CIBCB Paper Outline?

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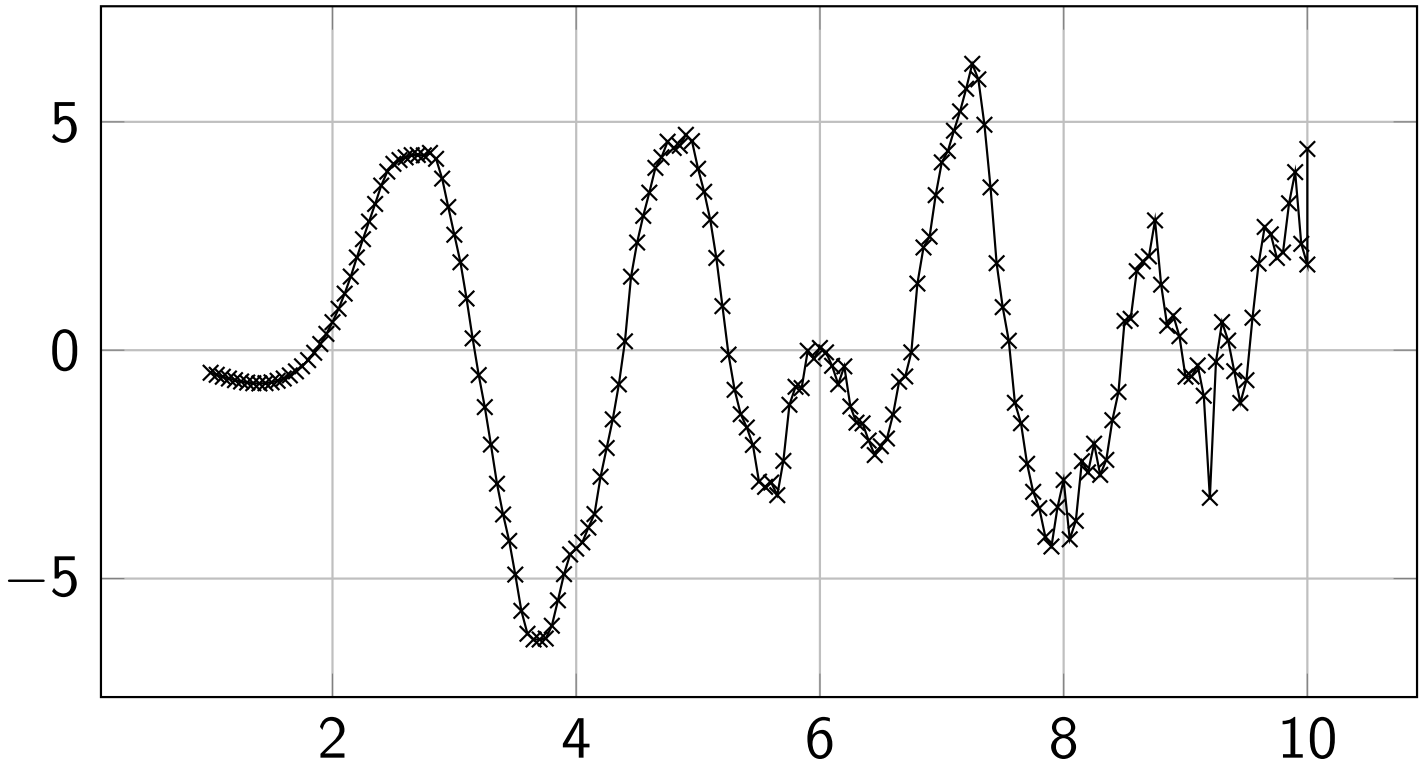
December 1, 2013

EXAFS

- X-Ray Absorption Fine Structure (XAFS) is a method used to measure the absorption coefficient of a material as a function of energy.
- EXAFS can be use to identifying properties of a molecule but they do not provide enough detail.
- We can identify how far atoms are from each other but we do not know their dihedral angles.
- The energy spectra given off by the molecule is unique for its structure meaning that we can create our own atomic structure and obtain an EXAFS spectra and compare the results.
- IFEFFIT application is used to simulate an EXAFS experiment.

Sample EXAFS Spectra



Baseline Atomic Structure

- Initial atomic structure is put into a simulation.
- Atoms are allowed to move freely to minimize energy.
- Generates baseline atomic structure.

Initial Population Generation

- A second simulation is run with baseline atomic structure.
- Atoms are heated up to cause them to move rapidly.
- Atoms begin to oscillate.
- Snapshots(10000) of atomic strcture are recorded.
- Top(300) atomic structures are used.

Chromosome Representation

- List of 3-dimensional coordinates.
- The actual positions of each atom is not relevant because we are only concerned with the position each atom relative to each other.

X	Y	Z
14.451	-13.346	1.133
15.336	-13.488	2.014
13.005	-13.364	1.452
0.019	0.011	0.045
7.816	-10.174	3.906
12.724	-10.266	4.814
13.506	-13.217	5.94
15.394	-10.779	6.204

Recentering

if population has converged to minimum diversity **then**
  remove all duplicate individuals;
  while population not full **do**
    insert random draw from generated individuals into population;
  end while
end if

Crossover

- Single-point.

