Function Reconstruction via Maximum Entropy Approach: Application to Electronic Structure

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Introduction

- Classical Moment Problem as an Inverse Problem:
  - How to construct a solution from an incomplete set of data
- Moments:
  - A mathematical way to express the properties of a distribution.

$$\mu_n^p = \int_a^b p(x) f(x) dx \qquad n = 0, 1, 2, 3, \ldots$$

$$f(x) \in [a, b]$$

$$\mu_n < \infty \qquad \text{for} \qquad n \to \infty$$

- Classical Moment Problem (CMP):

Given a set of finite moments $\{\mu_n\}$, construct an approximate density distribution function $f^A(x)$ that satisfies the moments

(Akheizer 1965, Shohat and Tamarkin 1963)

- Maximum Entropy
  - Provides an unbiased solution of CMP.

For finite moments, multiple solutions exist

- Maximum Entropy Method:
  - Shannon entropy functional

$$S[f] = -\int f(x)\ln[f(x)]dx$$

MaxEnt provides a ***least biased*** solution consistent with the moments by maximizing the entropy [Jaynes 1957, Kullback-Libler 1951]

Mead and Papanicolaou (JMP 1984); Turek (JPC 1988); Silver (PRB 1997); Bandyopadhyay, Biswas, et. al. (PRE 2006)

