Transfer from Discrete to Continuous Inner-Products in a Computational Course

DUE 1836604

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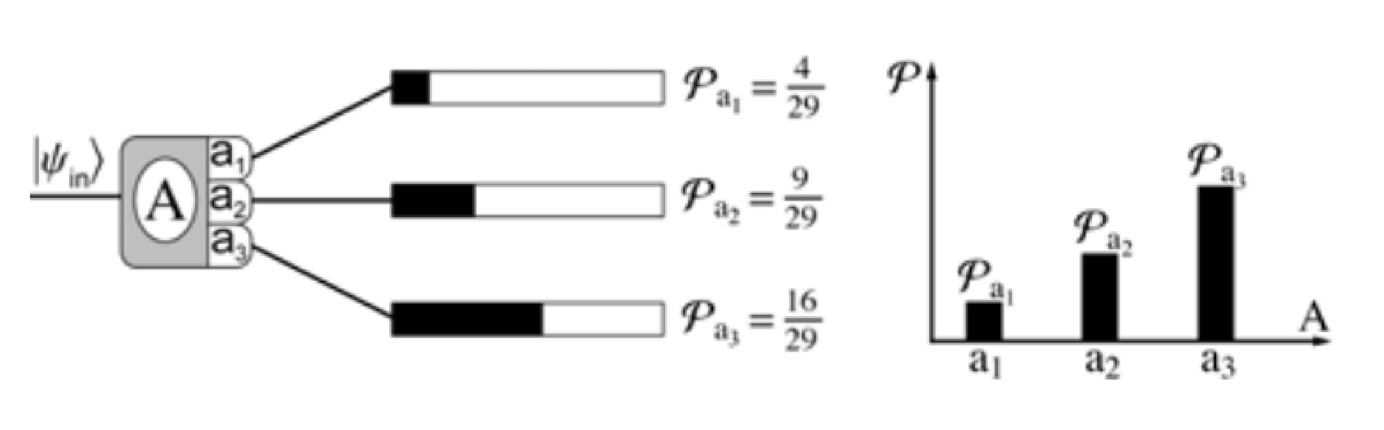
A Spins-First Approach at OSU

- Introductory Quantum course starts with spin systems
  - Introduces Dirac and matrix notation early
  - Emphasis on histograms of probabilities
  - Ends with a particle in a box



Manogue et al. PERC 2011 Proceeding **1413**, 55-58 (2011)

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RQ: What resources about discrete inner products are students using for continuous inner products?

The connection

$$\langle \alpha | \beta \rangle = \sum_i \alpha_i^* \beta_i = \alpha_1^* \beta_1 + \alpha_2^* \beta_2 + ...$$

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$$\langle \phi_n | \psi \rangle = \sum_{i=0} \phi_n^*(i) \psi(i) \Delta x \rightarrow \int_0^L \phi_n^*(x) \psi(x) dx$$

Supporting with Computation

- Wavefunctions are necessarily discretized in computation

$$\psi(x) = Ax(x - L)$$

Supporting the transition with Computation

- Wavefunctions are necessarily discretized in computation

$$\psi(x) = Ax(x - L)$$

$$\Downarrow$$

$$\psi(x) \rightarrow \psi(0), \psi(\Delta x), \psi(2\Delta x), ...\psi(L)$$

Computational Physics Lab

Physics 365

Winter 2020

Office hours: David Roundy: F 12-1, 401B Weniger
Zoom: Link for the last class class
Zoom: Instructions for the final exam

1 Introduction

Static fields

1 Potential due to charges
2 Electric field
3 Vector potential

Quantum fundamentals

1 Mean position
2 Sinusoidal basis set
3 Position operator
4 Kinetic energy

Computational Lab Course

- Taken with the associated intro quantum course
- Students practice pair programming
- Designed to compliment what is being learned in the quantum course

