This paper shows the way from a (real) function $f(x)$ to a function in an infinite dimensional Hilbert space $|f\rangle$ suitable for the inner product $\langle\hat{o}|f\rangle$ and the Dirac delta. It can be seen as a supplement to the paper Hilbert space you find on this website.

It follows Andrea Aiello:

https://mpl.mpg.de/fileadmin/user_upload/Marquardt_Division/Teaching/Lecture_13.pdf

Hope I can help you with learning Quantum mechanics.

Contents

Prerequisites

Vector notation

We write vectors in bra-ket notation.

$|u\rangle$ corresponds to a column vector. We assume the vector $\vec{u}$ has n dimensions and write:

$$|u\rangle = \begin{pmatrix} u_1 \\ \dots \\ u_n \end{pmatrix}$$

$\langle u|$ corresponds to a row vector. We assume the vector $\vec{u}$ has n dimensions and write:

$$\langle u| = (u_1 \dots u_n)$$

Note: For real vectors we have $|u\rangle = \langle u|$. For complex valued vectors we need to use the complex conjugated: $|u\rangle = \langle u^*|$.

We write the inner product $\vec{u} \cdot \vec{v}$ as:

$$\vec{u} \cdot \vec{v} = \langle u|v\rangle$$

We write the orthonormal standard basis:

$$(1,0,\dots) \coloneqq |e_0\rangle, \qquad (0,1,0,\dots) \coloneqq |e_1\rangle, \qquad (0,0,1,0,\dots) \coloneqq |e_2\rangle, \qquad \dots$$

We can decompose every vector into a sum:

$$|u\rangle = \langle u|e_0\rangle + \dots + \langle u|e_{n-1}\rangle = \sum_{j=0}^{n-1} \langle u|e_j\rangle$$

Note: $\langle u|e_i\rangle$ can be seen as the projection of the vector $\langle u|$ onto the basis vector $|e_i\rangle$.

Note: any other set of orthonormal basis vectors would work the same way.

Length of a vector

In order to describe the length of a vector $\vec{u}$ we use the l^2 norm $||\vec{u}||$ to get its length:

$$||\vec{u}|| \coloneqq \sqrt{\langle u|u\rangle}$$

If the vector space is of finite dimension n then the length is finite:

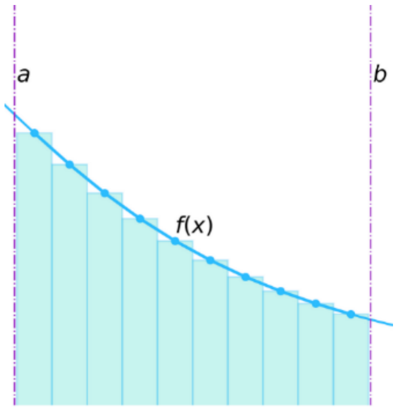
$$||\vec{u}|| \le n \cdot max(|u_i|^2)$$

Riemann integral

We remember the task calculating the area below a continuous function $f(x)$ between the boundaries a and b.[1]

We start by quantizing the function $f(x) \to f(x_i)$ and calculate the area as the sum of rectangles $\Delta x \cdot f(x_i)$:

$$A_{f(x)} \cong \sum_i \Delta x \cdot f(x_i)$$



[1] *Graphic by Vladimir Ilievski, https://isquared.digital/blog/2020-05-27-riemann-integration/*

By refining the partition, the number of rectangles grows and the width shrinks but the product $i \cdot \Delta x$ remains constant:

$$i \cdot \Delta x = b - a$$

We get:

$$\lim_{n \to \infty} \sum_{i=0}^{n} f(x_i) \cdot \Delta x = \int_a^b f(x) dx$$

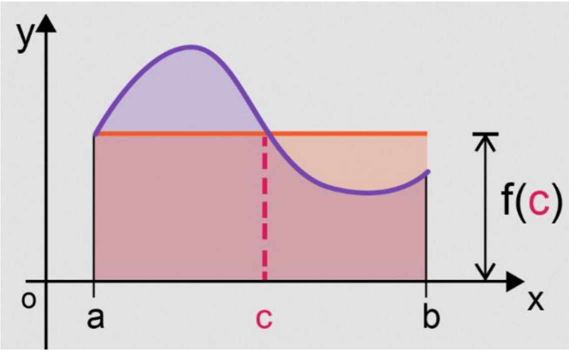
Note: What we need is that an infinite sum gives a finite value.

