
Reflection, Refraction, and Hamiltonian Monte Carlo

SUPPLEMENTARY MATERIAL

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In the supplementary material, we carry out more experiments on our test model.

- In Figures 1 to 16 *error vs iteration* and *error vs time* plots are depicted for a range of (leapfrog) parameter configurations. Namely all combinations of $L \in \{20, 50, 100, 200\}$ and $\epsilon \in \{0.05, 0.1, 0.2, 0.4\}$ are tested on 2, 10 and 50 dimensional models. The worst mean absolute error (WMAE) over all dimensions is taken as the error measurement of a Markov chain. (In the paper, the model and error measure formulas should be corrected as bellow:)

$$U(\mathbf{q}) = \begin{cases} \sqrt{\mathbf{q}^\top A \mathbf{q}} & \text{if } \|\mathbf{q}\|_\infty \leq 3 \\ 1 + \sqrt{\mathbf{q}^\top A \mathbf{q}} & \text{if } 3 < \|\mathbf{q}\|_\infty \leq 6 \\ +\infty, & \text{otherwise} \end{cases}$$
$$\text{WMAE} \left(\mathbf{q}^{(1)}, \dots, \mathbf{q}^{(k)} \right) = \frac{1}{k} \max_{d=1,\dots,n} \left| \sum_{s=1}^k q_d^s \right|$$

The figures show that

1. The proposed reflective HMC (RHMC) remains superior to the baseline HMC over a large range of L and ϵ and in no setting it performs worse.
 2. Compared to the basic HMC, the performance of reflective HMC is less sensitive to parameter tuning.
 3. Regardless of the tuning, in high dimensional models, reflective HMC performs significantly better than the basic HMC and tuned Metropolis-Hastings.
- Finally, the rejection rates of the basic and reflective HMC algorithms as well as the reflections and refraction rates of the latter sampler are depicted in Tables 1 to 3.

An interesting observation is that in high dimensions (as in Table 3), the number of refractions is significantly less than reflections. The reason is that the studied model consists of two positive-probability (hyper-cubic) partitions one of which is inside the other. In high dimensions, the internal hyper-cube is rarely sampled since most of the mass is concentrated near the outer surface of the external one.

Based on this observation, we predict that in general, due to the effect of *reflection*, the performance of our proposed method on high dimensional truncated/finite-support model should be remarkable. The reason is that in such high-dimensional models, the density mass is concentrated near the manifolds that mark the external surfaces of the density function and reflection prevents the leapfrog mechanism to enter the zero-probability ambient space.

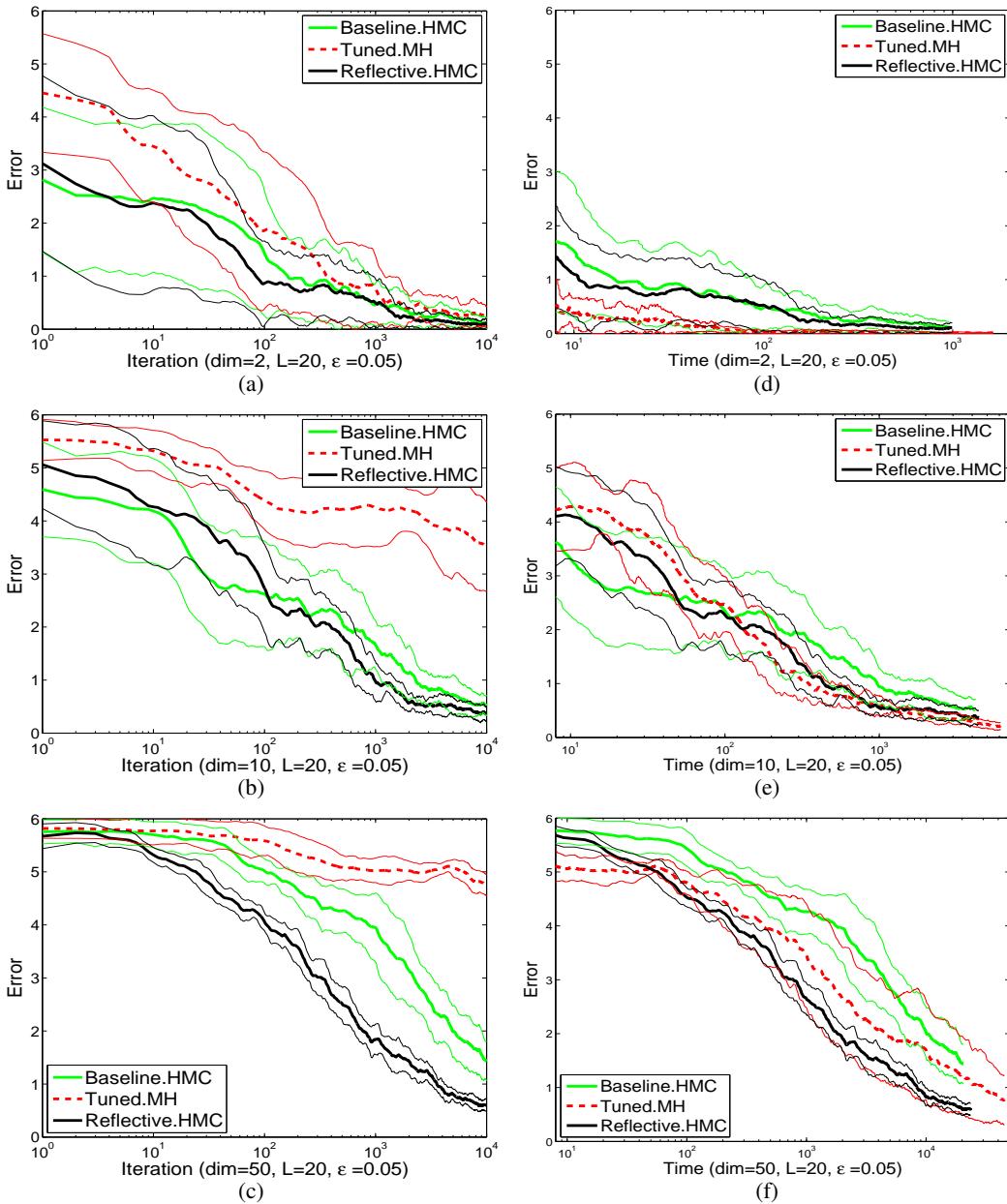


Figure 1: Error (worst mean absolute error per dimension) versus iterations (left) and time (right) (ms). Results correspond leapfrog parameters $L = 20$, $\epsilon = 0.05$.

