Adaptive error control for diffusion Monte Carlo

John Jumper

31 July 2008

Multiple time scales in DMC

- Typical DMC has a single time step for all electrons and moves
- Some electron configurations are problematic for fixed time steps
  - Near nodes, the drift vector must diverge
  - Local energy near nuclei is badly behaved
  - Core electrons have different time scales than valence electrons
- Time step should adapt based on the region of simulation space

Continuous-time DMC

- Continuous-time DMC
  - Generate paths of length τ from a random walk with a drift velocity $v = \nabla \log \Psi_T$
  - Weight each path $R(t)$ by $w(R) = \exp\left[-\int_0^\tau (E_{loc}(R(t)) - E_{ref})dt\right]$
- Standard DMC is one discretization of this method
- Non-constant drift vector and local energy causes time step bias

Measuring the error

- Position error is approximately $\frac{\tau}{2} |v(R_1) - v(R_0)|$
- Weight error is approximately $\frac{\tau}{2} |E_{loc}(R_1) - E_{loc}(R_0)|$
- These quantities are available for free in a DMC simulation

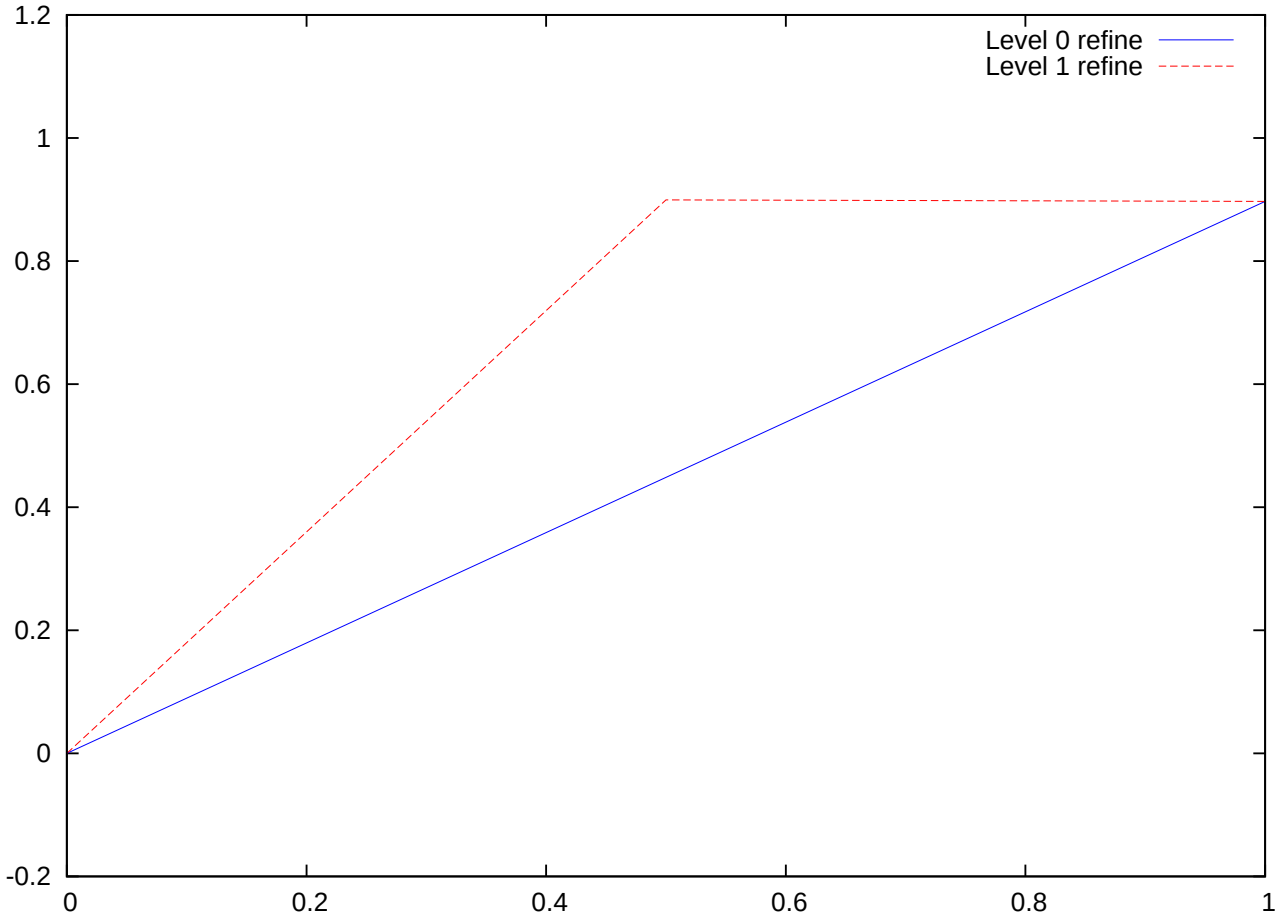
Refining poor moves

- What if drift vector or local energy varies significantly over a move?
- Rejection enforces detailed balance but does not eliminate bias
- Poor moves should be split in two by a *Brownian bridge*