Power and Chebyshev Moments

- Power moments

$$\mu_n = \int x^n f(x) dx$$ ✗

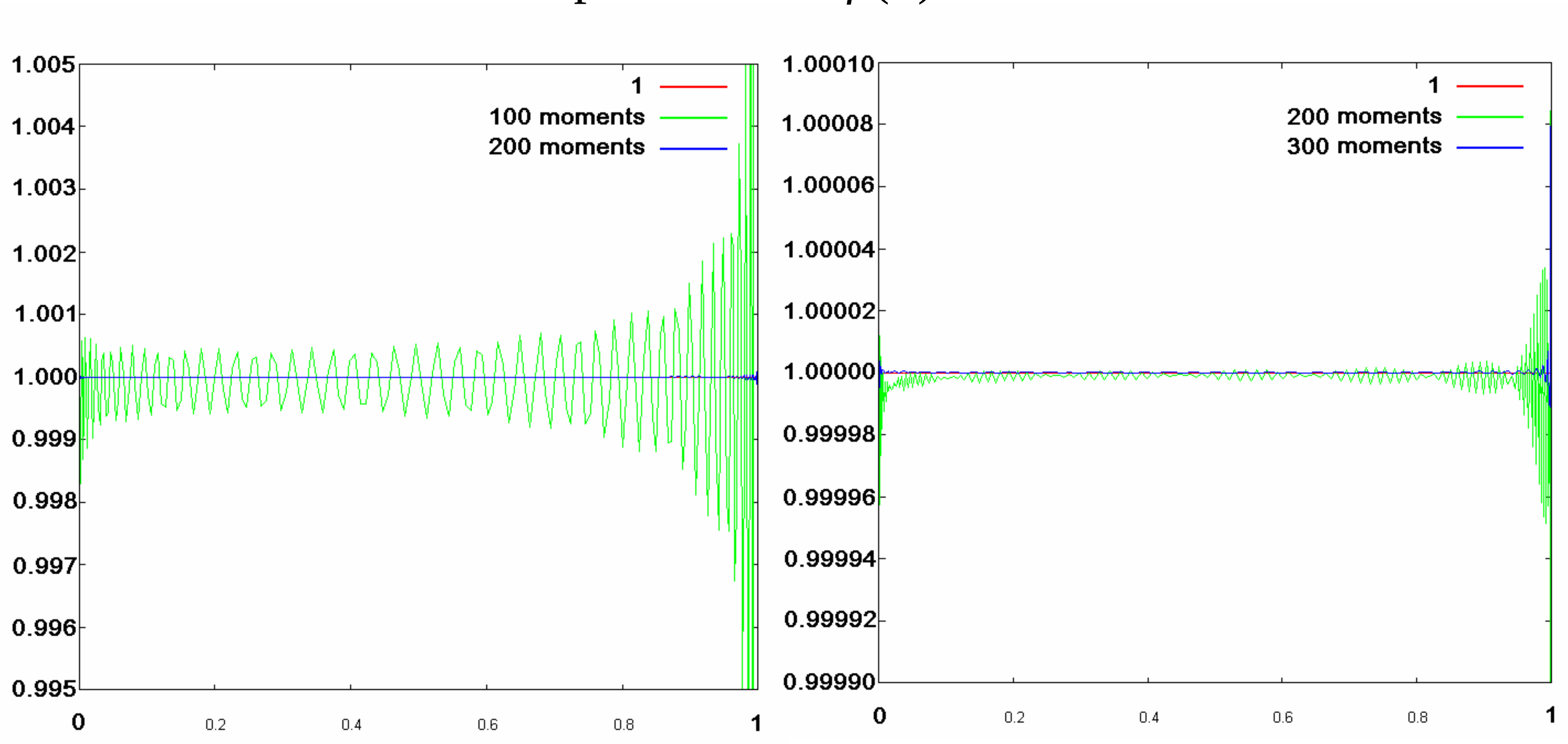
- Chebyshev moments

$$\mu_n = \int T_n(x) f(x) dx$$ ✓

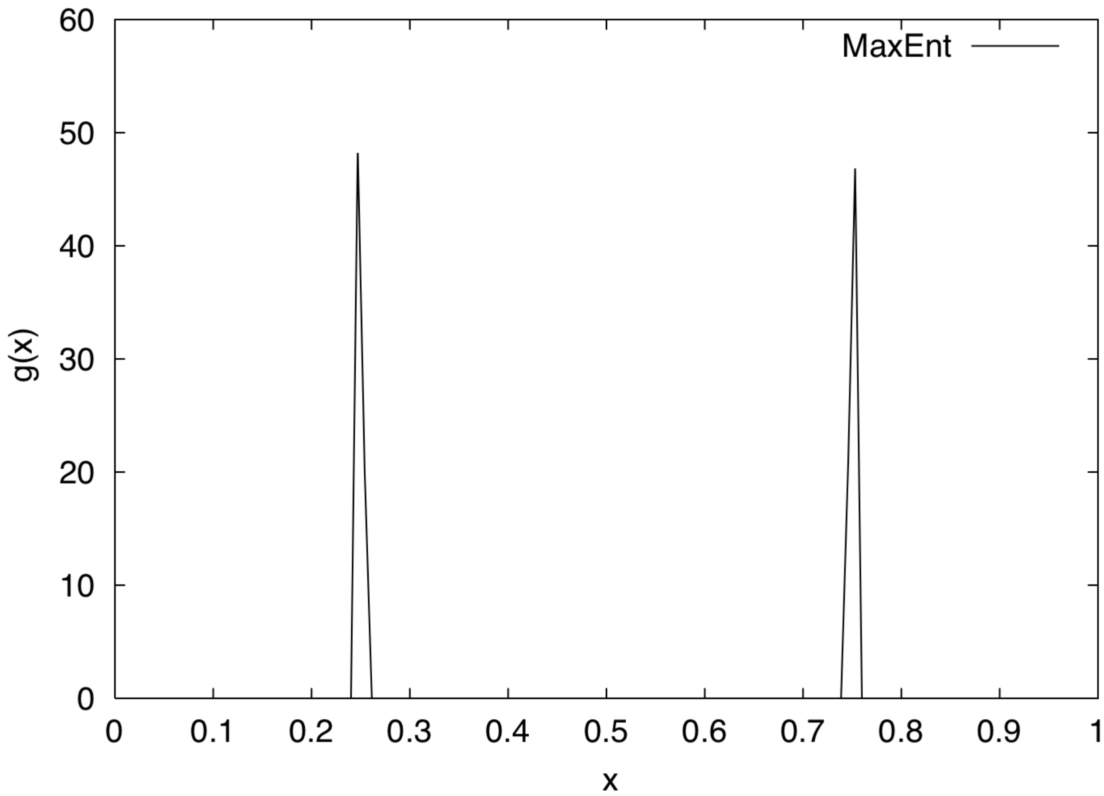
  - Chebyshev polynomials
    - A minmax polynomial
    - More accurate results
    - But somewhat slower than power moment