Methods – Remote Interviews

- Asked six students to participate in the study
- Conducted interviews over Zoom using screen-sharing
- Interview included
  - Pseudo-code component
  - Code interpretation Component

https://www.creativefabrica.com/wp-content/uploads/2019/12/18/Laptop-icon-vector-Graphics-1.png

https://blog.zoom.us/wordpress/wp-content/uploads/2020/02/Zoom-Logo.jpg

Interview Prompts

Psuedo-Code Section: Spin-1 System

- How would you describe in pseudo-code computing the inner product (IP) of these two spin-1 states?

$$|\alpha\rangle = \frac{2}{\sqrt{14}}|-1\rangle + \frac{1}{\sqrt{14}}|0\rangle + \frac{3}{\sqrt{14}}|1\rangle$$

$$|\beta\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle$$

Pseudo-Code Section: Particle in a Box

- How would you describe in pseudo-code computing the inner product of the wavefunction below and an energy eigenstate of a particle in a box (PIB)?

$$\psi(x) = Ax(x-L)^4$$

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

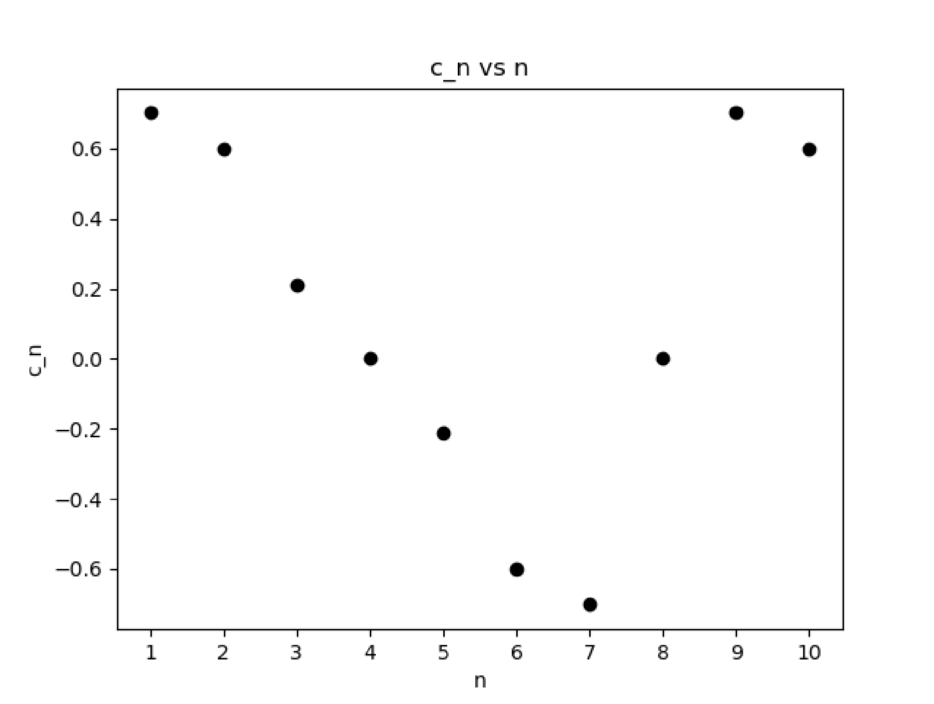
Code Interpretation