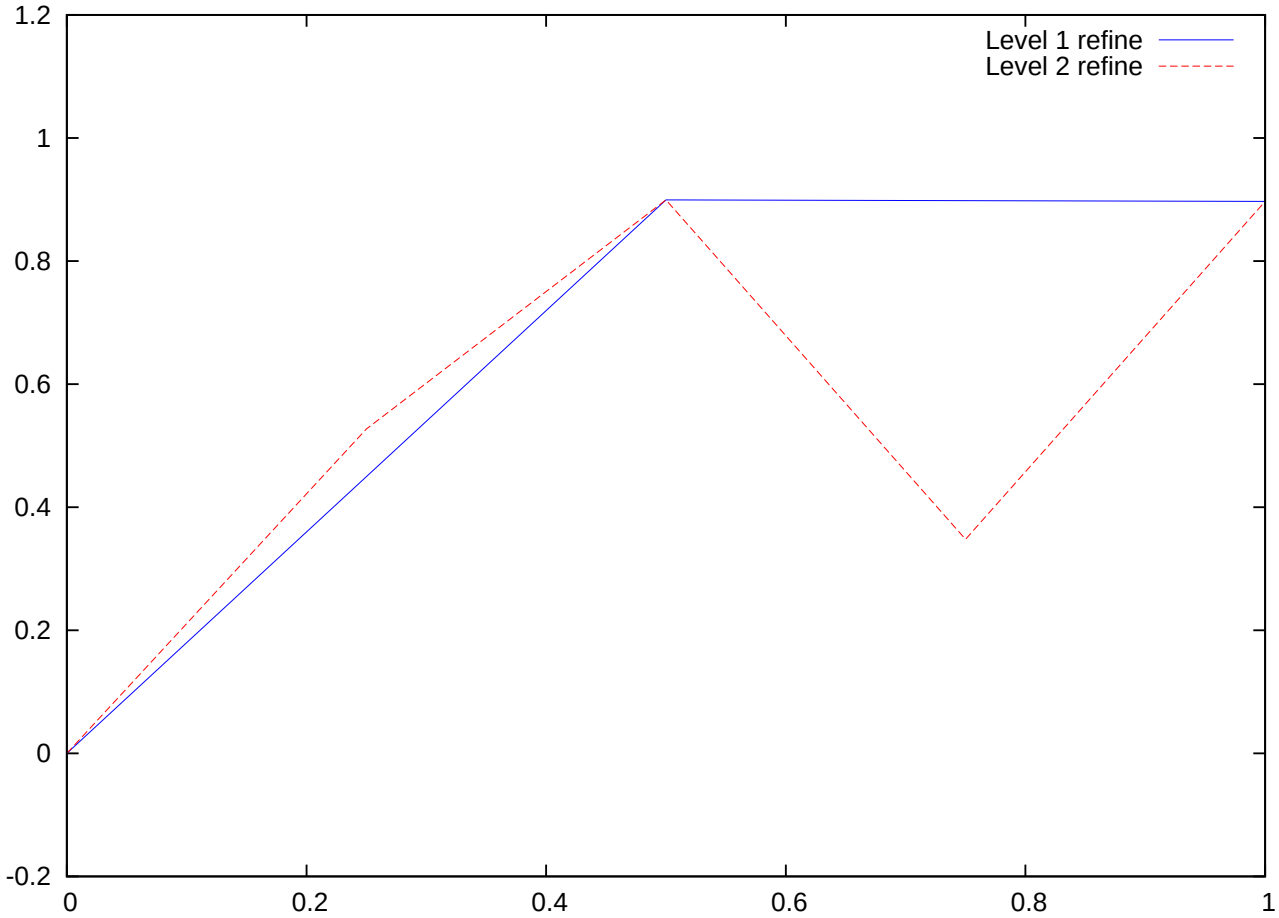
Brownian bridge

- Midpoint of a random walk with known ends is a Gaussian centered at the average of the ends with 1/4 the variance
- Drifted random walks are improved by refining the underlying random walk
- Refinement is recursive