X	Y	Z	X	Y	Z
14.451	**-13.346**	**1.133**	14.451	-13.346	1.133
15.336	**-13.488**	**2.014**	15.336	-13.488	2.014
13.005	**-13.364**	**1.452**	13.005	-13.364	1.452
0.019	0.011	0.045	**0.019**	**0.011**	**0.045**
7.816	-10.174	3.906	**7.816**	**-10.174**	**3.906**
12.724	-10.266	4.814	**12.724**	**-10.266**	**4.814**
13.506	-13.217	5.94	**13.506**	**-13.217**	**5.94**
15.394	-10.779	6.204	**15.394**	**-10.779**	**6.204**

Mutation

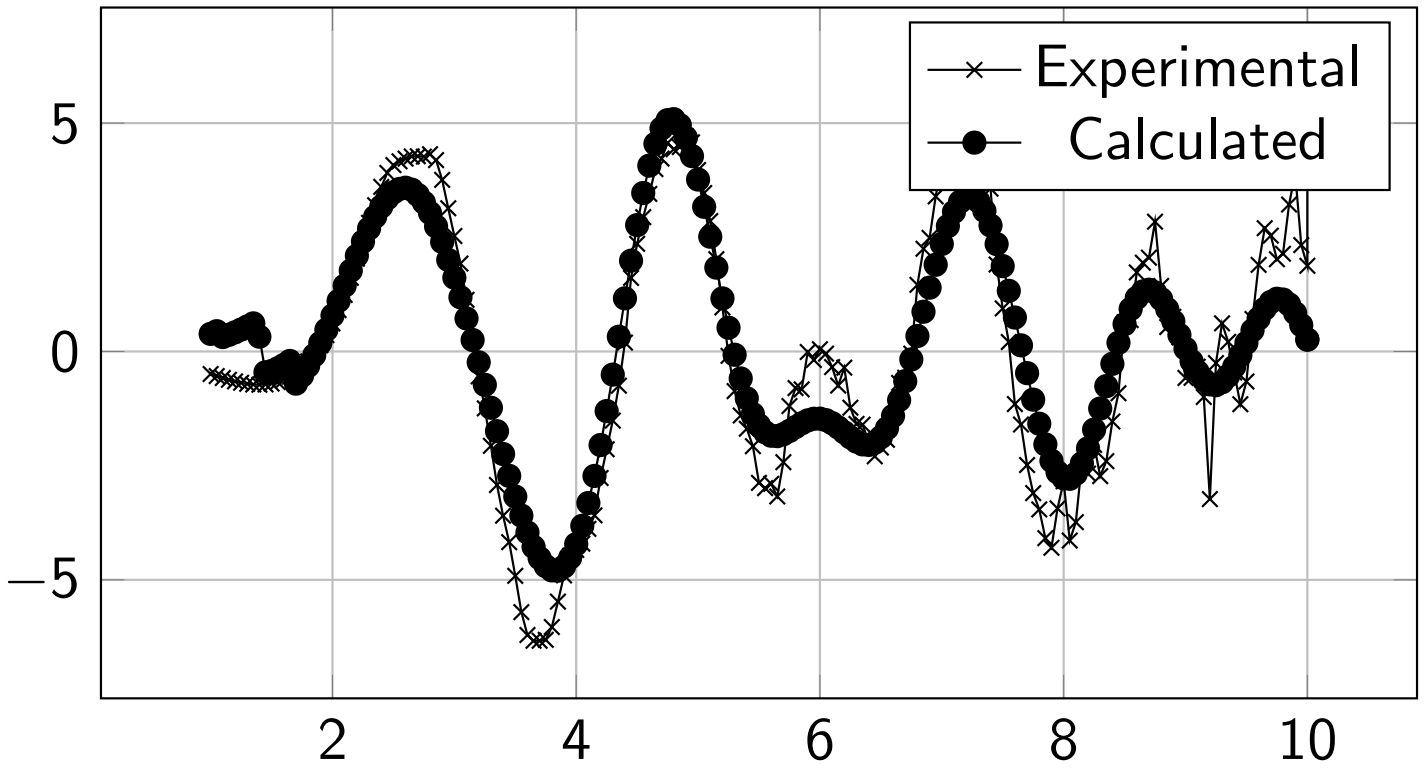
- Single point from chromosome is selected.
- Point is moved randomly by 0.05.
- 0.05 was selected after determining that it was the minimum move required to make a difference in the EXAFS spectra.

Selection

- 3-tournament selection.

Fitness

- root-mean-square deviations(RMSD) between the two spectras.