Mean value theorem for integrals

If $f(x)$ is continuous over an interval $[a, b]$, then there is at least one point $c \in [a, b]$ such that

$$f(c) = \frac{1}{b - a} \int_a^b f(x) dx$$

Graphically:



https://chitowntutoring.com/wp-content/uploads/mean-value-theorem-for-integrals1-1200x675.png

You may find more information at:

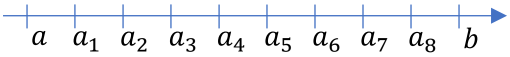
https://math.libretexts.org/Courses/Cosumnes_River_College/Math_401%3A_Calculus_II_-_Integral_Calculus/01%3A_Applications_of_Integration/1.09%3A_The_Mean_Value_Theorem_for_Integrals

End prerequisites

Quantizing functions

We use a real function $f(x)$ defined over the interval $[a, b]$.

We build an equal distributed partition of $[a, b]$:



Note: we could rename $a \rightarrow a_0$, $b \rightarrow a_n$ with $n = 9$ in the case shown above.

The length of one partition depends on the number n of intervals:

$$\Delta x = a_i - a_{i-1} = \frac{b-a}{n}$$

With an equal distribution we get the center x_i of the intervals:

$$x_i = a_i + \frac{\Delta x}{2}$$

We use $a_i = a_0 + i \cdot \Delta x, i = 0, \ldots, n-1$.

We get:

$$x_i = a_0 + i \cdot \Delta x + \frac{\Delta x}{2} = a_0 + \frac{2 \cdot i \cdot \Delta x + \Delta x}{2} =$$

$$a_0 + \frac{(2i+1)}{2} \cdot \Delta x$$

We get a discrete representation of $f(x)$:

$$f(x) \rightarrow f(x_0), f(x_1), \ldots, f(x_{n-1})$$

We can interpret this as a vector. The finer the decomposition the more dimensions.

We name the vector $|f_d\rangle$:

$$|f_d\rangle = \big(f(x_0), f(x_1), \ldots, f(x_{n-1})\big)$$

The vectors $|f_d\rangle$ are vectors with a finite number of dimensions.

We define basis vectors $|e_i\rangle, i = 0, \ldots, n-1$:

$$|e_i\rangle \coloneqq (0, \ldots, 0,1,0, \ldots, 0)$$

Every basis vector $|e_i\rangle$ has a 1 at position i and 0 else.

The basis vectors $|e_i\rangle$ form an orthonormal basis of the vector space.

The basis vectors represent the discrete x-coordinates

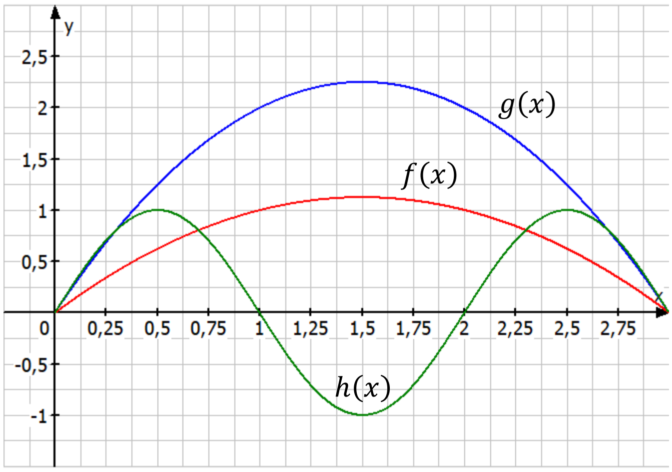
By help of the basis vectors we can rewrite $f(x)$ as a sum of projections of the vector $|f_d\rangle$ onto each basis vector:

$$|f_d\rangle = \sum_{j=0}^{n-1} f(x_j)|e_j\rangle$$

Similar functions should produce similar vectors.