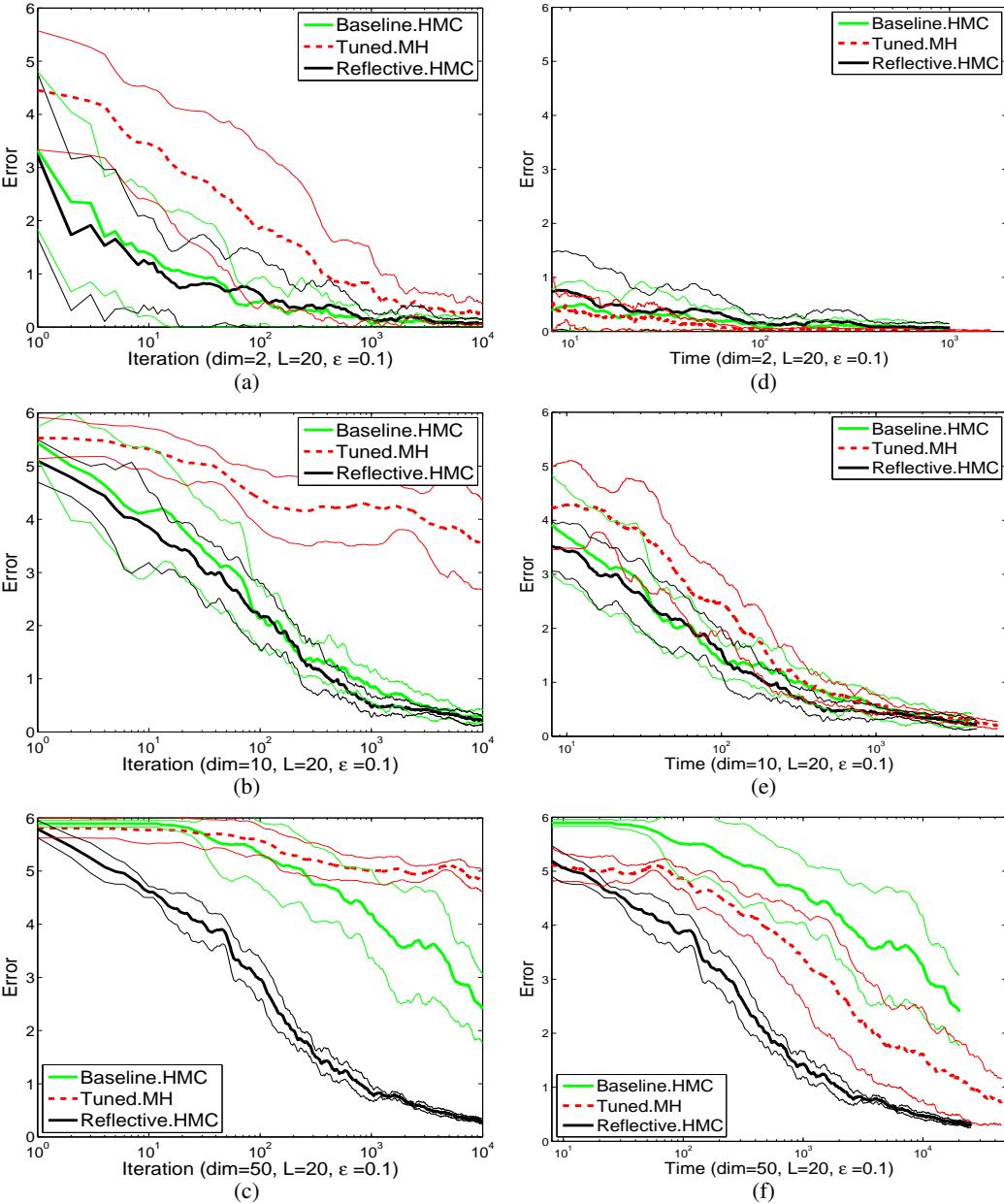


Figure 2: Error (worst mean absolute error per dimension) versus iterations (left) and time (right) (ms). Results correspond leapfrog parameters $L = 20$, $\epsilon = 0.1$.

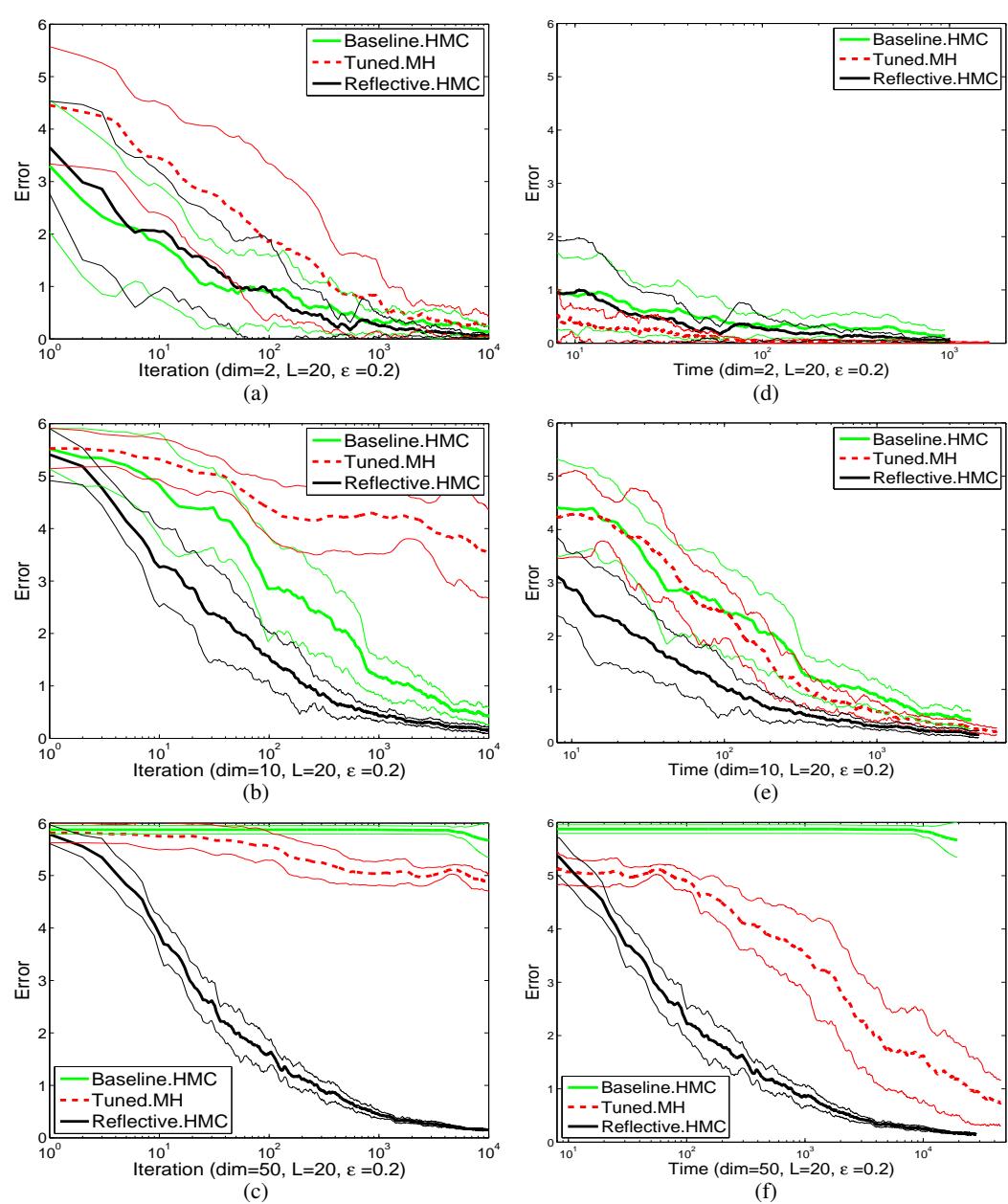
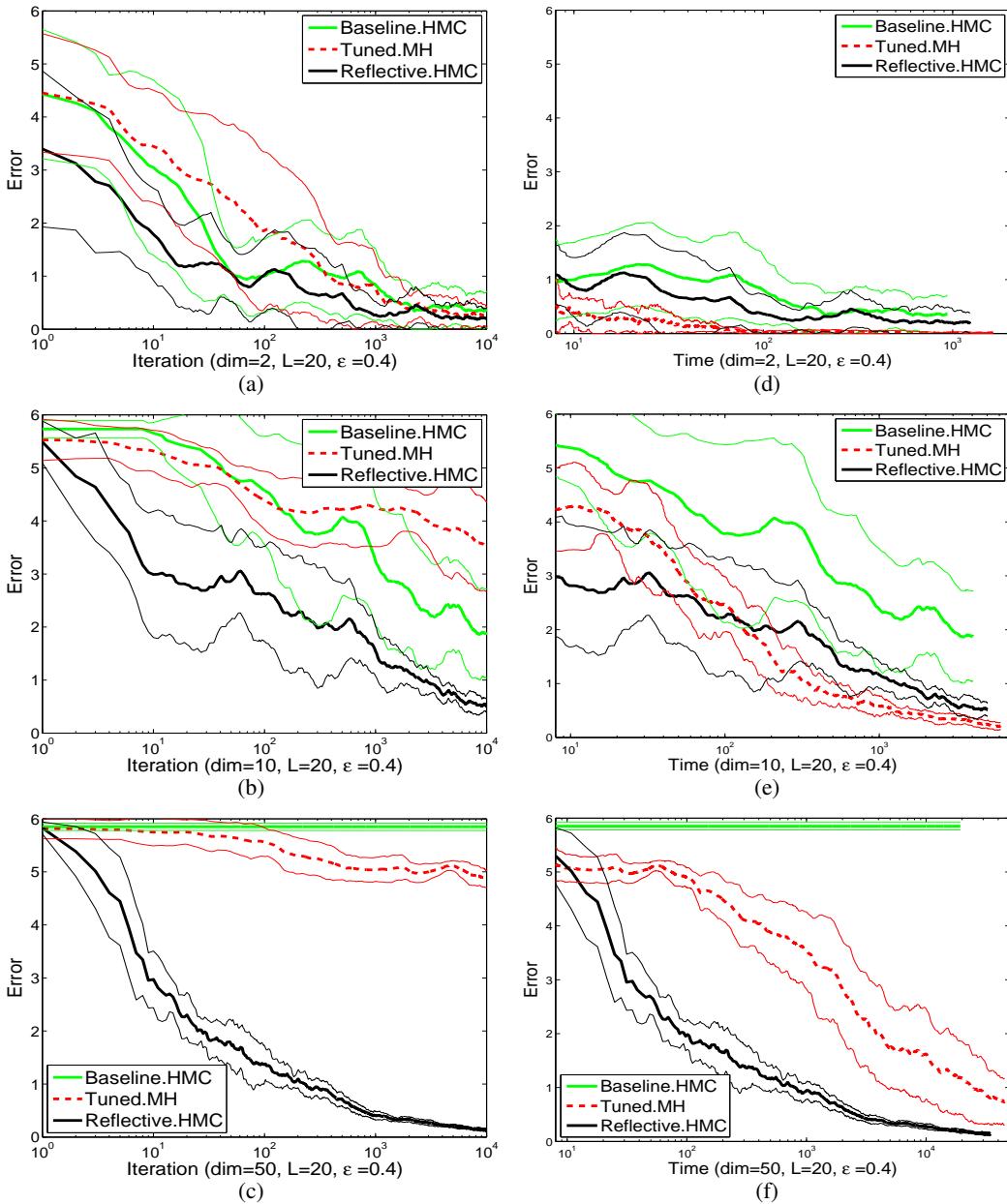