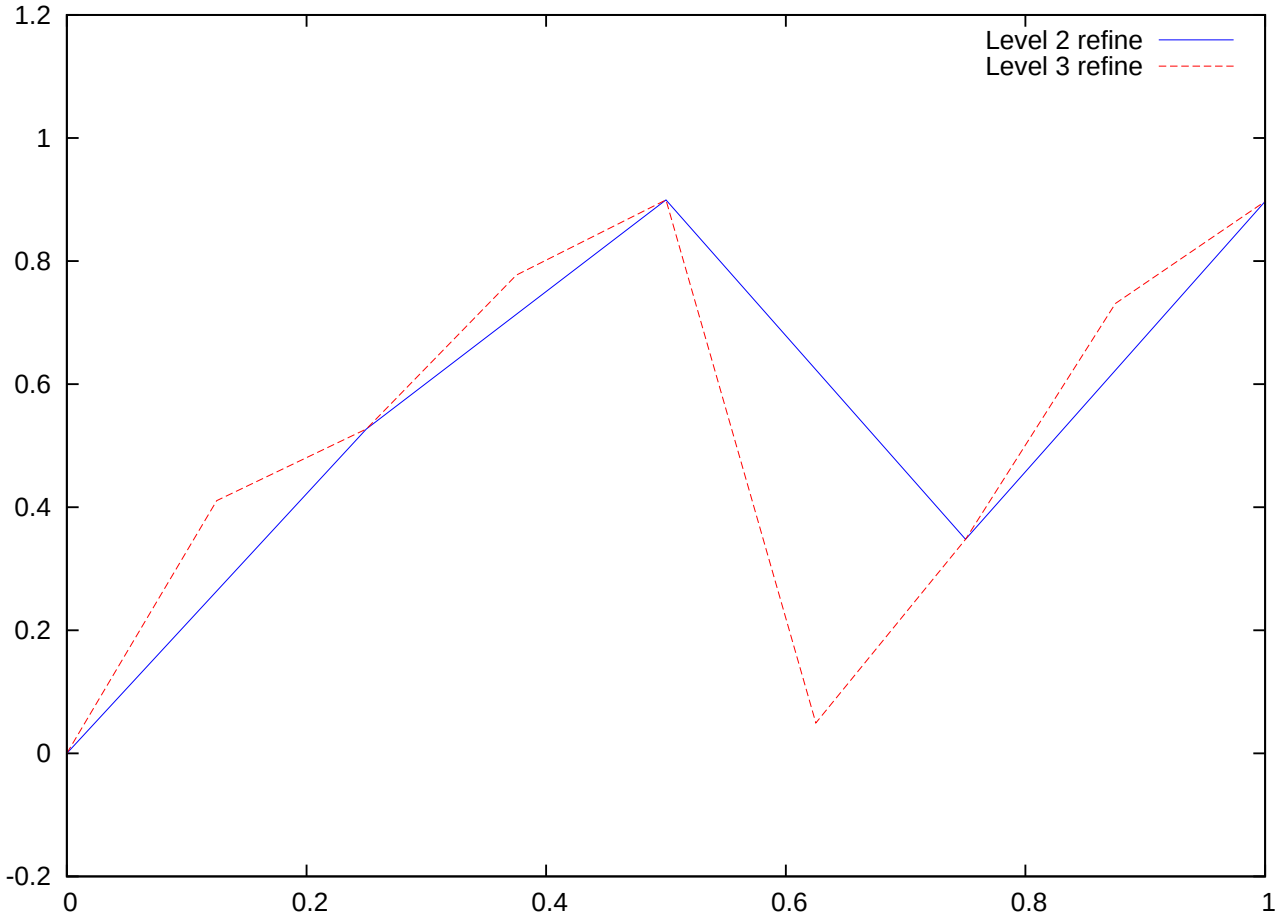
Random walk refinement



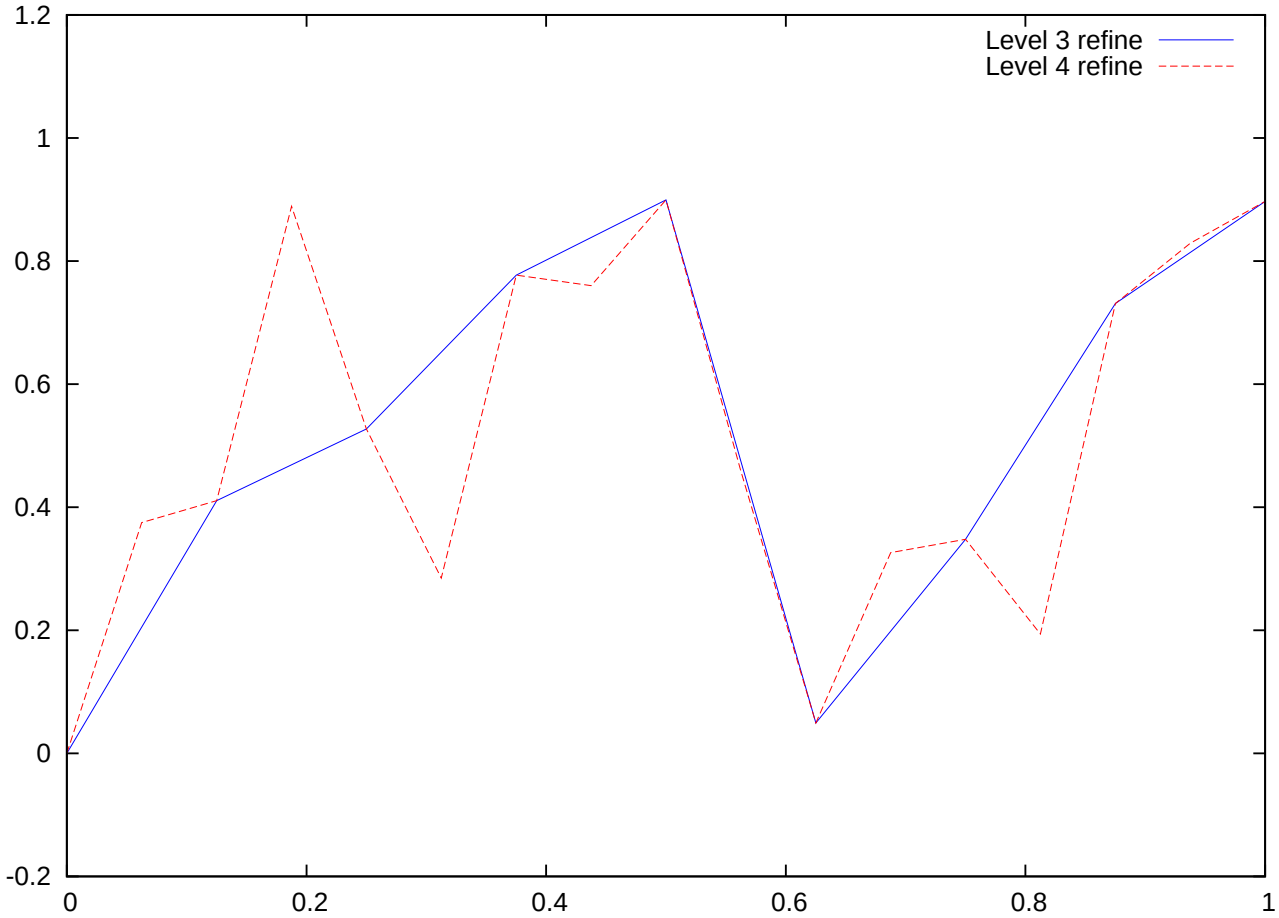
