Improvement of Metropolis-Hastings Algorithm on Manifold

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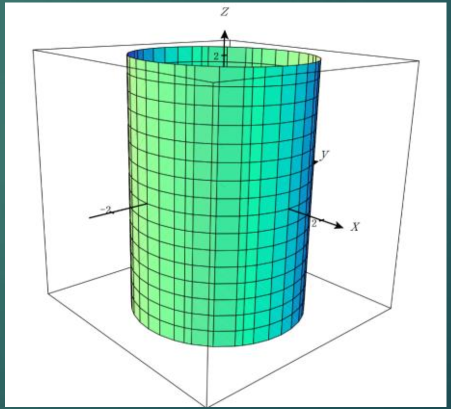
Motivation

- Markov Chain Monte Carlo is a widely applied sampling technique to generate random variables from any given probability distribution.
- Its basic idea is to generate random walk in the space by accepting or rejecting a proposed move.
- In the real case, what if we have constraints? These constraints form a manifold in the space.

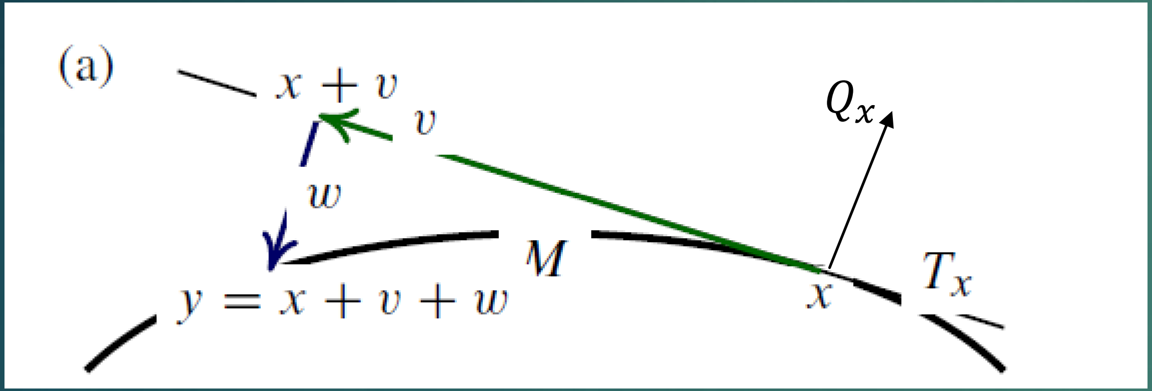
$$M = \{q_i(x) = 0\}$$

Where q_i represents the ith constraints.



$$x^2 + y^2 - 2 = 0$$

The usual approach: Take a random point and project it back to manifold



[1]

- Random point is taken on the tangent space of x

- The projection process is solving a system of equation.

$$\{q_i(x + v + Q_x a) = 0\}$$

  - where columns of Q_x is the gradient of constraints at x
  - $Q_x a = w$ on the graph

- Analytical solution may not exist.

[1] Zappa, E., Holmes-Cerfon, M.C., & Goodman, J. (2017). Monte Carlo on manifolds: sampling densities and integrating functions. arXiv: Numerical Analysis.

Newton's Method

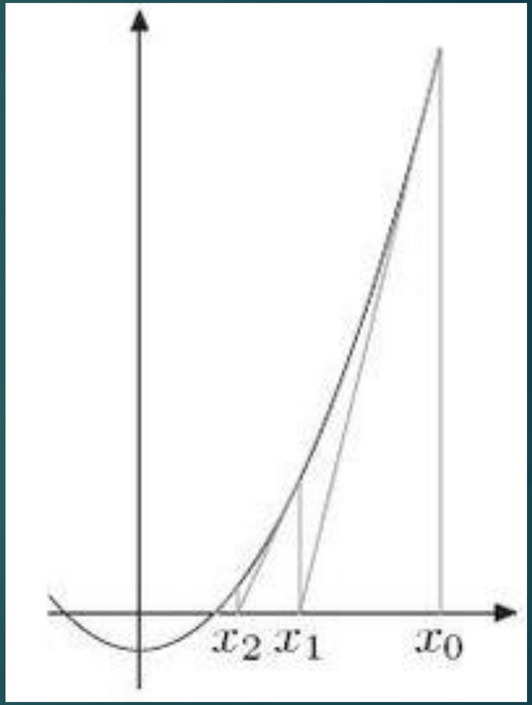
- Newton's method is an iterative method to generate a sequence of x find the x such that $f(x) = 0$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

- In multi-dimensional case, instead of $f'(x_n)$, we have Jacobian matrix $J_{ij} = \frac{\partial f_i}{\partial x_j}$

- Then we are going to solve a for $J(z_n)a + f(z_n) = 0$
  - Where $z_n = x + v + Q_x a_n$

- In this case, we simply have $J(z_n) = {Q_{z_n}}^T Q_x$



Bottlenecks of Newton’s method

- However, Newton’s method is sometimes slow.
  - Calculate Jacobian Matrix on each iteration
  - Need to solve a system of linear equations on each iteration