We check this with three examples and a very coarse partition of three intervals.

$$f(x) = \frac{-x^2 + 3x}{2}, \qquad g(x) = -x^2 + 3x, \qquad h(x) = sin(x \cdot \pi)$$



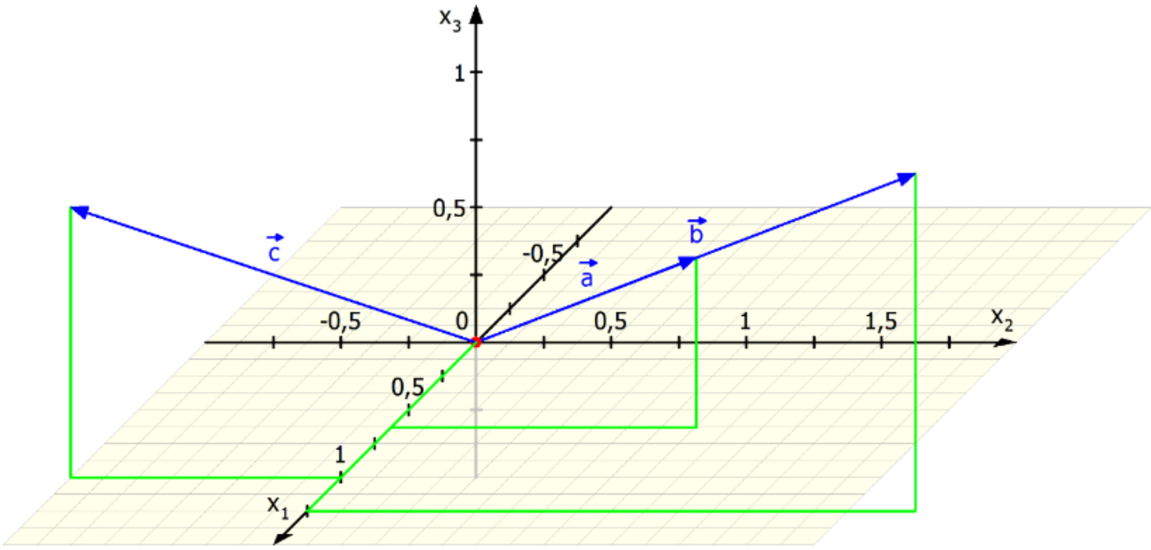
We set $n = 3$ in order to be able to display this in a $3D$ model and set the interval $[a, b]$ to $[0,3]$.

We get the quantized functions:

$$|f_3\rangle \rightarrow f(0.5); f(1.5); f(2.5) \rightarrow 0.625,1.125,0.625$$

$$|g_3\rangle \rightarrow g(0.5); g(1.5); g(2.5) \rightarrow 1.25,2.25,1.25$$

$$|h_3\rangle \rightarrow h(0.5); h(1.5); h(2.5) \rightarrow 1, -1,1$$



Note: $\vec{a}$ represents $|f_3\rangle$, $\vec{b}$ represents $|g_3\rangle$, $\vec{c}$ represents $|h_3\rangle$.

The picture shows that functions f and g are similar. The values of function g are twice the values of function f. In Hilbert space this shows as vector $\vec{b}$ being twice vector $\vec{a}$.

Vector $\vec{c}$, representing the sin- function, is different in size and direction.