Results

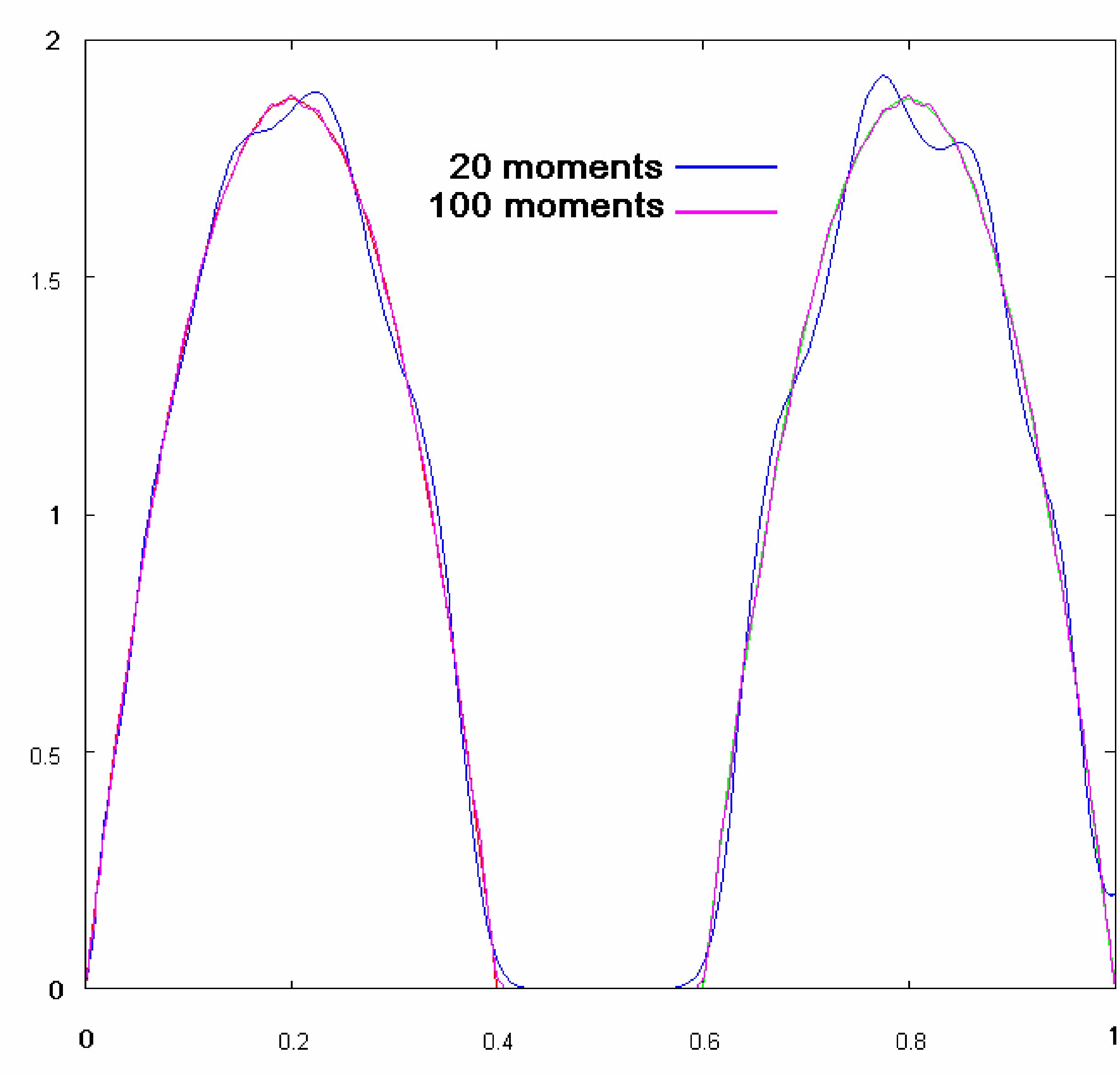
Step Function $f(x) = 1$



MaxEnt Construction of Delta Function



$$f(x) = \delta(x - \frac{1}{4}) + \delta(x - \frac{3}{4})$$



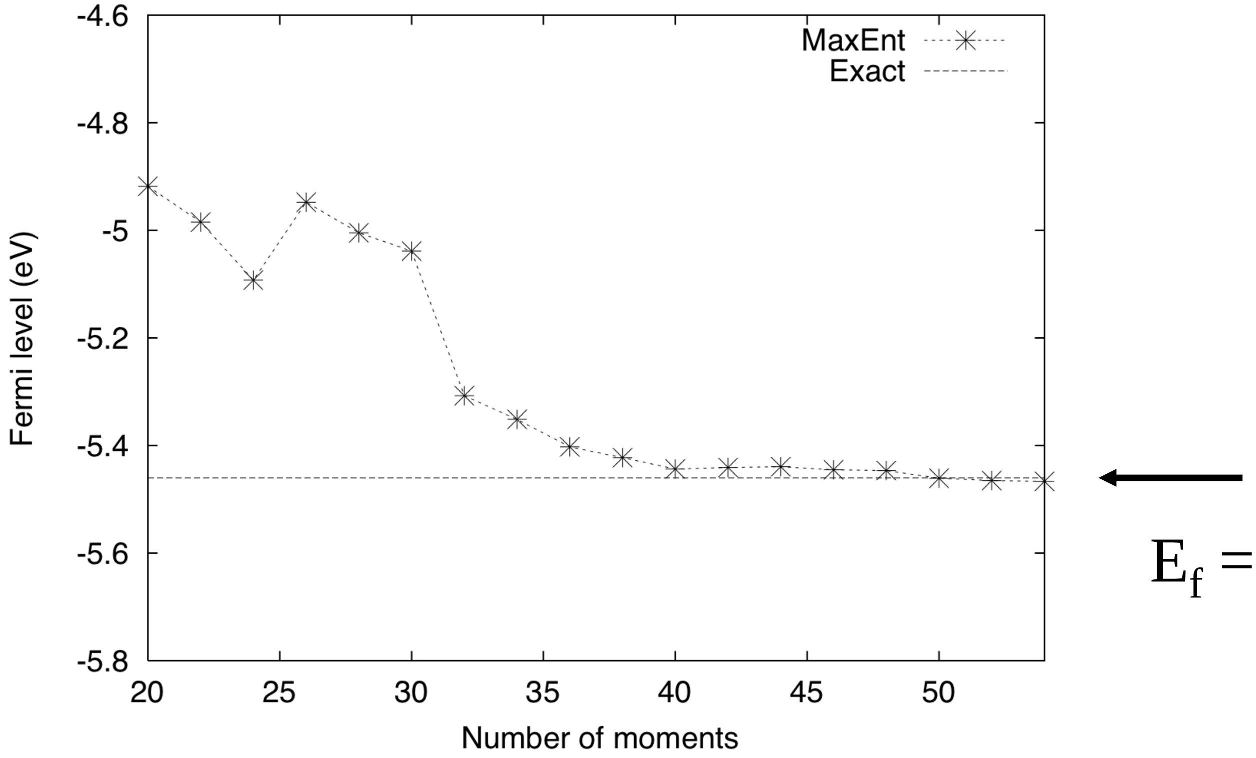
$$f(x) = Ax(x - x_1)$$

$$\begin{cases} A = \dfrac{3}{x_1^3} \\ x_1 = 0.4 \\ 0 \le x \le 0.4 \end{cases}$$

$$f(x) = B(x - x_2)(1 - x)$$

$$\begin{cases} B = \dfrac{3}{(1 - x_2)^3} \\ x_2 = 0.6 \\ 0.6 \le x \le 1.0 \end{cases}$$

