Observations

on

Gaussian Basis Functions

for

Schrödinger's Equation

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Outline

- Some problems in computational QM
- Spatial discretization - choosing basis functions
- Distributed Gaussian bases
- Observations on Gaussian basis functions
- Conclusions and prospects

Computational quantum mechanics

Hamiltonian: $\hat{H} = -\frac{\partial^2}{\partial x_1^2} \ldots - \frac{\partial^2}{\partial x_d^2} + \hat{V}_{sys}(x_1, \ldots, x_d)$

Examples of system potentials

- n atom molecules, $d = 3n - 6$ d.o.f.
- n electron quantum dots $d = 2n$ d.o.f.

Schrödingers eigenproblem:

- $\hat{H}\psi = E\psi$ find energies/eigenfunctions

Dynamics - Schrödingers equation:

- $\psi(x_1, \ldots, x_d, 0) = \psi_0(x_1, \ldots, x_d)$
- $i\frac{\partial \psi}{\partial t} = [\hat{H} + \hat{V}(x_1, \ldots, x_d, t)]\psi$

Examples of external potentials $\hat{V}$

- Lasering an electron trapped in a 2D quantum dot $\hat{V}(t) = I(t)\cos(\omega t)(x_1 + x_2)$
- Electrodes with potentials $f_i(x)$ effecting trapped particles $\hat{V}(x, t) = \sum I_i(t) f_i(x)$
- Time dependent switching between different $\hat{V}_{sys}$ induced by short laser bursts

Problems we want to solve

- Eigenproblems - spectrum, structure, properties, of molecules and nano structures

- Understand and control molecular dynamics

- Manipulate trapped particles (quantum computers), $e.g.$ transport between traps

Presently consider only bound problems

Hard calculations!

- High dimensional domains, with non trivial geometry

- Space oscillations

- Time oscillations

Presently can calculate

Dynamics: d.o.f. ≤ 6 (say the physicists)

Eigenproblem: d.o.f. ≤ 9 (e.g. Carrington et. al. 2005)

Spatial discretization

- Choose basis functions $\varphi_1, \ldots, \varphi_n$
- Calculate matrix approximations for operators $H_{ij} = \langle \varphi_i | \hat{H} \varphi_j \rangle$, $V_{ij}(t) = \langle \varphi_i | \hat{V}(x,t) \varphi_j \rangle$
- Solve $H\psi = E\psi$, $\dot{\psi} = -i[H + V(t)]\psi$

Standard basis functions

In 1D: Eigenfunctions of an $\hat{H}_0$, $e.g.$ weighted polynomials $\varphi_i(x) = \mathrm{e}^{-x^2} H_i(x)$, trigonometric polynomials $\varphi_i(x) = \mathrm{e}^{ikx}$

