{V}{n}\sum_{i=1}^{n} \phi(\mathbf{x}_i). \quad (16)$$

This implies that

$$\frac{V}{n} \approx \frac{1}{\sum_{i=1}^{n} \phi(\mathbf{x}_i)}. \quad (17)$$

To give an example, ϕ could be a normalized weight function like $\phi(\mathbf{x}) = exp(-\pi\,\mathbf{x}^T\mathbf{x})$. Note that it also holds for higher-order (normalized) Hermite functions. By putting (17) into (15), the integral $\tilde{I}_{\mathbb{R}^3}$ can be approximated with

$$\tilde{I}_{\mathbb{R}^3} \approx \tilde{S}_n = \frac{1}{\sum_{i=1}^{n} \phi(\mathbf{x}_i)}\sum_{i=1}^{n} g(\mathbf{x}_i)\phi(\mathbf{x}_i)\,, \quad (18)$$

which does not contain an explicit reference to the volume V of the integration domain anymore. However, quite a large number of sample points are required to reduce noise. In fact, the error is cut in half by taking four times more sample points into account. Therefore, many samples are required to obtain an accurate result. In the next section, we present the least-squares method that is slightly more complex but yields better results if only a handful of samples are provided.

6. Least-Squares Fitting of Hermite Polynomials

The goals is to approximate the function f with a finite set of N multivariate Hermite polynomials (see section 4.1 in [SSH14]) as basis functions $\phi_i : \mathbb{R}^3 \to \mathbb{R}$ for $i \in 1,...,N$ such that

$$f(\mathbf{x}) \approx \mathbf{w}^T\phi(\mathbf{x}). \quad (19)$$

where $\mathbf{x} \in \mathbb{R}^3$ and $\mathbf{w} = [\mathbf{w}]_i \in \mathbb{R}^N$ is called the weight vector with a dimension that matches the number N of basis functions. The basis functions themselves are stacked in the basis vector $\phi(\mathbf{x}) : \mathbb{R}^3 \to \mathbb{R}^N = [\phi_1(\mathbf{x}),...,\phi_N(\mathbf{x})]^T$ is obtained by putting the ϕ_i for $i \in 1,...,n$ in a vector. In other words, $\phi(\mathbf{x})$ contains the evaluation of all the basis functions for the vector $\mathbf{x}$.

The main task is to determine the unknown weights in $\mathbf{w}$. For this reason, we introduce the difference function

$$d(\mathbf{x}) := \mathbf{w}^T\phi(\mathbf{x}) - f(\mathbf{x}) \quad (20)$$

that can be used to define the squared approximation error e as

$$e := ||d(\mathbf{x})||_H^2 = \langle d(\mathbf{x}), d(\mathbf{x})\rangle_H = \int_{\mathbb{R}^3} d(\mathbf{x})^2\omega(||\mathbf{x}||_2)dV \quad (21)$$

where $\langle\cdot,\cdot\rangle_H$ is the Hermite inner-product (see equation (4) in [SSH14]) that utilizes the Gaussian bell curve $\omega(r) := (2\pi)^{-\frac{3}{2}}\exp(-0.5\,r^2)$.

Formally, $\mathbf{w}$ is the solution of an unconstrained quadratic minimization problem

$$\mathbf{w} = \arg\min_{\mathbf{w}}(e) \quad (22)$$

that we solve by setting the derivative $\frac{d}{d\mathbf{w}}e = \mathbf{0}$ by using the zero vector $\mathbf{0} = [0,...,0] \in \mathbb{R}^N$.

If f is now sampled $n \geq N$ times one obtains n pairs of the form $(\mathbf{x}_i, f(\mathbf{x}_i))$ for $i \in 1,...,n$ which leads to a discrete version based on equation (21):

$$\frac{d}{d\mathbf{w}}\left(\sum_{i=1}^{n}\left(\mathbf{w}^T\phi(\mathbf{x}_i) - f(\mathbf{x}_i)\right)^2\omega(||\mathbf{x}_i||_2)\right) = \mathbf{0} \quad (23)$$

Interestingly, this equation corresponds to the *moving least squares* approach. By taking the derrivative and reordering terms it can be written in matrix-form as the following linear equation

$$\Phi^T\Phi\mathbf{w} = \Phi^T\mathbf{f} \quad (24)$$

where the matrix

$$\Phi \in \mathbb{R}^{n\times N} := \left[\phi(\mathbf{x}_1)\,\omega(\frac{1}{2}||\mathbf{x}_1||_2),...,\phi(\mathbf{x}_n)\,\omega(\frac{1}{2}||\mathbf{x}_n||_2)\right]^T \quad (25)$$

contains the weighted basis vectors. An element-wise definition of Φ is also possible and would read as $[\Phi]_{ij} := \phi_j(\mathbf{x}_i)\,\omega(\frac{1}{2}||\mathbf{x}_i||_2)$. Similarly, the $f(\mathbf{x}_i)$ are stacked into

$$\mathbf{f} \in \mathbb{R}^N := \left[f(\mathbf{x}_1)\,\omega(\frac{1}{2}||\mathbf{x}_1||_2),...,f(\mathbf{x}_n)\,\omega(\frac{1}{2}||\mathbf{x}_n||_2)\right]^T. \quad (26)$$

Note that, both times we use $\omega(\frac{1}{2}||\mathbf{x}_i||_2)$ with an additional factor of $\frac{1}{2}$ to accommodate the fact that they are multiplied back in the term $\Phi^T\Phi$ and $\Phi^T\mathbf{f}$.

Finally, one can solve for $\mathbf{w}$ by using inverse of $\Phi^T\Phi$ that leads to the well-known Moore-Penrose inverse $(\Phi^T\Phi)^{-1}\Phi^T$ which is the expected solution for a sum of quadratic error terms:

$$\mathbf{w} = (\Phi^T\Phi)^{-1}\Phi^T\mathbf{f}. \quad (27)$$

After obtaining $\mathbf{w}$, the approximation to f can be used to solve other problems, like computing the indefinite integral

$$\int_{\mathbb{R}^3} f(\mathbf{x})\,\omega(||\mathbf{x}||_2)\,dV \approx [\mathbf{w}]_0. \quad (28)$$

Stated differently, the first weight $[\mathbf{w}]_0$ of the weight vector $\mathbf{w}$ corresponds directly to indefinite integral of f in the weighted window of ω.

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References

[SSH14] SEILER M., SPILLMANN J., HARDERS M.: Efficient transfer of contact-point local deformations. *Vriphys 2014* (2014). 3

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