Remarks

What we have so far – we can describe any continuous real function $f(x)$ by a quantized counterpart $|f_d\rangle$, a vector in a finite dimensional Hilbert space.

The finer the quantization the closer the function $|f_d\rangle$ to its continuous counterpart $f(x)$.

Properties of continuous functions $f(x)$ are slope, area.

Properties of quantized functions $|f_d\rangle$ are direction and length.

We describe the quantized function by a set of basis vectors and the projection of the function vector onto this basis vectors with their eigenvalues.

The basis vectors represent the x-coordinates.

In the process of refining $|f_d\rangle$ the number of dimensions of the Hilbert space grow, length and direction change.

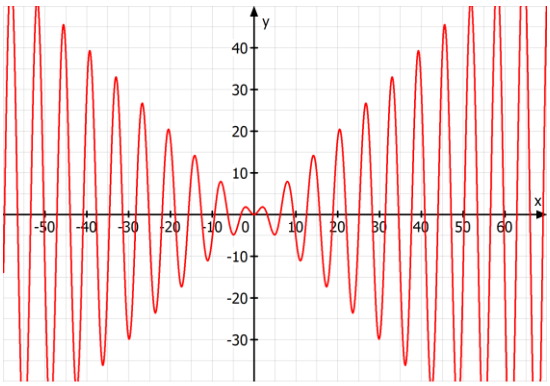
Multiplying a function

Multiplying a function $f(x)$ with a constant c changes the amplitude of the function.

In Hilbert space it changes the length of the corresponding vector.

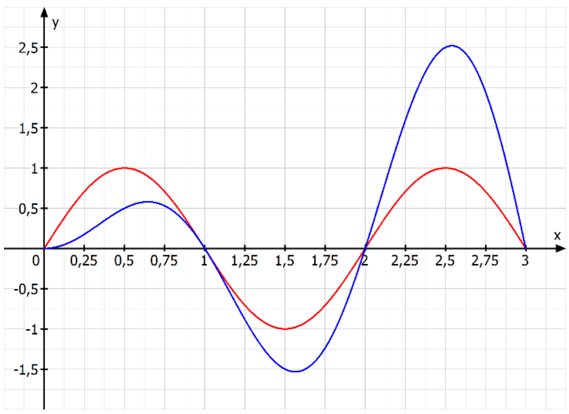
Multiplying $f(x)$ with x changes the shape of the function.

Example: $f(x) = x \cdot sin(x)$



In Hilbert space it changes length and coordinates of the corresponding vector.

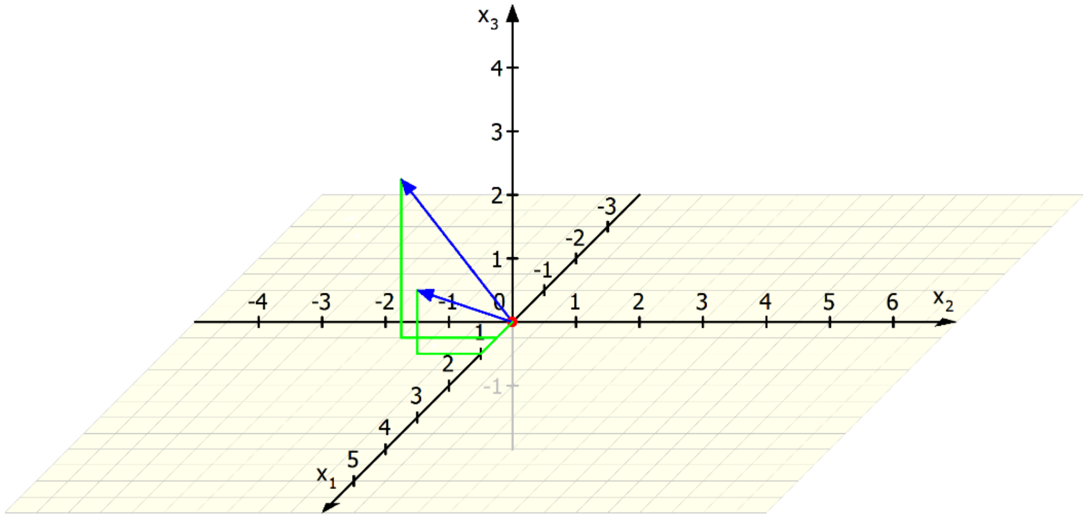
We check this by the graphs of the functions $f(x) = sin(x \cdot \pi), g(x) = x \cdot sin(x \cdot \pi)$.