Figure 3: Error (worst mean absolute error per dimension) versus iterations (left) and time (right) (ms). Results correspond leapfrog parameters $L = 20$, $\epsilon = 0.2$.



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Figure 4: Error (worst mean absolute error per dimension) versus iterations (left) and time (right) (ms). Results correspond leapfrog parameters $L = 20$, $\epsilon = 0.4$.

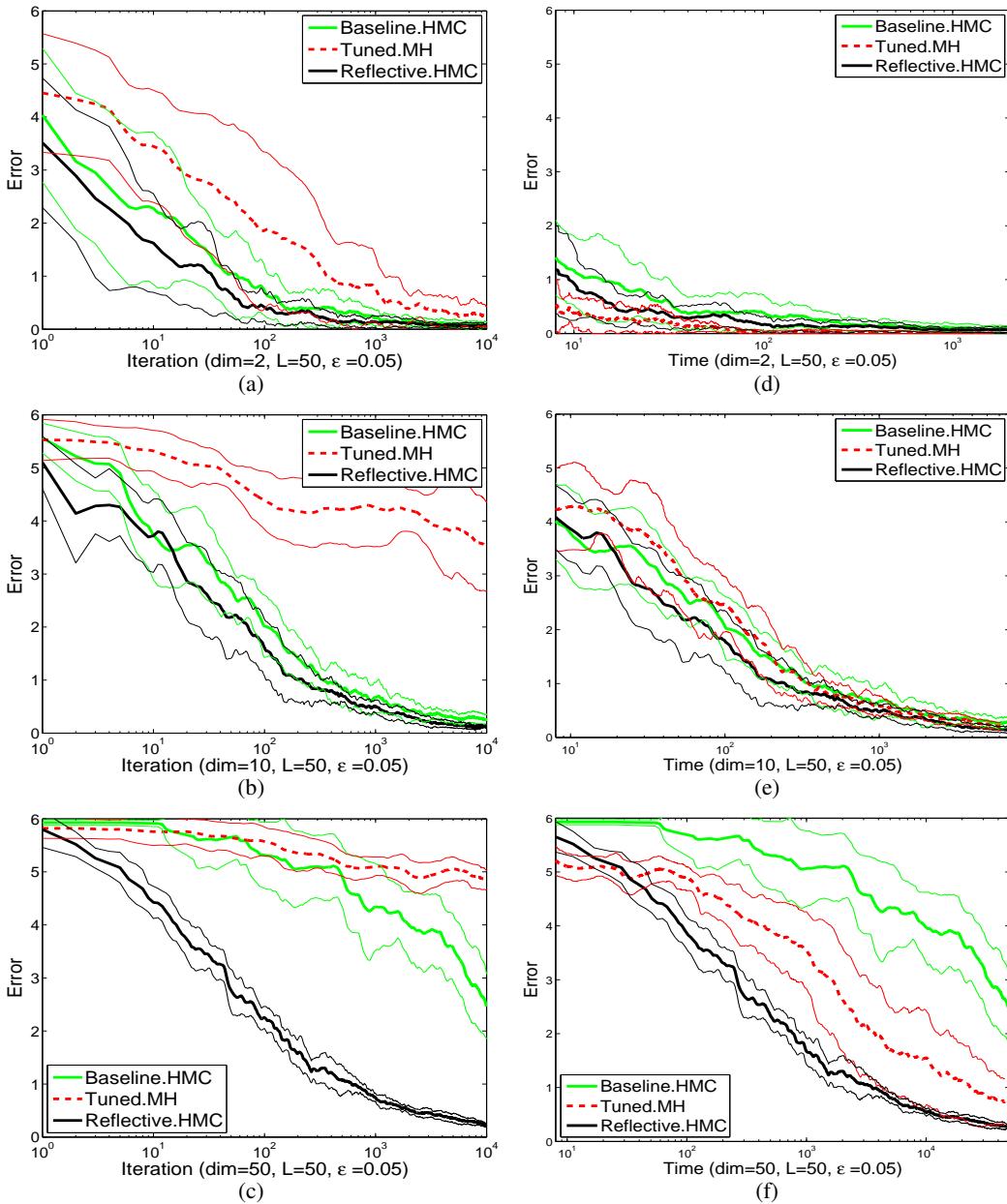


Figure 5: Error (worst mean absolute error per dimension) versus iterations (left) and time (right) (ms). Results correspond leapfrog parameters $L = 50$, $\epsilon = 0.05$.