Random walk refinement



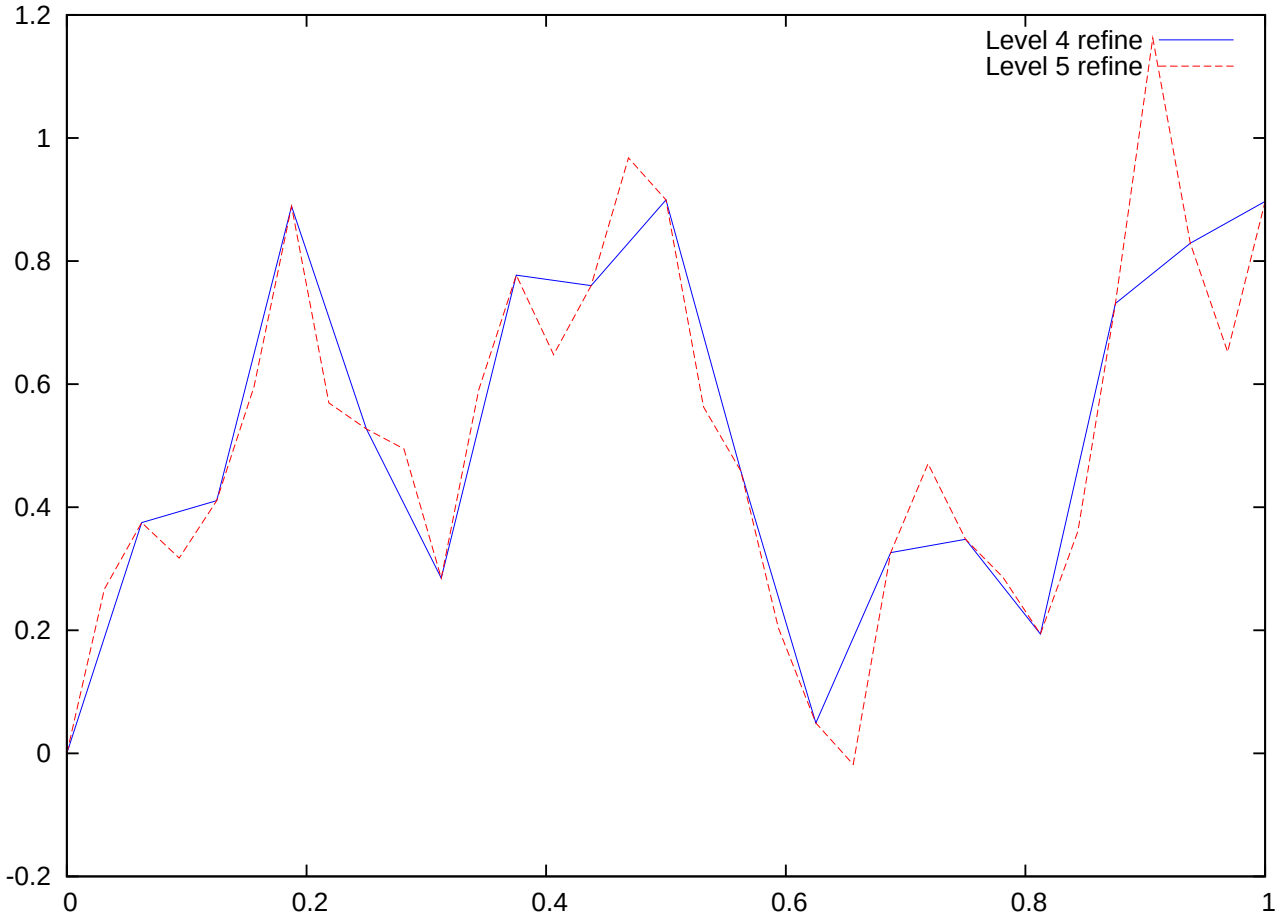
Random walk refinement