$$|f_3\rangle \rightarrow f_3(0.5); f_3(1.5); f_3(2.5) \rightarrow 1, -1, 1$$

$$|g_3\rangle \rightarrow g_3(0.5); g_3(1.5); g_3(2.5) \rightarrow 0.5, -1.5, 2.5$$

The representation in Hilbert space shows two vectors different in direction and length:



Multiplying by position

We describe the process of multiplying a function with x by help of an operator $\hat{x}$:

$$(\hat{x}f)x \coloneqq x \cdot f(x)$$

Its discrete counterpart is $\hat{x}|f_d\rangle$.

We can represent the operator $\hat{x}$ by a $n \times n$ matrix. We name the matrix X and get:

$$\hat{x}|f_d\rangle = X|f_d\rangle$$

The matrix X is a diagonal matrix containing the x-positions:

$$X = \begin{pmatrix} x_0 & 0 & \dots & 0 \\ 0 & x_1 & \dots & 0 \\ \dots & \dots & \dots & \dots. \\ 0 & 0 & \dots & x_{n-1} \end{pmatrix}$$

For this matrix holds:

$$\langle e_i|X|e_j\rangle = x_i\delta_{ij}$$

The basis vectors $|e_i\rangle$ are eigenvectors of the matrix X with eigenvalue x_i.

We build the inner product of $\hat{x}|f_d\rangle = X|f_d\rangle$ with $\langle e_i|$:

$$\langle e_i|\hat{x}|f_d\rangle = \langle e_i|X|f_d\rangle$$

We check:

Left side $\langle e_i|\hat{x}|f_d\rangle$:

$$\langle e_i|\hat{x}|f_d\rangle = \langle e_i|x_0 \cdot f(x_0)|e_0\rangle + \langle e_i|x_1 \cdot f(x_1)|e_1\rangle + \dots + \langle e_i|x_{n-1} \cdot f(x_{n-1})|e_{n-1}\rangle =$$

$$x_0 \cdot f(x_0)\langle e_i|e_0\rangle + x_1 \cdot f(x_1)\langle e_i|e_1\rangle + \dots + x_{n-1} \cdot f(x_{n-1})\langle e_i|e_{n-1}\rangle =$$

$$x_i \cdot f(x_i)$$

Right side $\langle e_i|X|f_d\rangle$:

$$\langle e_i|X|f_d\rangle = (0 \dots 0\ i\ 0 \dots 0)\begin{pmatrix} x_0 & 0 & \dots & 0 \\ 0 & x_1 & \dots & 0 \\ \dots & \dots & \dots & \dots . \\ 0 & 0 & \dots & x_{n-1} \end{pmatrix}\begin{pmatrix} f(x_0) \\ f(x_1) \\ \dots \\ f(x_{n-1}) \end{pmatrix} =$$

$$(0 \dots 0\ x_i\ 0 \dots 0)\begin{pmatrix} f(x_0) \\ f(x_1) \\ \dots \\ f(x_{n-1}) \end{pmatrix} = x_i \cdot f(x_i)$$

We remember $|f_d\rangle$:

$$|f_d\rangle = \sum_{j=0}^{n-1} f(x_j)|e_j\rangle$$

We remember the position matrix:

$$\langle e_i|X|e_i\rangle = x_i\delta_{ij}$$

With this we can write the quantized function $x_i|f_d(x_i)\rangle$:

$$x_i|f_d(x_i)\rangle = \sum_{j=0}^{n-1} \langle e_i|X|e_j\rangle\, |f_d(x_i)\rangle$$

Length in an infinite dimensional space

We replace the function $f(x)$ by $\coloneqq \sqrt{\Delta x} \cdot f(x)$.