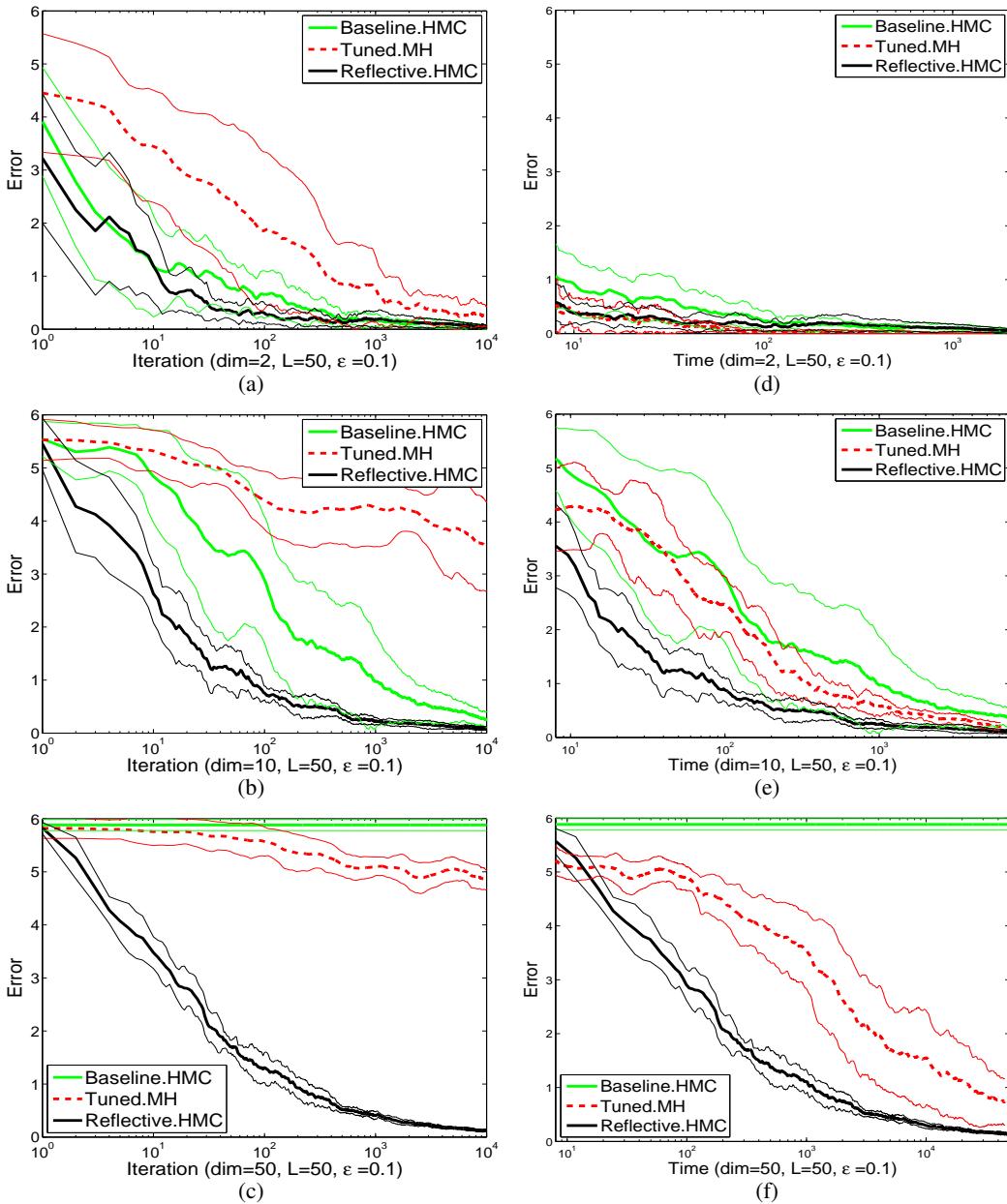


Figure 6: Error (worst mean absolute error per dimension) versus iterations (left) and time (right) (ms). Results correspond leapfrog parameters $L = 50$, $\epsilon = 0.1$.

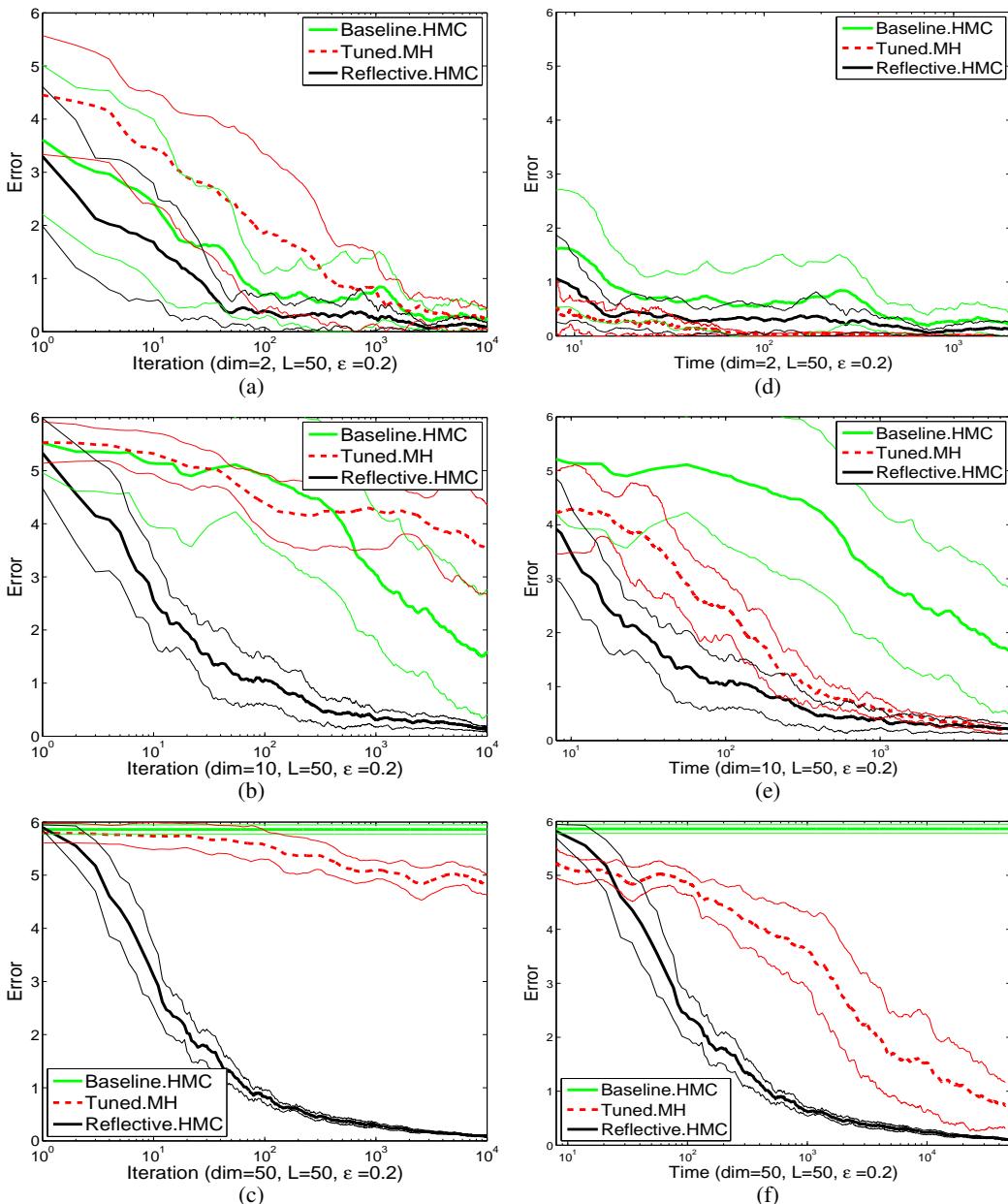


Figure 7: Error (worst mean absolute error per dimension) versus iterations (left) and time (right) (ms). Results correspond leapfrog parameters $L = 50$, $\epsilon = 0.2$.