Key Observation

- Newton’s method can converge even when we are not using the exact Jacobian Matrix.
- Choose approximation of Jacobian Matrix

Two Alternative methods

CCMA [1]

- Fix the Jacobian matrix to be $J(z_1) = {Q_z}^T Q_x$ (i.e. the first Jacobian matrix).
- On each iteration always use this Jacobian Matrix to solve system of equation

Symmetric Newton Iteration [2]

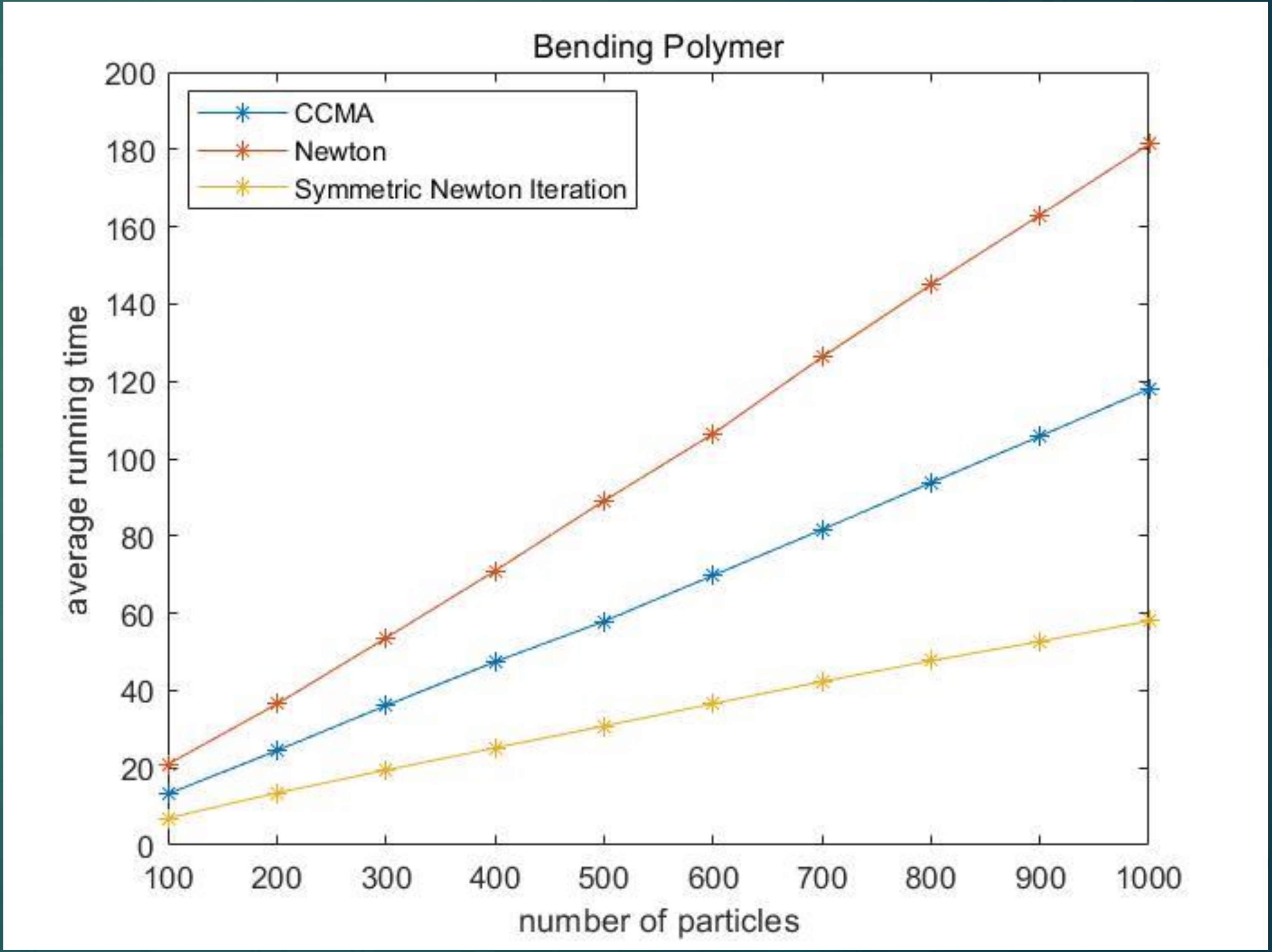
- Fix the Jacobian matrix to be ${Q_x}^T Q_x$ instead of ${Q_z}^T Q_x$.
- Additional advantage:
  - Cholesky decomposition can be applied to solve system of equation
  - Cholesky decomposition can also be used to calculate v.

[1] Eastman, P., & Pande, V. S. (2010). *Constant Constraint Matrix Approximation: A Robust, Parallelizable Constraint Method for Molecular Simulations*. https://pubs.acs.org/doi/pdf/10.1021/ct900463w.

[2]Barth, E., Kuczera, K., Leimkuhler, B., & Skeel, R. D. (2004, September 7). *Algorithms for constrained molecular dynamics*. Wiley Online Library. https://onlinelibrary.wiley.com/doi/pdf/10.1002/jcc.540161003.