This leads to a replacement of the quantized function $|f_d\rangle$ by $\sqrt{\Delta x}|f_d\rangle$.

We calculate the l^2-norm of $\sqrt{\Delta x}|f_d\rangle$:

$$\left\|\sqrt{\Delta x}|f_d\rangle\right\| = \sum_{j=0}^{n-1} |f(x_i)|^2 \cdot \Delta x$$

Note: Δx is a positive value.

We take the limes:

$$\lim_{\Delta x \to 0} \left\|\sqrt{\Delta x}|f_d\rangle\right\| = \lim_{\Delta x \to 0} \sum_{j=0}^{n-1} |f(x_i)|^2 \cdot \Delta x$$

Note: By $\Delta x \to 0$ we perform the transition from the discrete to the continuous case.

This resembles the Riemann integral:

$$\lim_{\Delta x \to 0} \sum_{i=1}^{n} f(x_i) \cdot \Delta x = \int_a^b f(x)dx$$

We need that the infinite sum converges to a finite value.

We get:

$$\lim_{n\to\infty}\sum_{j=0}^{n-1}|f(x_i)|^2\cdot\Delta x=\int_a^b|f(x)|^2dx=\|f\|^2$$

Note: $\|f\|^2$ is the l^2-norm of $f(x)$.

Note: Functions that allow this transition are called square integrable functions. You may find more information at:

https://chem.libretexts.org/Courses/Grinnell_College/CHM_364%3A_Physical_Chemistry_2_(Grinnell_College)/04%3A_Postulates_and_Principles_of_Quantum_Mechanics/4.01%3A_The_Wavefunction_Specifies_the_State_of_a_System

Note: Square integrable functions often have no analytic antiderivative. The integral then can be solved only numerically.

Note: By multiplying $f_d(x_i)$ with $\sqrt{\Delta x}$ we got the new function $\sqrt{\Delta x}|f_d\rangle$. For this function holds:

$$\left\|\sqrt{\Delta x}|f_d\rangle\right\|^2\xrightarrow{\Delta x\to 0}\|f\|^2$$

Rescaling

We work with the scaled function $\sqrt{\Delta x}|f_d\rangle$:

$$\sqrt{\Delta x}|f_d\rangle=\sqrt{\Delta x}\cdot f(x_0)|e_0\rangle+\sqrt{\Delta x}\cdot f(x_1)|e_1\rangle+\cdots+\sqrt{\Delta x}\cdot f(x_{n-1})|e_{n-1}\rangle$$

The "old" scalar product was:

$$\langle e_i|f_d\rangle=f(x_i)$$

Now we get:

$$\left\langle e_i\middle|\sqrt{\Delta x}f_d\right\rangle=\sqrt{\Delta x}\cdot f(x_i)$$

In order to correct this, we rescale the basis vectors:

$$|e'_i\rangle=|e_i\rangle\cdot\frac{1}{\sqrt{\Delta x}}\to|e_i\rangle=\sqrt{\Delta x}|e'_i\rangle$$

With this rescaling of the basis vectors by we rewrite $\sqrt{\Delta x}|f_d\rangle$:

$$\sqrt{\Delta x}|f_d\rangle=\sum_{j=0}^{n-1}\sqrt{\Delta x}\cdot f(x_j)|e_j\rangle=\sum_{j=0}^{n-1}\Delta x\cdot f(x_j)|e'_j\rangle$$

We have a new inner product:

$\left\langle e'_i\middle|e'_j\right\rangle=\frac{\delta_{ij}}{\Delta x}$t

Note: δ_{ij} is the Kronecker delta. In the limes $\lim_{\Delta x\to 0}\frac{\delta_{ij}}{\Delta x}$ this becomes the Dirac δ.