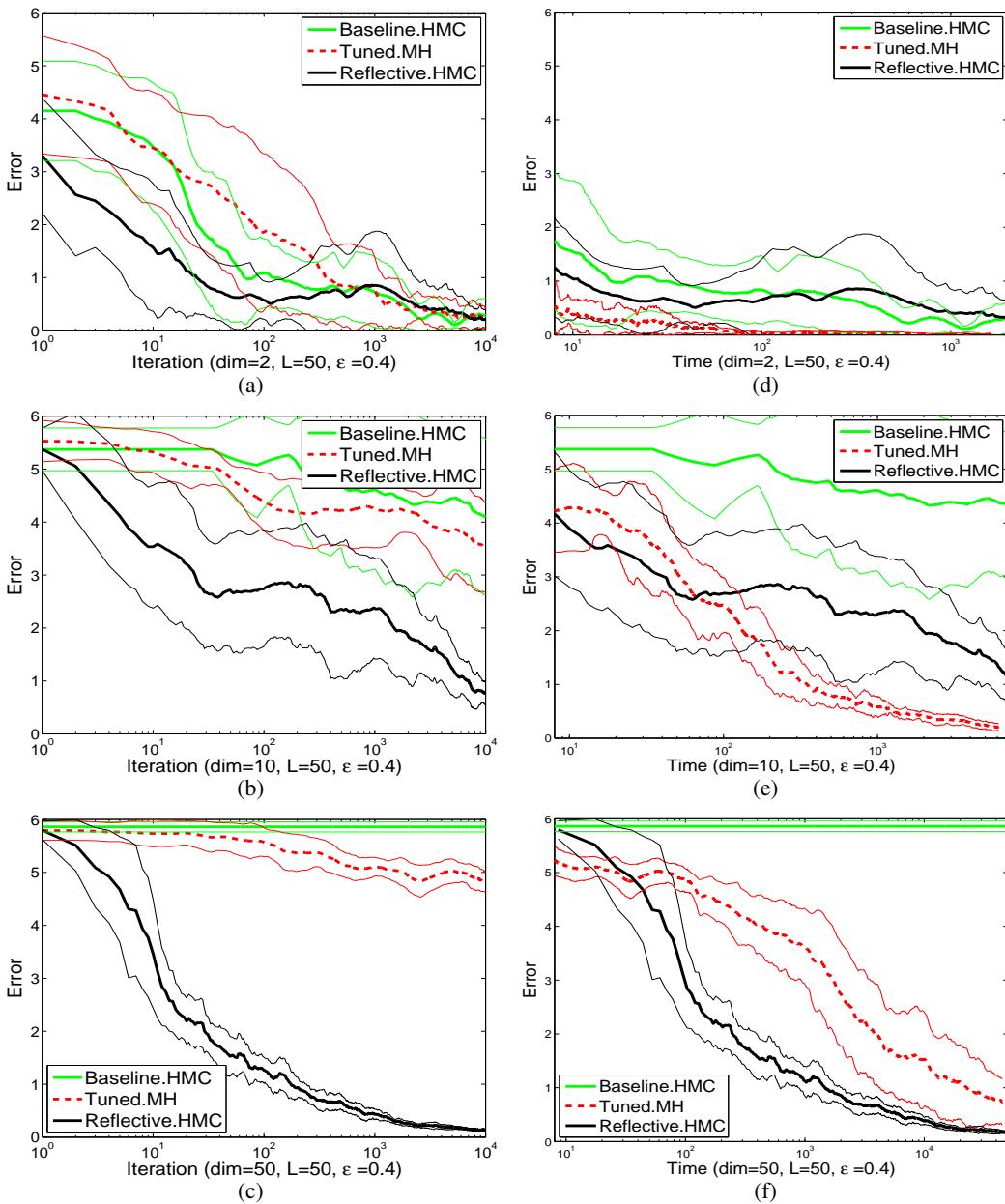


Figure 8: Error (worst mean absolute error per dimension) versus iterations (left) and time (right) (ms). Results correspond to leapfrog parameters $L = 50$, $\epsilon = 0.4$.