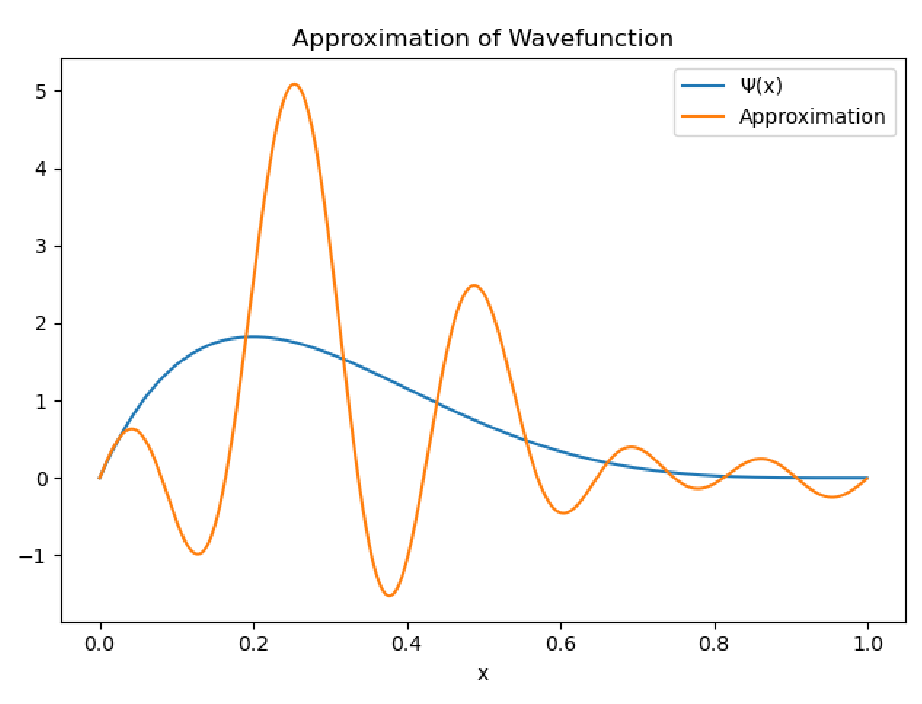
- Buggy code approximates a wavefunction of a particle in a box

$$f_{n_{max}}(x) = \sum_{n=0}^{n_{max}} \langle \phi_n | \psi \rangle \phi_n(x)$$

```python
import numpy as np
L=1
n_max = 10
dx = .25

def psi(x):
    return np.sqrt(495)/L**5/np.sqrt(L)*x*(x-L)**4

def phi_n(n, x):
    return np.sqrt(2/L)*np.sin(n*np.pi*x/L)

def c_n(n):
    sum = 0
    for x in np.arange(0,L,dx):
        sum += np.conjugate(phi_n(n,x))*psi(x)*dx
    return sum

def f_nmax(x):
    f=0
    for n in list(range(1, n_max+1,1)):
        f += c_n(n)*phi_n(n,x)
    return(f)

import matplotlib.pyplot as plt

plt.figure()
for n in list(range(1, n_max+1, 1)):
    print("c_"+str(n)+" = "+str(c_n(n)))
    plt.scatter(n,c_n(n), color='black')
plt.xlabel("n")
plt.ylabel("c_n")
plt.title("c_n vs n")
plt.xticks(list(range(1, n_max+1, 1)))

plt.figure()

xvals = np.arange(0,L,0.001)

plt.plot(xvals, psi(xvals), label='Ψ(x)')
plt.plot(xvals, f_nmax(xvals), label="Approximation")
plt.plot(xvals, c_n(9)*phi_n(9,xvals), label="c9*φ_n(x)")
plt.xlabel("x")
```