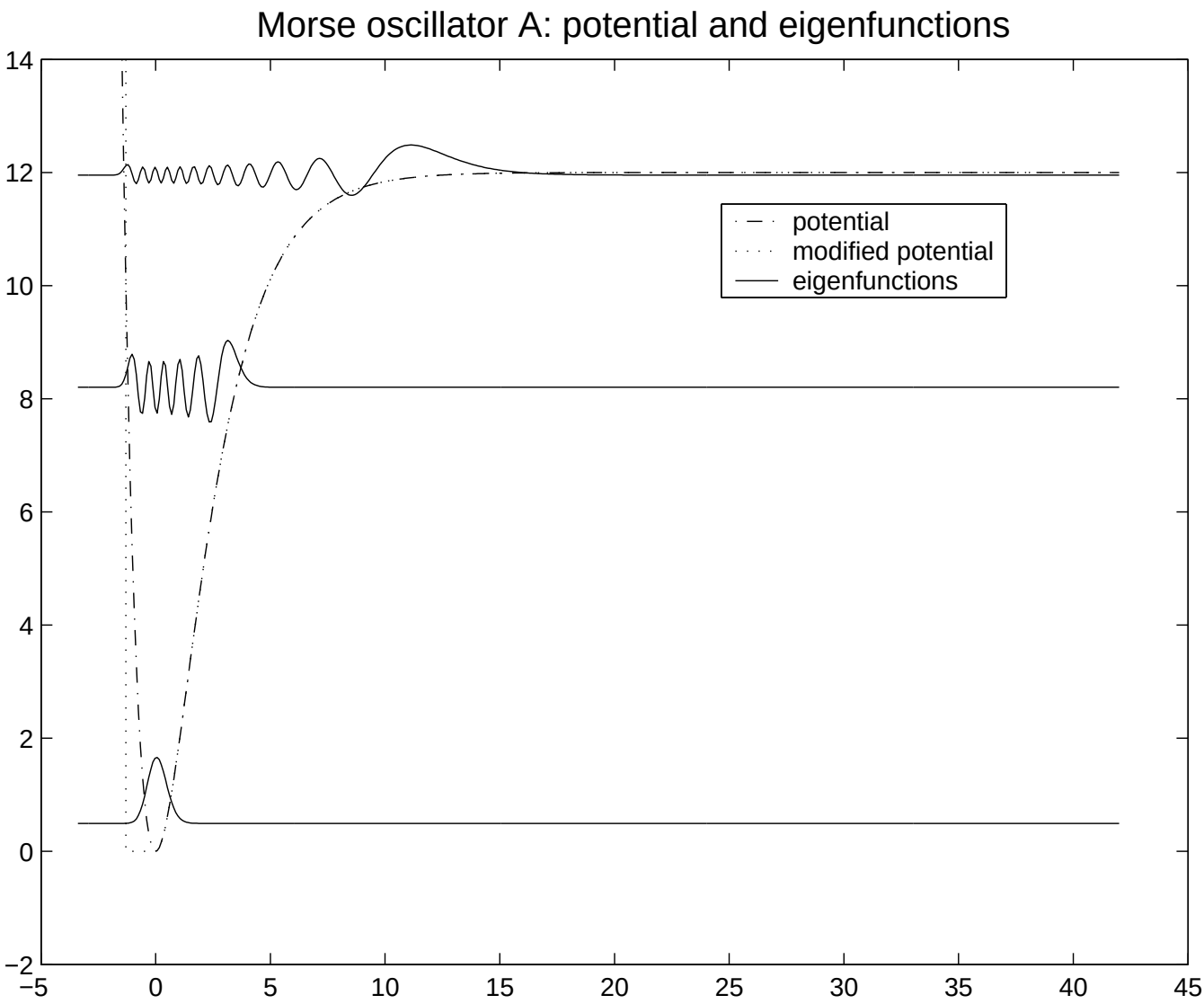
In multi-D: tensor products of such spaces

Problem - product cubature formulae, grids with $\approx 10^d$ points, rectangular layout un-related to system

Partial solution - Transform to DVR basis of "δ functions" peaked on quadrature nodes. Prune un-needed basis functions and nodes.

Ideally -

Construct basis functions that will "capture" properties of our system



Morse potential $V(x) = 12(1 - \mathrm{e}^{-0.5x})^2$ with 0th, 10th, and 23rd eigenfunctions

Gaussian Radial Basis Functions

Hamilton-Light 1986, Poirier-Light 2000
Garashcuk-Light 2001

$\varphi_i(x) = \mathrm{e}^{-cw_i(x-x_i)^2}$

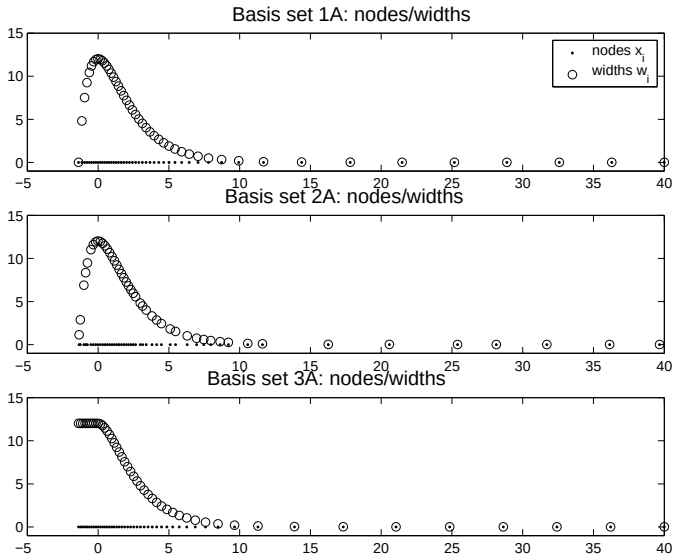
- quasi randomly distributed x_i with density $\sim \sqrt{E_{max} - V(x)}$
- width parameter $w_i \sim E_{max} - V(x_i)$
- accuracy improves as c gets smaller (but not too small)