Performance test: Bending Polymer

- Constraints: $||y_i - y_{i+1}|| - 1 = 0$
  - Where y_i is ith particle on the bending polymer.
- More particles than constraints.
- In order to prevent the bending polymer from collapsing, we applied an energy potential.
- Average running time is calculated by running algorithm to generate 1e5 time of iterations.



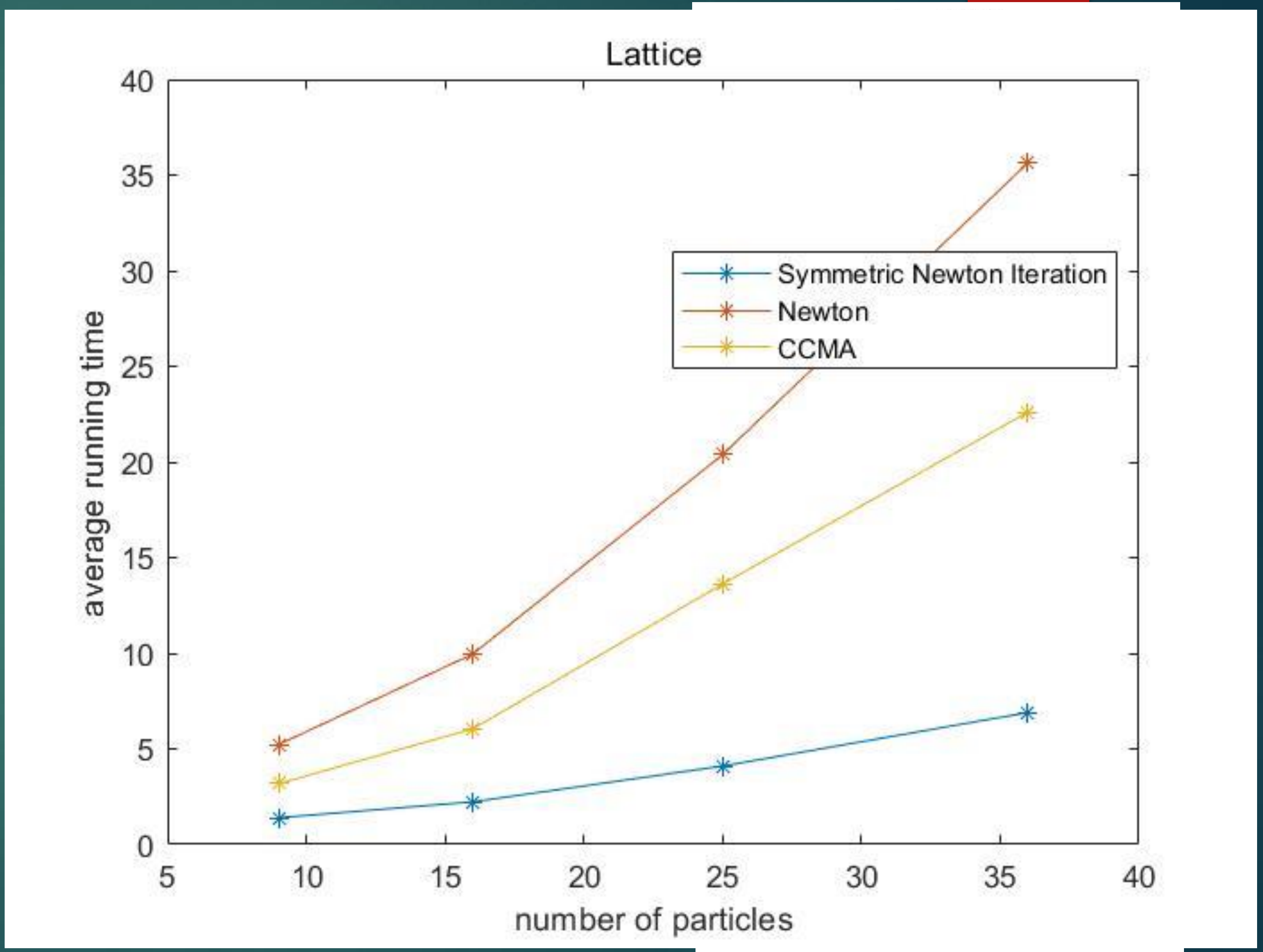
Performance test: Lattice

- Constraints: $||y_i - y_i|| - 1 = 0$
  - Where there is a chain between y_i and y_i

- More constraints than particles.

- In order to prevent the lattice from collapsing, we applied an energy potential.

- Similarly, average running time is calculated by running algorithm to generate 1e5 time of iterations.



Analysis

- Saves time for calculating Jacobian Matrix and Matrix decomposition.
- May need more iterations to converge.
- when n gets larger, there is no significant increase in number of iteration for Symmetric Newton iteration method and CCMA method

Conclusion

- Symmetric Newton iteration method is a way to accelerate the Markov Chain Monte Carlo on Manifold.

- Future work: explore the performance of Symmetric Newton iteration on other manifold (e.g. polygon)

Thanks for Watching!