Code Interpretation

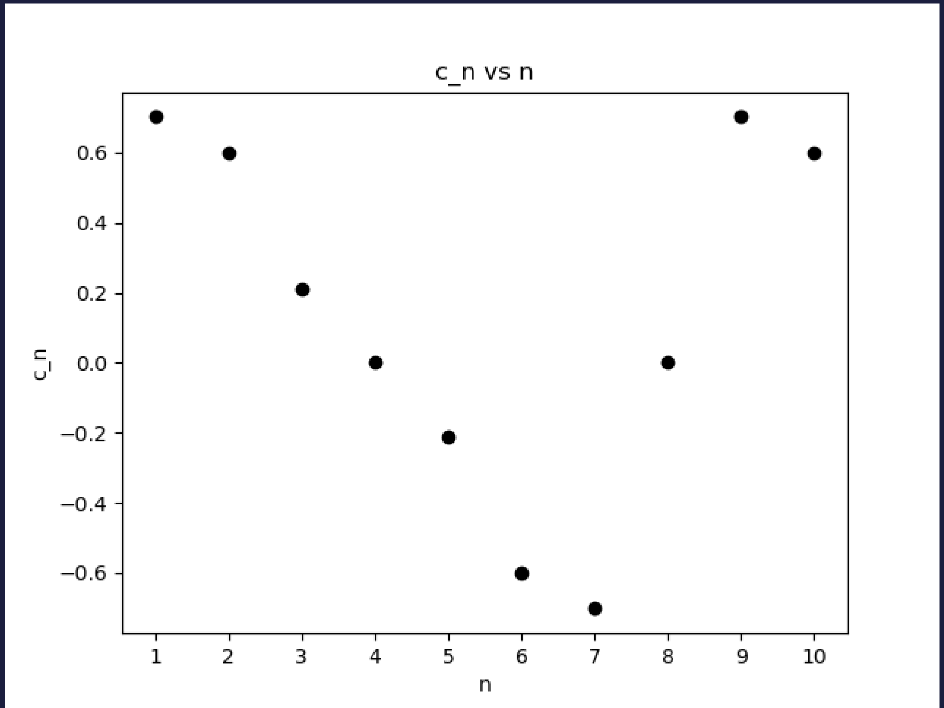


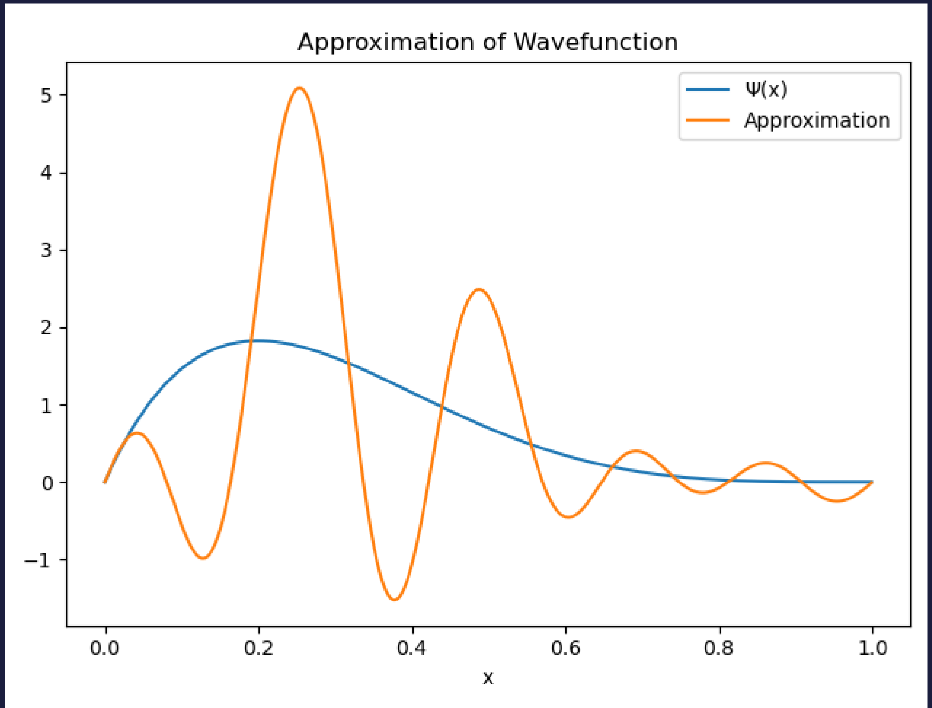


- Inner product c_n = <n|Ψ>
- Coefficients decrease past zero and then grow again

- Bad approximation
- More “wiggles” in the approximation than the wavefunction

Code Interpretation





- Plots generated from pre-written code
- Students are encouraged to manipulate the code
- Want to capture student’s reasoning and sense-making about the inner products