Best GA Parameters

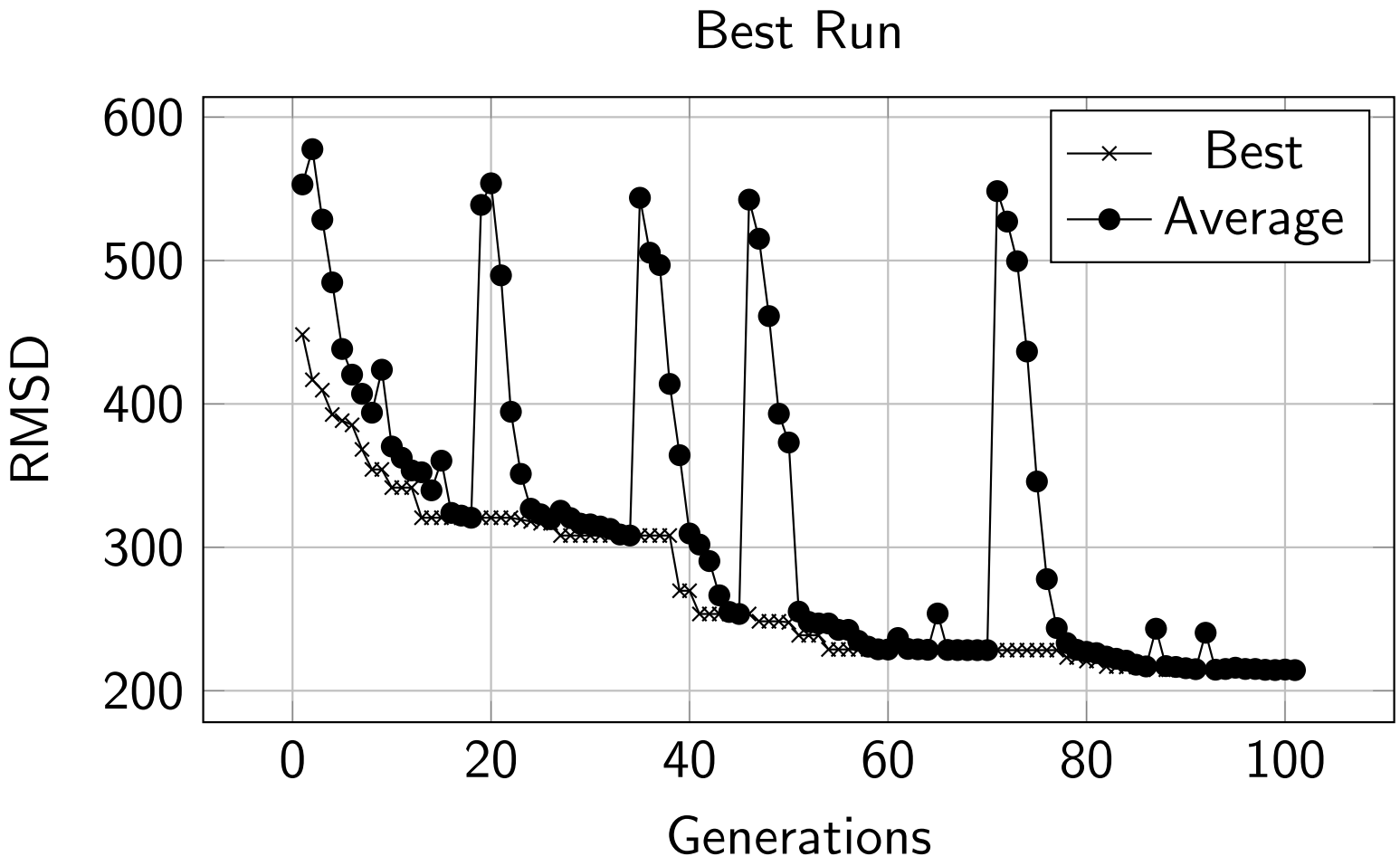
Table : GA Parameters

Population size	50
Crossover rate	0.8
Mutation rate	0.2
Elitism	True
Number of recentering attempts	5
Max convergence percentage before recentering	5%

Full GA Parameters

Name	Runs	Pop.	Gen.	Crossover	Mutation	Elitism	Conv. Rate	Recentering	Avg. Best
Test1	10	50	30	80%	20%	False	-	-	325.55
Test4	10	50	30	80%	10%	False	-	-	342.04
Test5	10	50	30	70%	30%	False	-	-	294.56
Test2	10	50	30	80%	10%	True	-	-	319.14
Test3	10	50	30	70%	30%	True	-	-	286.98
Test6	10	50	30	80%	20%	True	-	-	320.17
Test7	10	50	67	80%	20%	True	10%	3	271.49
Test8	10	50	81	80%	20%	True	5%	3	265.76
Test9	10	50	107	80%	20%	True	10%	5	263.36
Test10	10	50	124	80%	20%	True	5%	5	267.47
Test11	10	50	67	70%	30%	True	5%	5	**260.56**
Test12	10	50	81	70%	30%	True	10%	5	266.68

Best Run


Best Run
RMSD
600
500
400
300
200
0
20
40
60
80
100
Generations
Best
Average

Further Experiments

- Subsets of atoms. Currently using Ma, Ca, O, C, N, H.
- Reduce x-range in EXAFS spectra RMSD.
- CILIB - PSO
- Use PSO for local search at end?