Approximate Interacting Atomic Potentials by Analytic Functions Trained by Data Points

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A Quantum Mechanics Problem

Find a configuration of $N$ interacting atoms that minimizes the total potential energy of the system $E(x_1, x_2, \ldots, x_N)$

A system of $N$ interacting atoms  
Two-body Lennard-Jones potential $u(r)$  
$(r = \text{separation})$

Our proposed approach:

Step 1 -- approximation of potential function by simple functions in closed forms.  
Step 2 -- optimization of approximate potential functions.
Approximation of Total Potential Energy Function by Superposition of Basis Functions

\[ E(x) \sim \sum_{i} w_i b_i(x) \]

Nonlinear Function \( E(x) \)

Global optimizations
Vector space projections
Minimum Error
Space of Basis Functions
Approximate Function

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Approximation of Total Potential Function
by superposition of polynomials, radial basis functions, and neural networks
through global optimizations or vector space projections

Necessity of approximation: Quantum mechanics calculations are computationally too expensive to be used in optimization.

Simplest systems for testing: 2 atoms or 3 atoms
Input parameters: the coordinates or separations of atoms.
Output variable: the value of total potential function.
Training data set: generated by using a sum of known Lennard-Jones potential functions
Modeling objective: calibrate data driven function approximation models, and predict values of the output variable.

(Notation: tp = target pattern, op = model output, abserr = absolute error of prediction, idtp = indicator of the training patterns)
True unknown Lennard-Jones potential function recovered (2 atoms) if its structural information is known

AT1b_ANN_c03, by 1.0, P2-400, use 1 basis 101, Train minimum arrays

\[ u(r) \]

- tp[1]
- zp[1]
- abserr[1]
- idtp0

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Neural Network Model: Very good approximate model identified if special basis functions are used (2 atoms)

AT1b_Ann_tb.c04(partial arrays, 4 basis 101)
Neural Network Model: Good approximate model identified if generic basis functions are used (2 atoms)

AT1b_Ann_tb.c05(all w-r-s arrays, 4 basis 1)
One Lenard-Jones potential function

approximated by polynomial functions of degree 6
One Lenard-Jones potential function approximated by polynomial functions of degree 7
One Lenard-Jones potential function approximated by polynomial functions of degree 8
Neural Network Model: Very good approximate model identified if special basis functions are used (3 atoms)

AT3b_ANN_ci10, 1.0/2.0/5.0.P2-400, partial w-r-s-arrays for 3 basis 101
A Radial Basis Function Model ($v^*v^* \log v$): 3 atoms
AT3b_LLSp.c03, by -1.1, reordered, trimmed, P4(36,3,12)
Conclusions

1. These radial basis functions are satisfactory:

\[ \varphi(v) = v^2 \log(v), \quad v = \|x - \xi_i\|, \quad \beta > 0, \]
\[ \varphi(v) = v \exp\{-v^2/\beta\}, \quad v = \|x - \xi_i\|, \quad \beta > 0, \]
\[ \varphi(v) = \sin (\beta v), \quad v = \|x - \xi_i\|, \quad \beta > 0, \]

where \( \xi_i \) are selected from the training data set.

2. Polynomial functions of degrees 6 or higher are satisfactory.
3. Feedforward neural networks of flexible structures are also satisfactory.

Future Work

1. Test data driven models with data generated by traditional quantum mechanics calculations
2. Optimal design of atomic configurations based on trained data driven models
3. Realistic systems of atoms