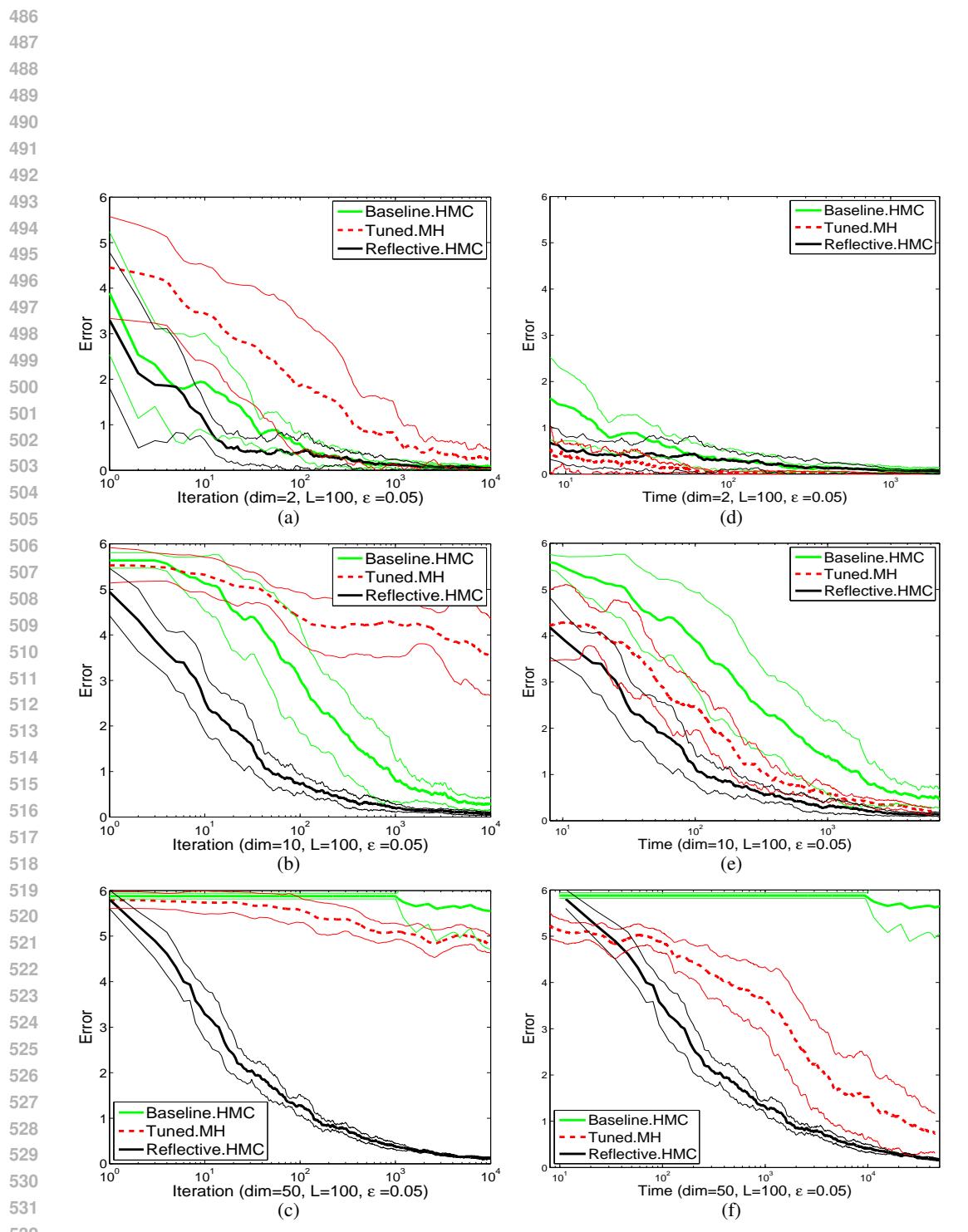
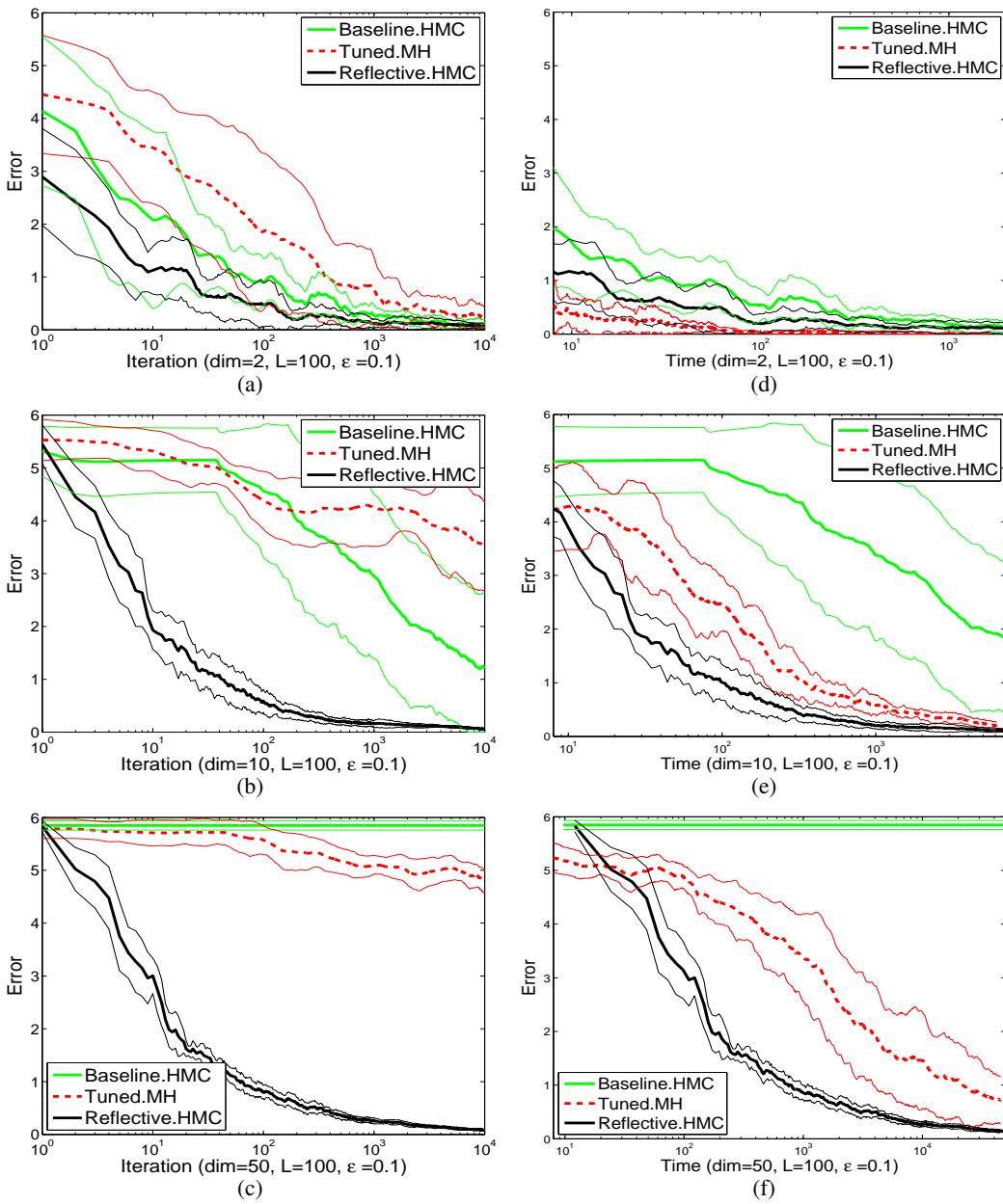
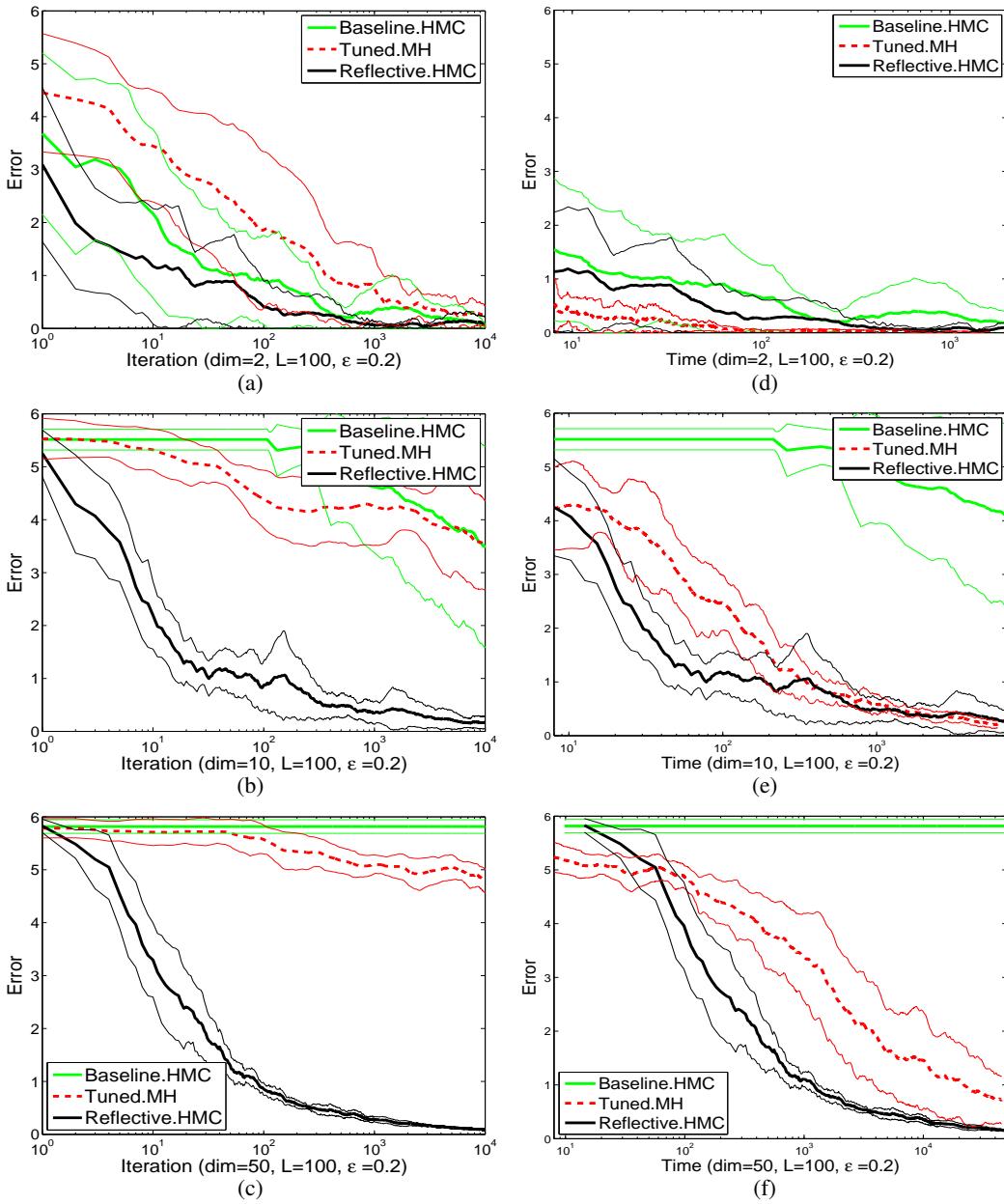


Figure 9: Error (worst mean absolute error per dimension) versus iterations (left) and time (right) (ms). Results correspond leapfrog parameters $L = 100$, $\epsilon = 0.05$.



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Figure 10: Error (worst mean absolute error per dimension) versus iterations (left) and time (ms).
Results correspond to leapfrog parameters $L = 100$, $\epsilon = 0.1$.