In eigenproblem - high accuracy with 2^d basis functions (10^d in standard approach)

Observations on Garashchuk-Light bases

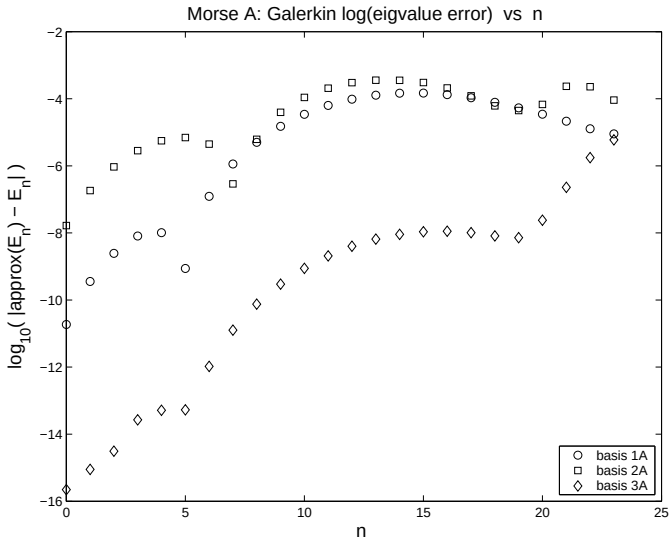
Narrower and denser Gaussians are needed in steep potential regions

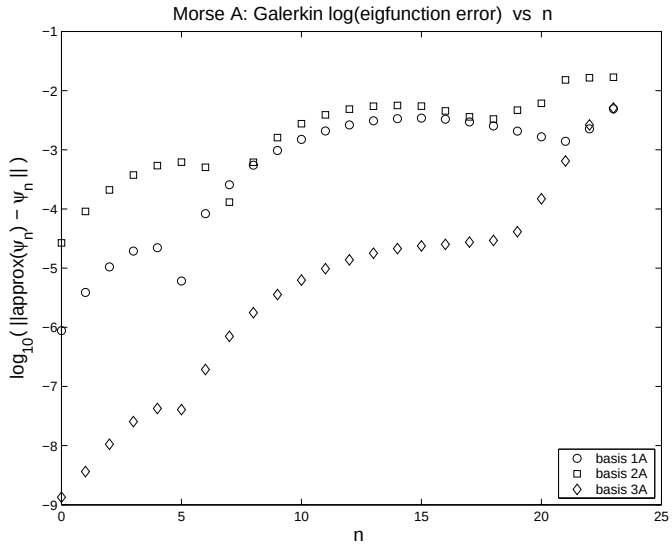
One way to achieve this: choose nodes/widths with modified potential



48 Nodes and widths chosen using different methods.

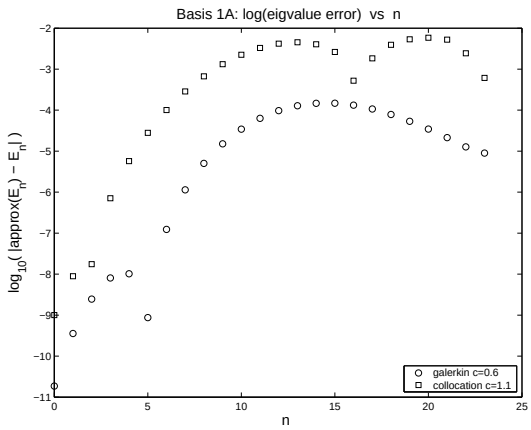
- Top: deterministically distributed nodes, density $\sim \sqrt{E_{max} - V(x)}$.
- Middle: quasi-randomly distributed nodes, density $\sim \sqrt{E_{max} - V(x)}$.
- Bottom: deterministically distributed nodes, density $\sim \sqrt{E_{max} - V_{modified}(x)}$.