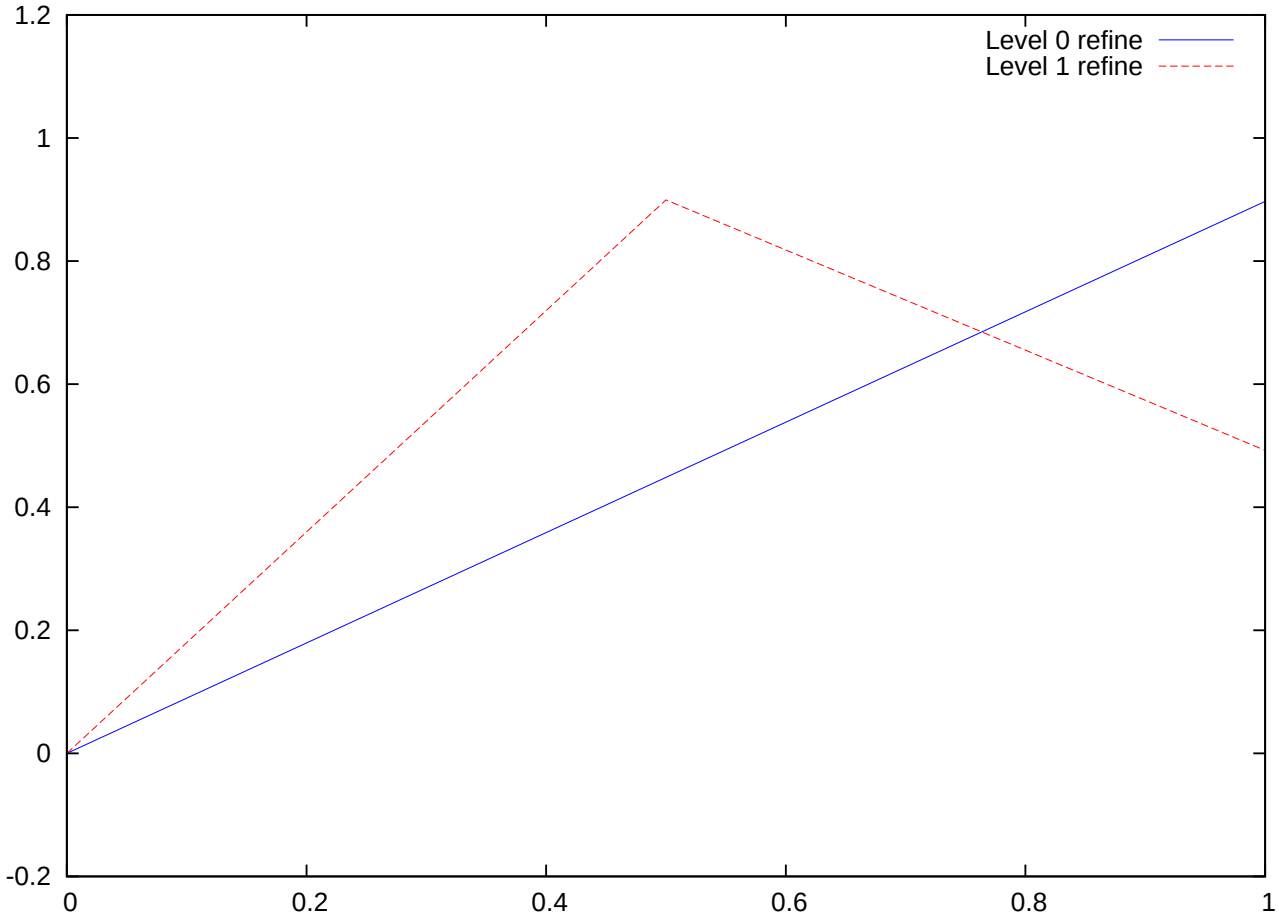
Random walk refinement



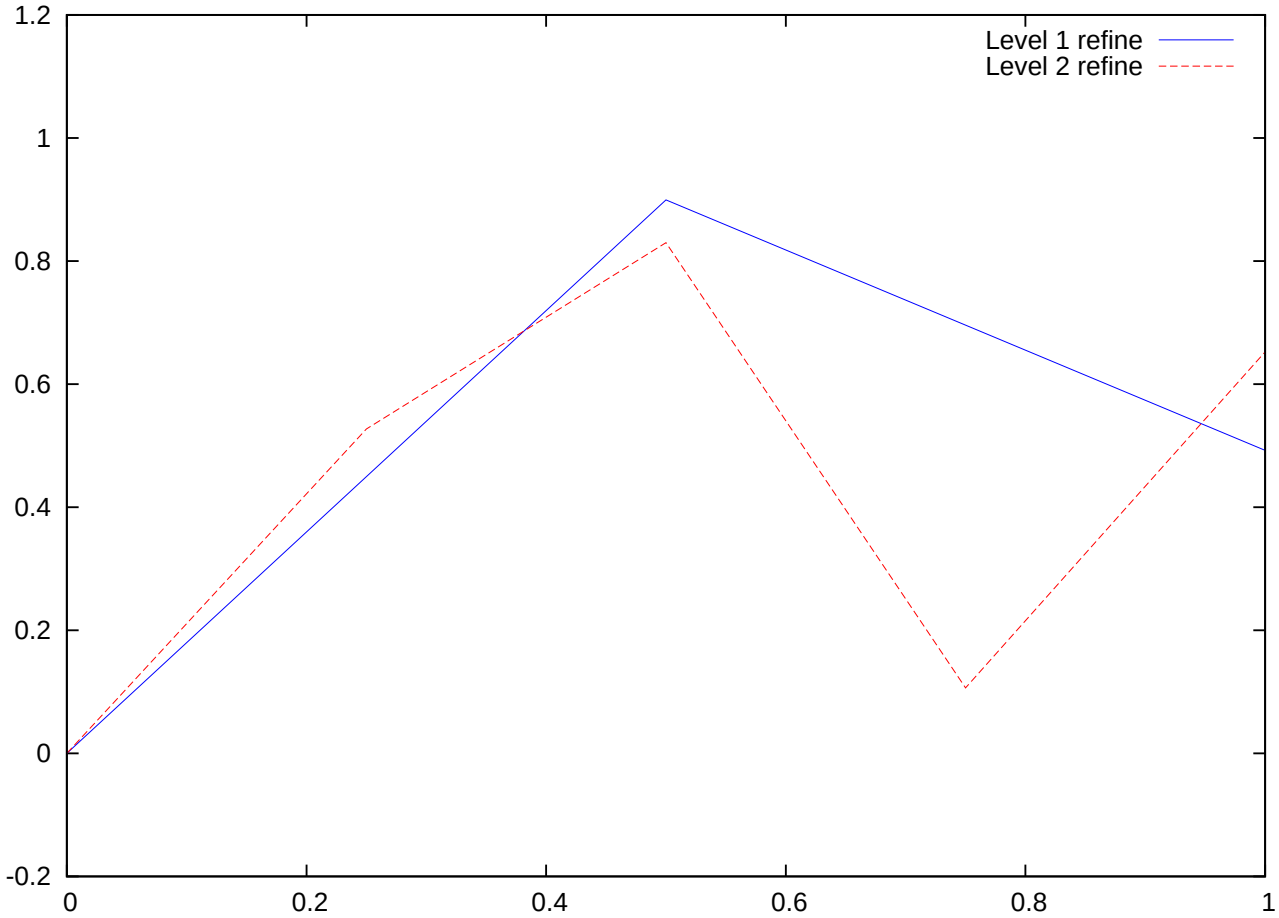