Application to Electric Structure: Calculation of Fermi Energy in a-SiO_2



$E_f = -5.46$ eV

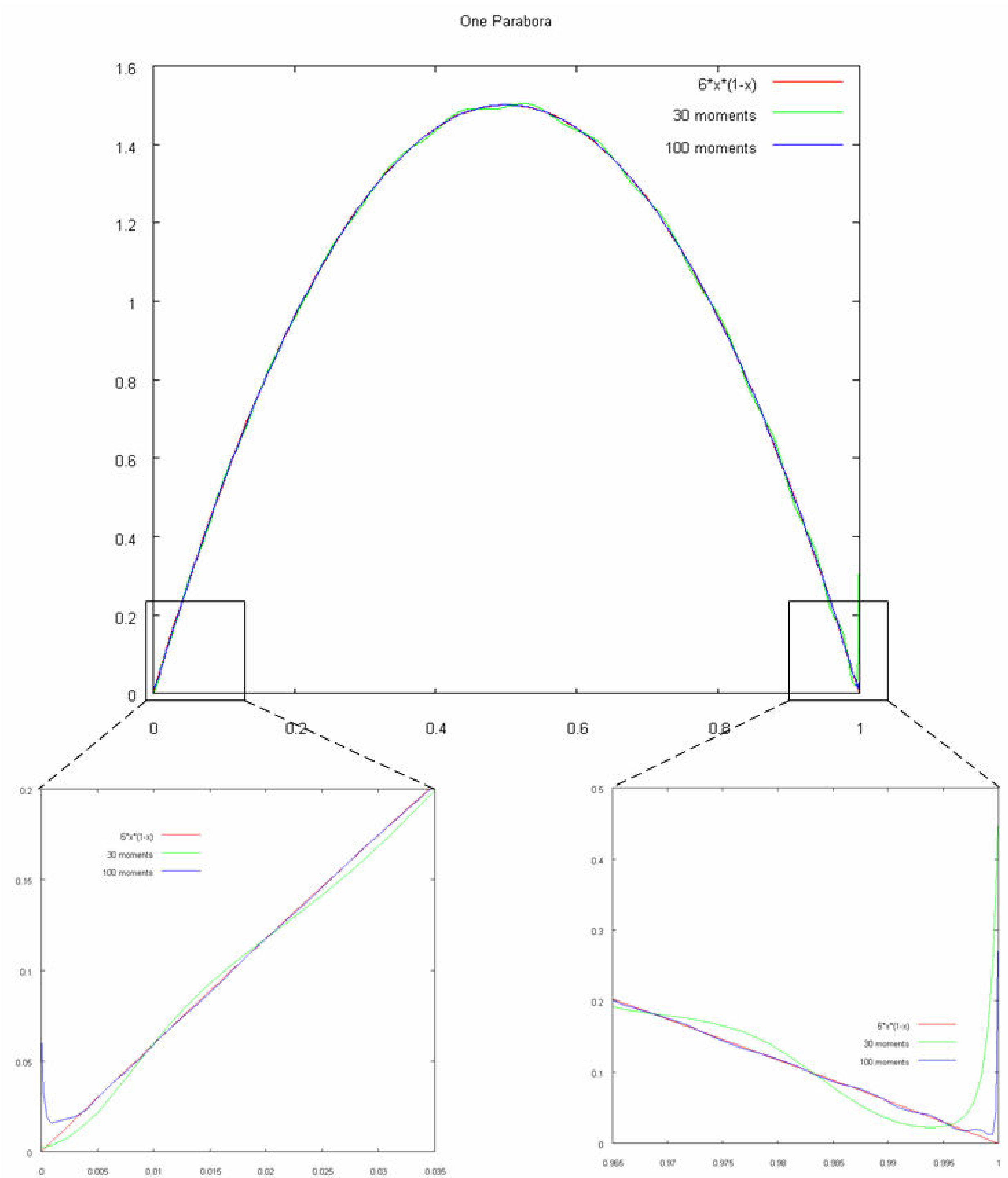
Electronic force from MaxEnt :1) MD Simulation