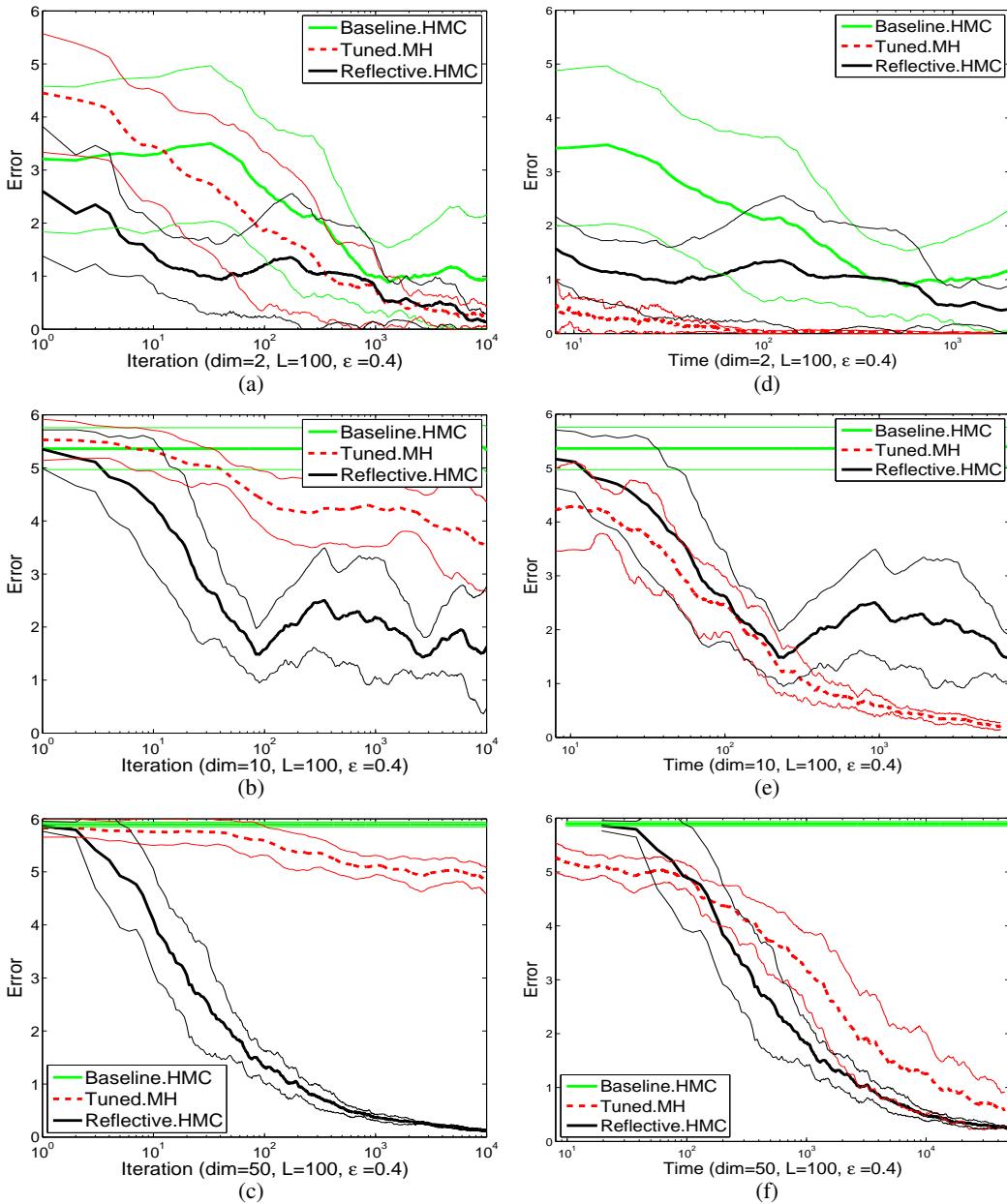


Figure 12: Error (worst mean absolute error per dimension) versus iterations (left) and time (ms) (right). Results correspond leapfrog parameters $L = 100$, $\epsilon = 0.4$.

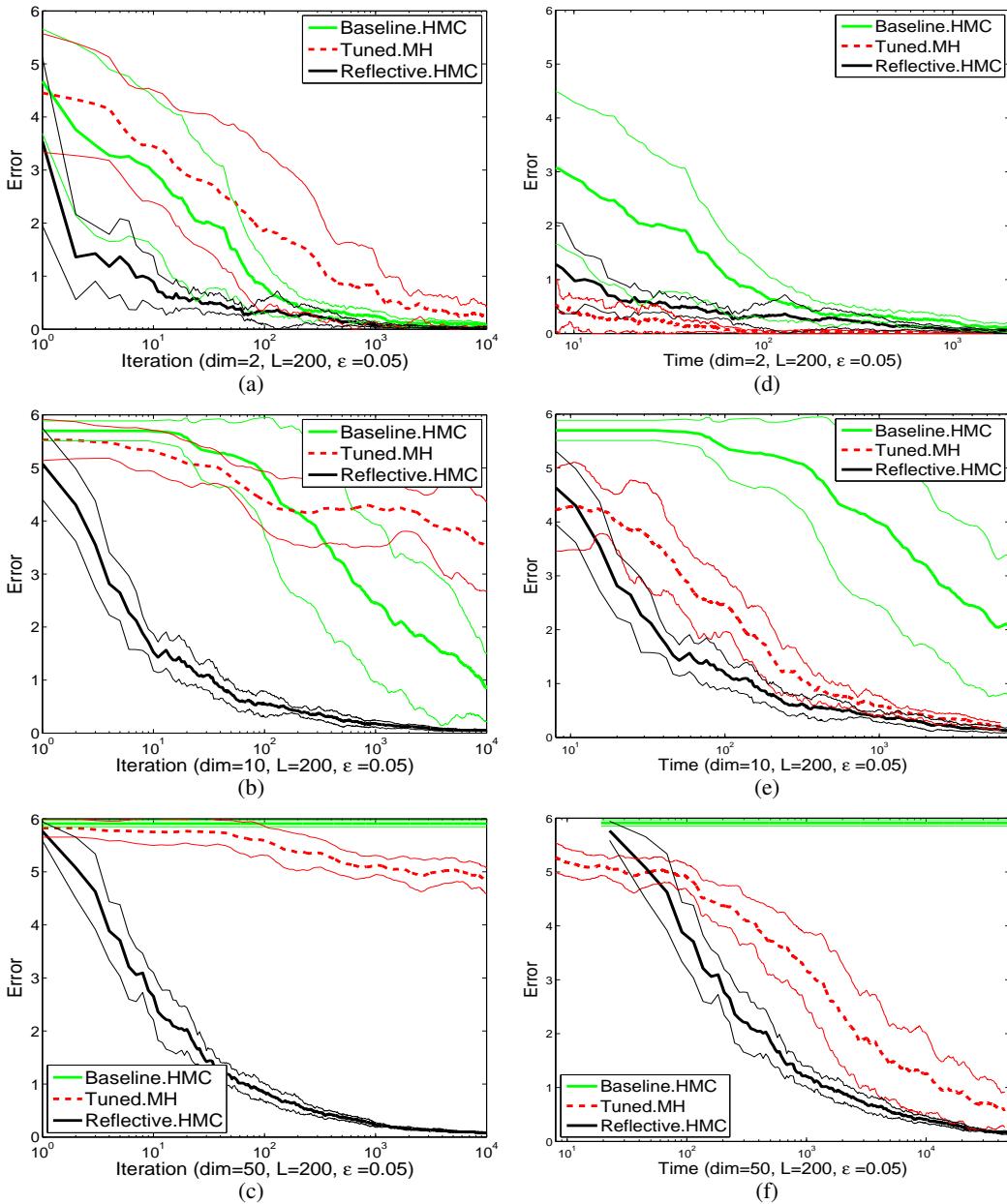


Figure 13: Error (worst mean absolute error per dimension) versus iterations (left) and time (ms) (right). Results correspond to leapfrog parameters $L = 200$, $\epsilon = 0.05$.