Random walk refinement



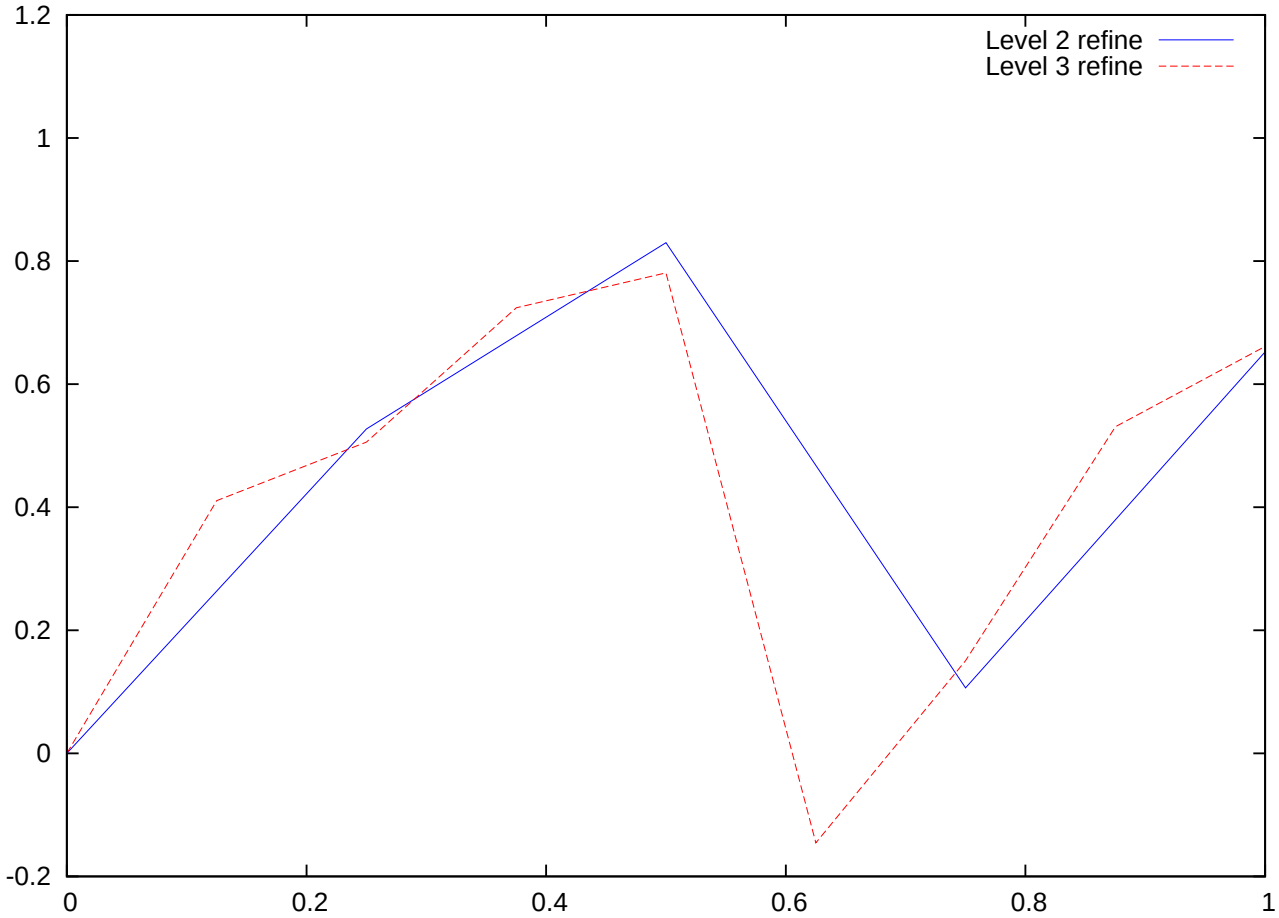
Drifted random walk refinement ($v = -x^2$)