Because of $\left\langle e'_i\middle|e'_j\right\rangle=\frac{\delta_{ij}}{\Delta x}$ and $e'_i\rangle=|e_i\rangle\cdot\frac{1}{\sqrt{\Delta x}}$ we get back the original function:

$$\left\langle e'_i\middle|\sqrt{\Delta x}f_d\right\rangle=f(x_i)$$

We remember that e'_i corresponds to the values on the x-axis.

In the limes $\Delta x \to 0$ resp. $n \to \infty$ we get:

$$\langle e'_i | \sqrt{\Delta x} f_d \rangle \to \langle x|f\rangle \to f(x)$$

Note: e'_i is x_i in the discrete case, in the continuous case this becomes x.

Note: $\sqrt{\Delta x} f_d$ gives the values of $f_d(x_i)$.

Note: In the limes this becomes $\langle x|f\rangle$ and this is a representation of $f(x)$.

According to Riemann we get in the limes:

$$\sqrt{\Delta x}|f_d\rangle = \sum_{j=0}^{n-1} \Delta x \cdot f(x_j)|e'_j\rangle \to \int_a^b f(\xi)|\xi\rangle d\xi$$

Continuous inner product

We take the limes case:

$$\sqrt{\Delta x}|f_d\rangle = \int_a^b f(\xi)|\xi\rangle d\xi$$

We build the inner product with $\langle x|$:

$$\langle x|f\rangle = \int_a^b \langle x|f(\xi)|\xi\rangle d\xi = \int_a^b f(\xi)\langle x|\xi\rangle d\xi$$

We remember $\langle e'_i | \sqrt{\Delta x} f_d \rangle \to \langle x|f\rangle \to f(x)$ and get for the left side:

$$\langle x|f\rangle = f(x)$$

On the right side we need $f(x)$ too.

We go back to the discrete case:

$$\sqrt{\Delta x}|f_d\rangle = \sum_{j=0}^{n-1} \Delta x \cdot f(x_j)|e'_j\rangle$$

$$\langle e'_i | e'_j \rangle = \frac{\delta_{ij}}{\Delta x}$$

We build the inner product:

$$\langle e'_i \sqrt{\Delta x} | f_d \rangle = \langle e'_i | \textstyle\sum_{j=0}^{n-1} \Delta x \cdot f(x_j)|e'_j\rangle\rangle =$$

$$\sum_{j=0}^{n-1} \Delta x \cdot f(x_j)\langle e'_i | e'_j \rangle =$$

$$\sum_{j=0}^{n-1} \Delta x \cdot f(x_j) \cdot \frac{\delta_{ij}}{\Delta x}$$

We keep Δx and use Riemann again:

$$\lim_{\Delta x \to 0} \sum_{i=0}^{n-1} \Delta x \cdot f(x_j) \cdot \frac{\delta_{ij}}{\Delta x} = \int_a^b f(\xi) \left(\lim_{\Delta x \to 0} \frac{\delta_{ij}}{\Delta x} \right) d\xi = \int_a^b f(\xi) \big(\delta(\xi - x) \big) d\xi = f(x)$$

Note: $\delta(\xi - x)$ is the Dirac delta.

Result

What we get is:

$$\langle x | f \rangle = f(x)$$

The inner product of position x and function $f(x)$ gives the value of the function at position x, both in the continuous and the discrete case.

We now have a vector representation $|f\rangle$ of the continuous function $f(x)$

Any square integrable function $f(x)$ may be interpreted as the projection of the vector $|f\rangle$ onto the basis vector $|x\rangle$ with the eigenvalue x.

$f(x)$ in this sense is the x-th coordinate of the vector $|f\rangle$ in an infinite dimensional vector space.