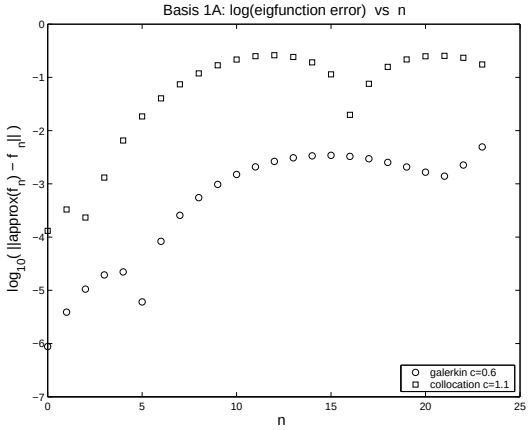


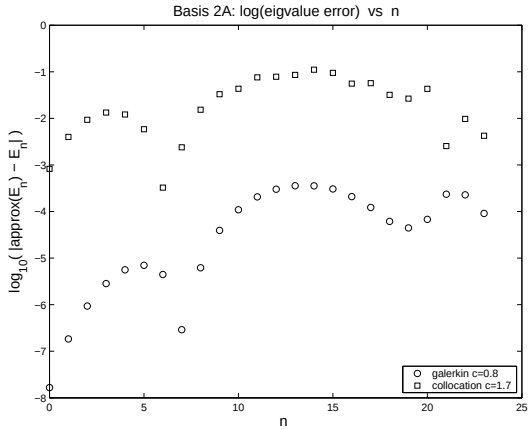


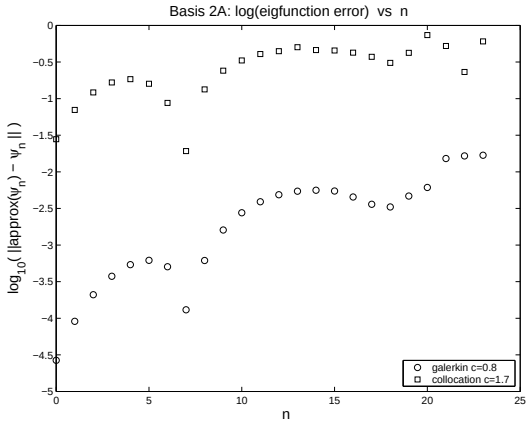
Comparing basis sets - log_{10} of eigenvalue/function errors vs index.

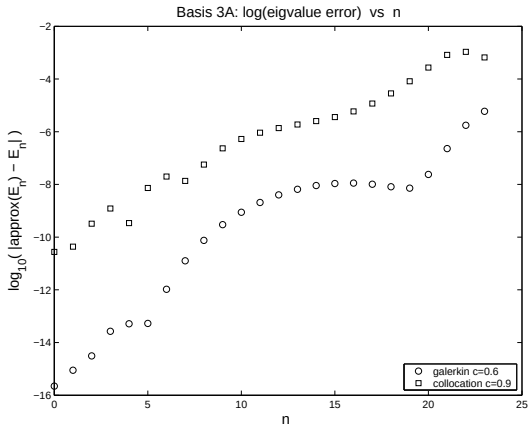
- Circles: deterministically distributed nodes, density $\sim \sqrt{E_{max} - V(x)}$.
- Squares: quasi-randomly distributed nodes, density $\sim \sqrt{E_{max} - V(x)}$.
- Diamonds: deterministically distributed nodes, density $\sim [E_{max} - V_{modified}(x)]^{1/2}$.

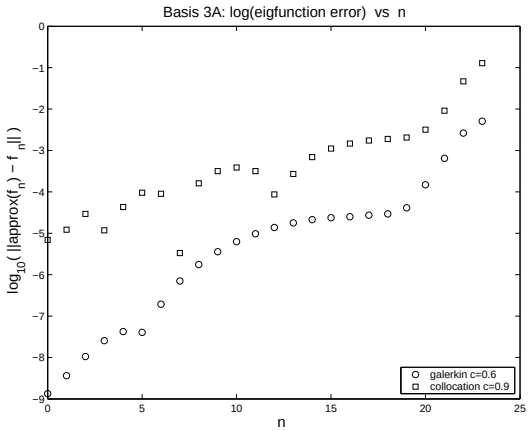












Comparing collocation and Galerkin - log_{10} of eigenvalue/function errors vs index.

Circles - Galerkin, squares - collocation.

Conclusions and prospects

- Basis function width should be compatible with highest oscillation in a neighborhood
- Collocation errors were greater than Galerkin
- Other (non random?) methods for distributing nodes?
- Using efficient basis functions (Gaussians?) in time dependent problems
- Error analysis?

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