Intriguing Results

(Chop,) Multiply, Add

"Well, an integral is just adding up a bunch of stuff so I guess that's where they're kind of similar. You can have a bunch of pieces in the [spin-1 case] and you just add them together and you do the same thing in the integral…"

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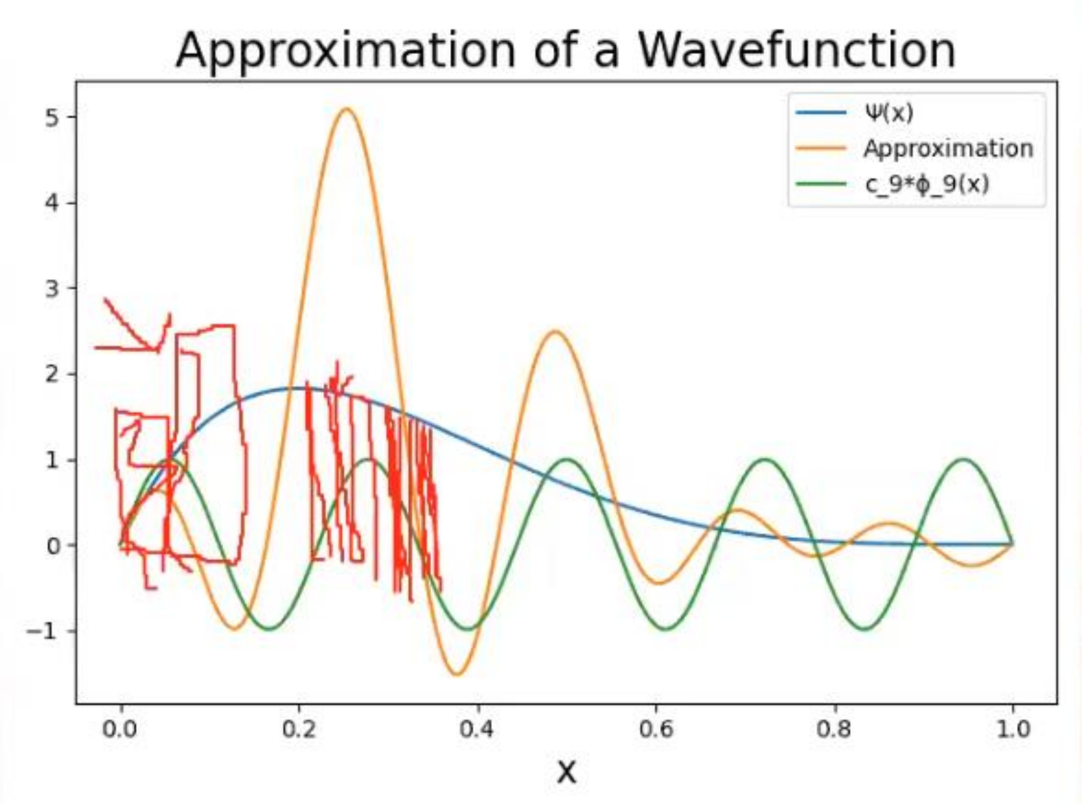
Riemann Sums

- Used Riemann sums to talk about the role of dx
- Transition from sums to integrals in calculus



F’s Riemann sum drawing

Projections

- The idea of projections was often used in intro quantum course

> "When you do an inner product, you're projecting that function onto that eigenstate so you're finding what amount of that function is along this eigenstate."
>
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Future Work

- Analysis is in progress – lots to consider!
- Finding a transfer framework
- In-class data of participants pair-programming

Summary

- RQ: What resources about discrete inner products are students using for continuous inner products?
- Designed an interview protocol for data collection during social distancing
- Ways participants related discrete and continuous Inner Products
  - Chop, Multiply, Add
  - Riemann Sums
  - Projections