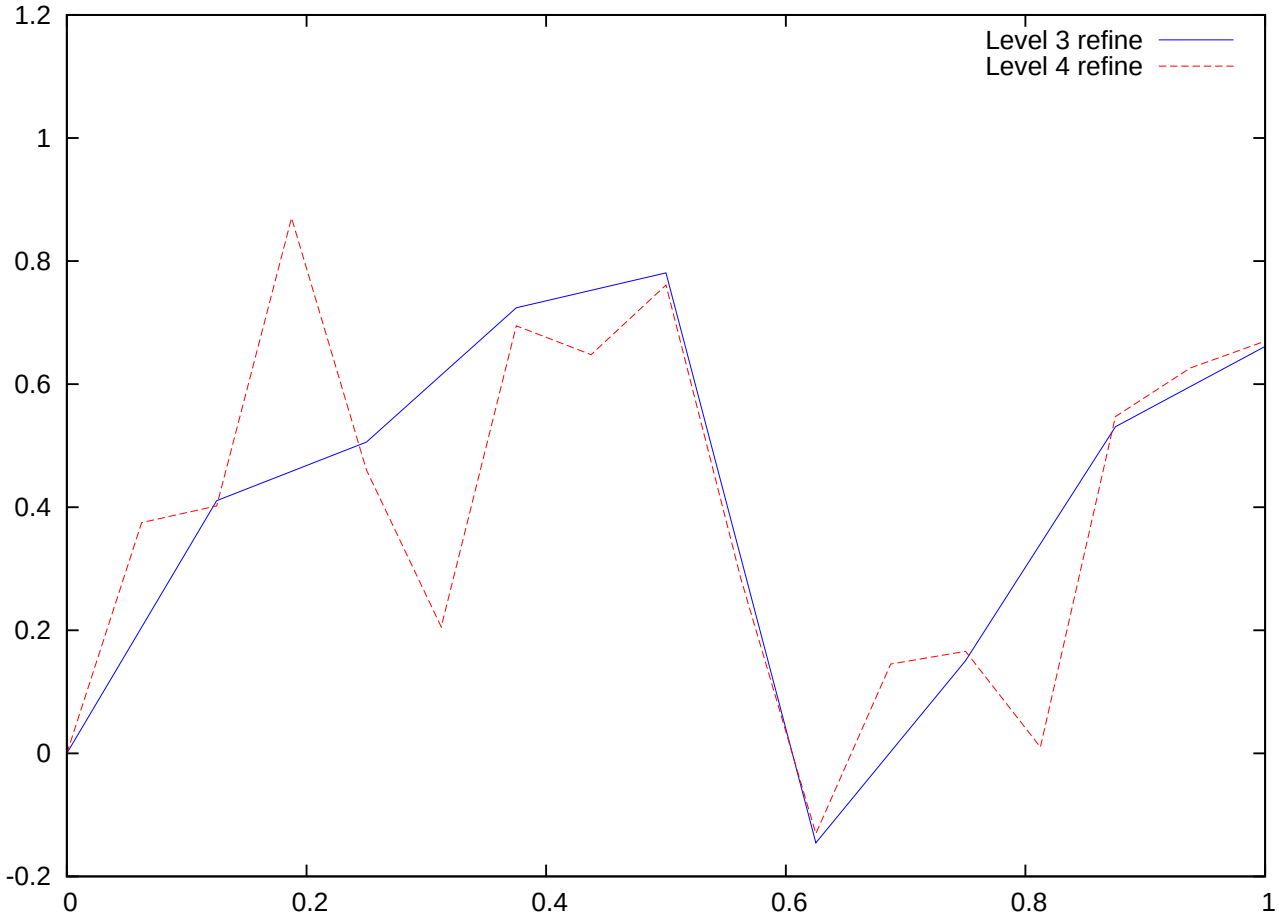
Drifted random walk refinement ($v = -x^2$)