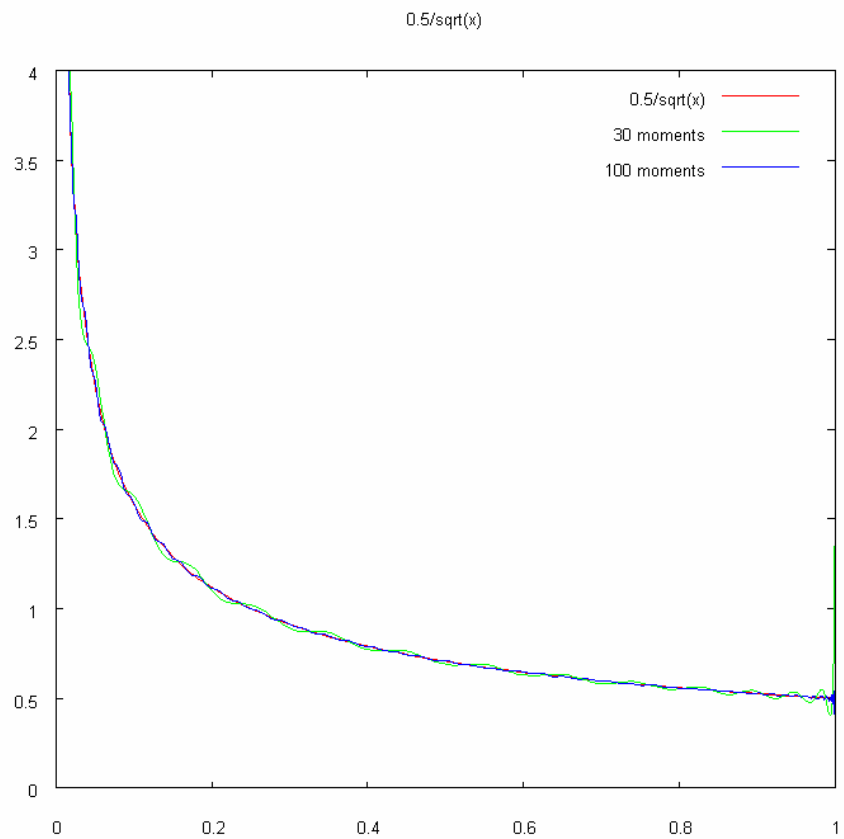
2) Effects of perturbing the moments

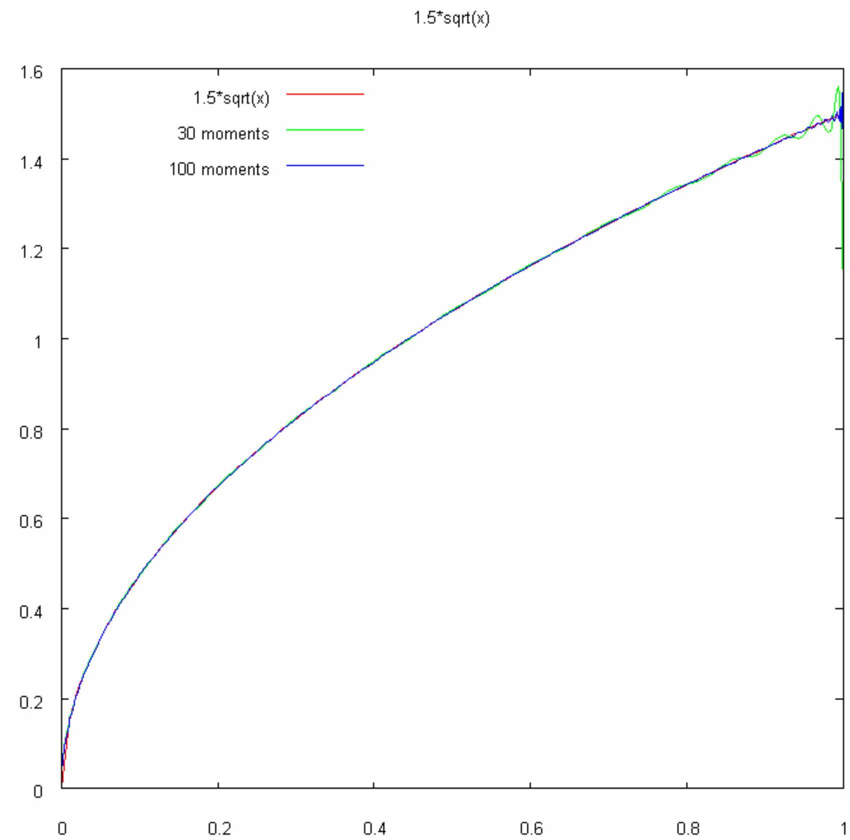
Conclusions

- Stable and accurate results from the Maxent Chebyshev iterative algorithm to the function reconstruction

- Leading to an accurate electronic structure (Fermi energy and band energy) with the systematic study of this scheme


One Parabora
6*x*(1-x)
30 moments
100 moments
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1
6*x*(1-x)
30 moments
100 moments
0.2
0.15
0.1
0.05
0
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035
6*x*(1-x)
30 moments
100 moments
0.5
0.4
0.3
0.2
0.1
0
0.965
0.97
0.975
0.98
0.985
0.99
0.995
1


0.5/sqrt(x)
0.5/sqrt(x)
30 moments
100 moments


1.5*sqrt(x)
1.5*sqrt(x)
30 moments
100 moments