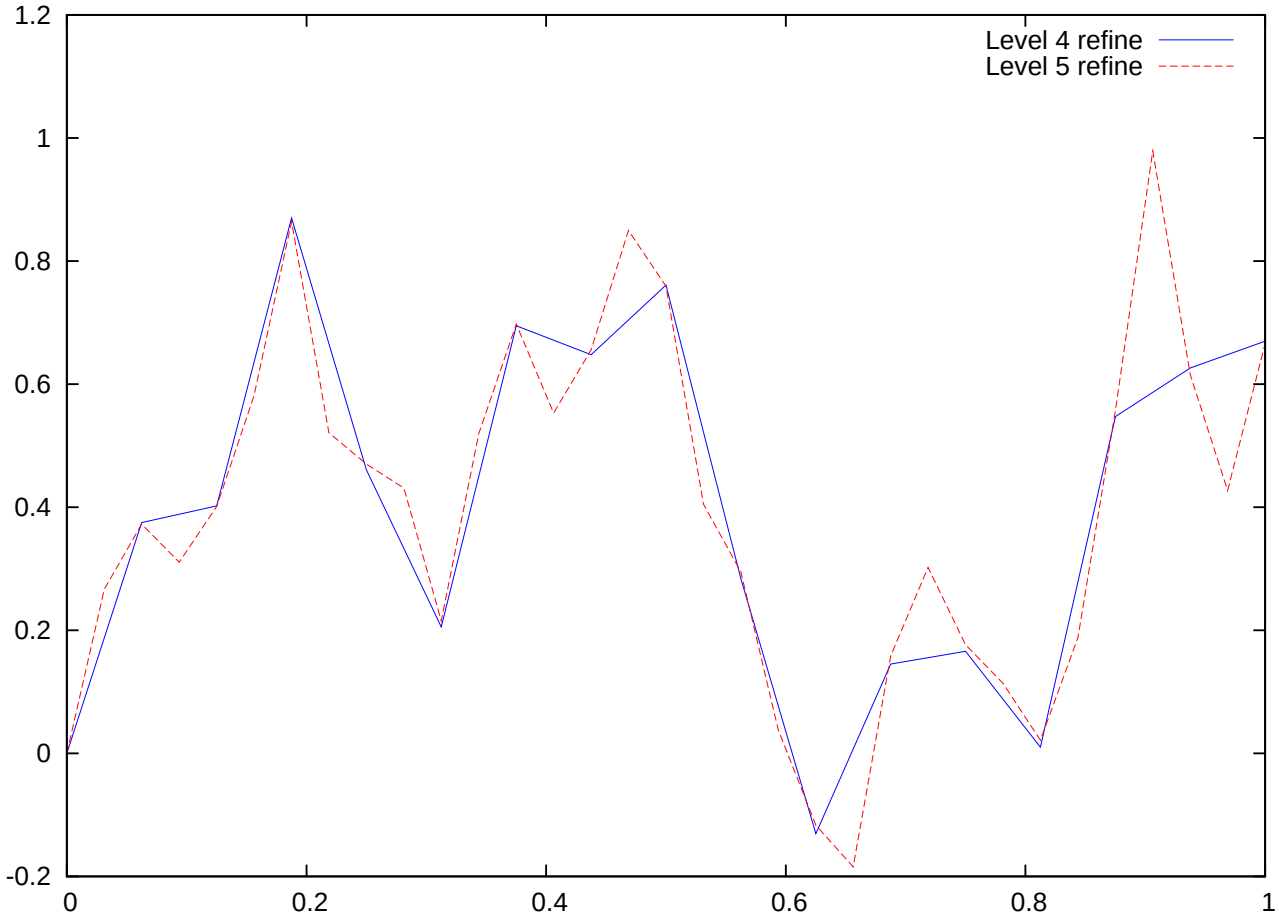
Drifted random walk refinement ($v = -x^2$)



Drifted random walk refinement ($v = -x^2$)



Drifted random walk refinement ($v = -x^2$)



Performance

- Time step bias goes to zero as error tolerances go to zero, *but only for whole-configuration moves*
- Unrefined moves have no time penalty over nonadaptive moves
- Refinement has a 50% time penalty
- Whole-configuration moves are inefficient for refining drift vectors
- Analogue of single-electron moves is needed for efficiency

Limitations

- Exact detailed balance lost
- Needs Heun propagator to retain approximate detailed balance
- Algorithm is useful only if time step error is dominated by relatively few configurations
- Whole-configuration refinement will scale poorly

Naive single-electron moves

- Exact single-electron propagation does not eliminate time step bias
- Single-electron move bias goes to zero as the time step goes to zero
- Can determine if electrons interact from wavefunction cross-derivatives

Cluster moves

- Two electrons e_1 and e_2 are *connected* in configuration R if $\partial_{e_1} v_{e_2}(R)$ is large
- Connected electrons should be moved together to avoid single-electron move bias
- Connectedness is symmetric
- Connectedness divides the electrons in a given configuration into *clusters*
- Cluster moves avoid single-electron move bias

Adaptive cluster moves

- Adaptive cluster moves
  1. Move all electrons
  2. Look at magnitude of drift vector change for each electron
  3. Mark electron for refinement if drift vector change is above threshold
  4. Refine moves of all marked electrons
- Clusters are not explicitly determined but are always moved together
- All time step related bias should go to zero as error tolerance goes to zero

Conclusion

- Poor DMC moves can be systematically improved
- Adaptive moves should speed simulations when a variety of time scales is needed
- Cluster moves are needed to avoid single-electron move bias
- Future work
  - Testing algorithmic efficiency
  - Investigate optimum tolerances
  - Reincorporate detailed balance
  - Predict correct time step to reduce refinement penalty

Acknowledgements

Richard Needs and Neil Drummond for helpful advice and support.

Marshall Aid Commemoration Commission for financial support.