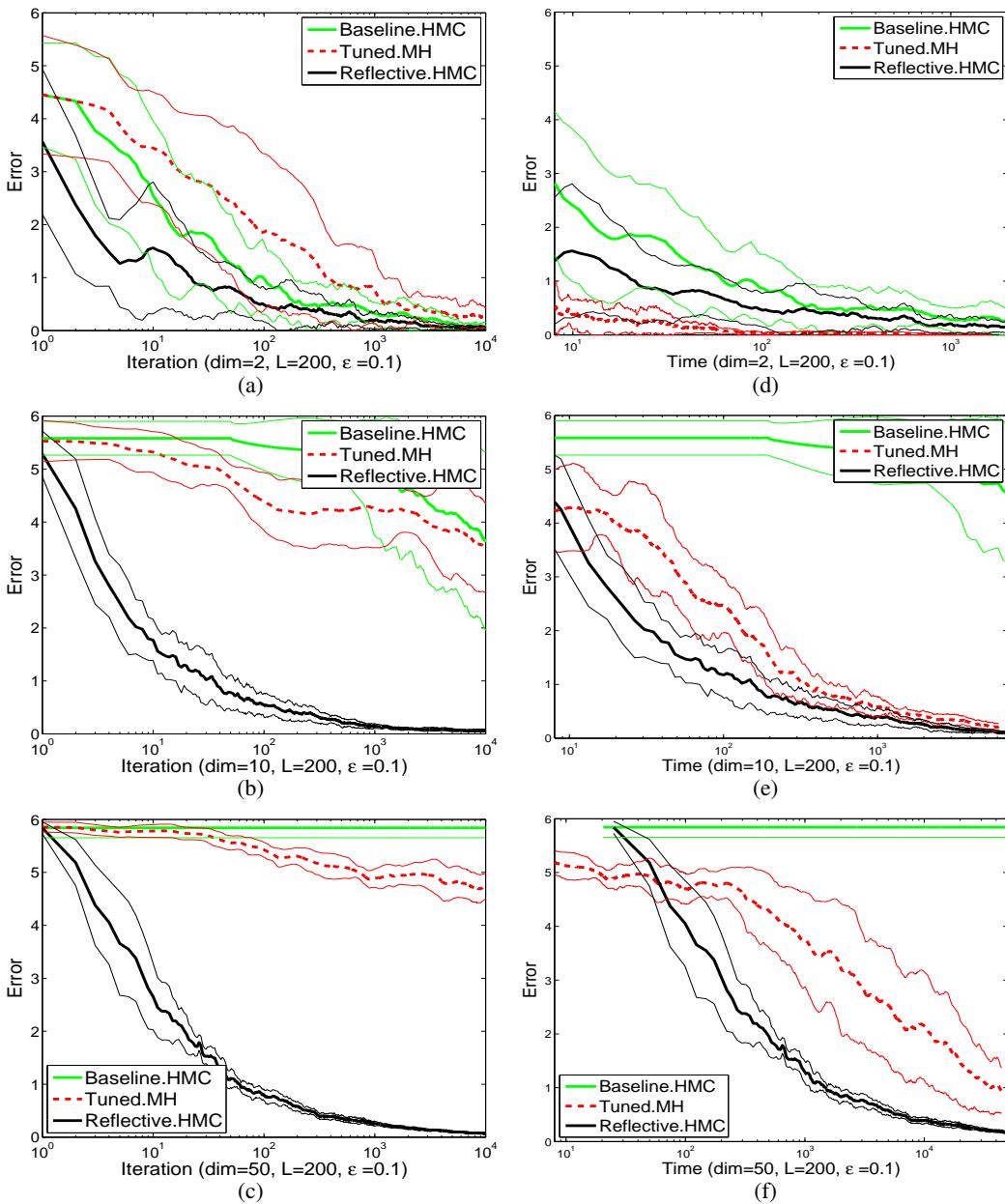


Figure 14: Error (worst mean absolute error per dimension) versus iterations (left) and time (ms) (right). Results correspond leapfrog parameters $L = 200$, $\epsilon = 0.1$.

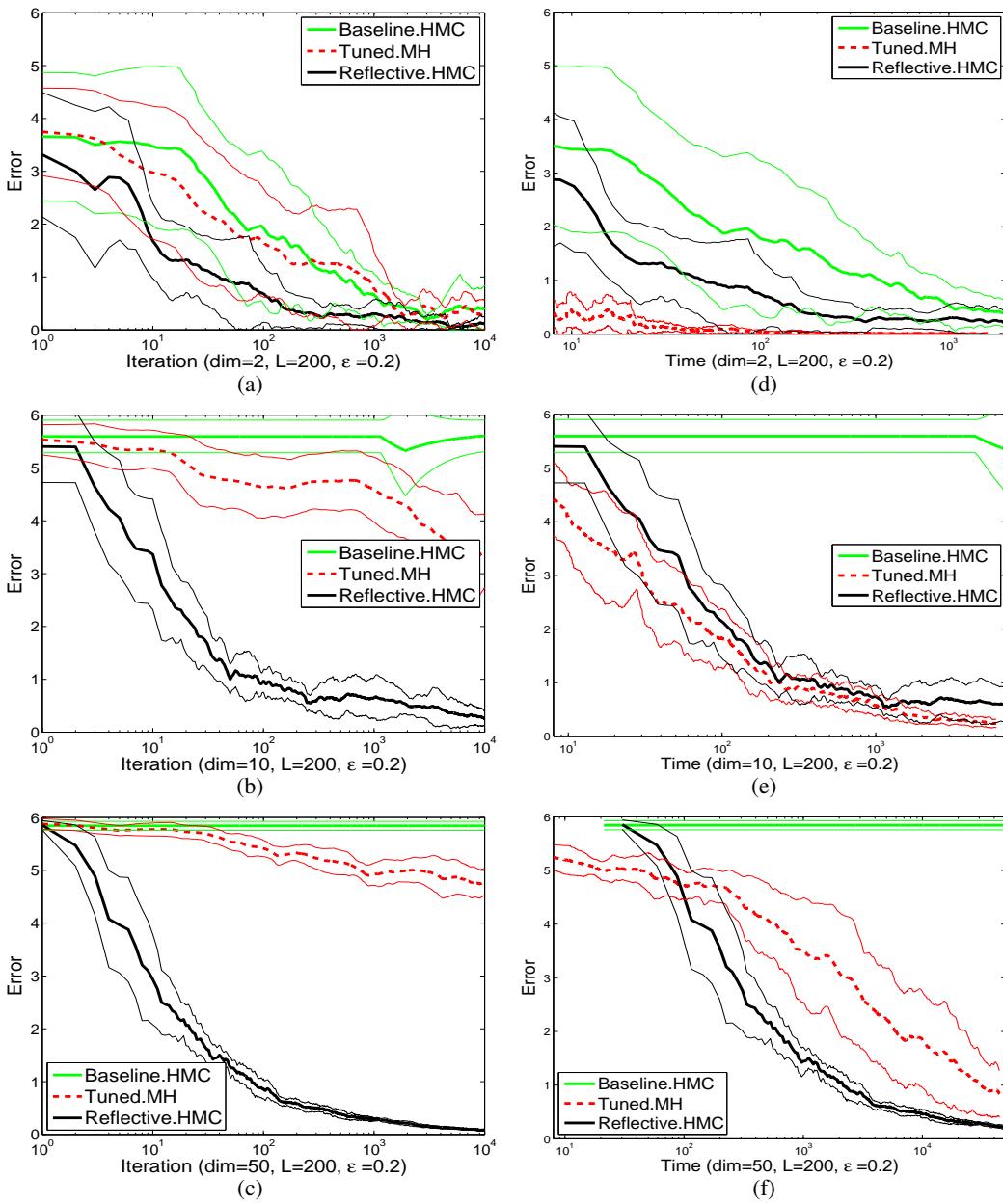


Figure 15: Error (worst mean absolute error per dimension) versus iterations (left) and time (ms) (right). Results correspond to leapfrog parameters $L = 200$, $\epsilon = 0.2$.

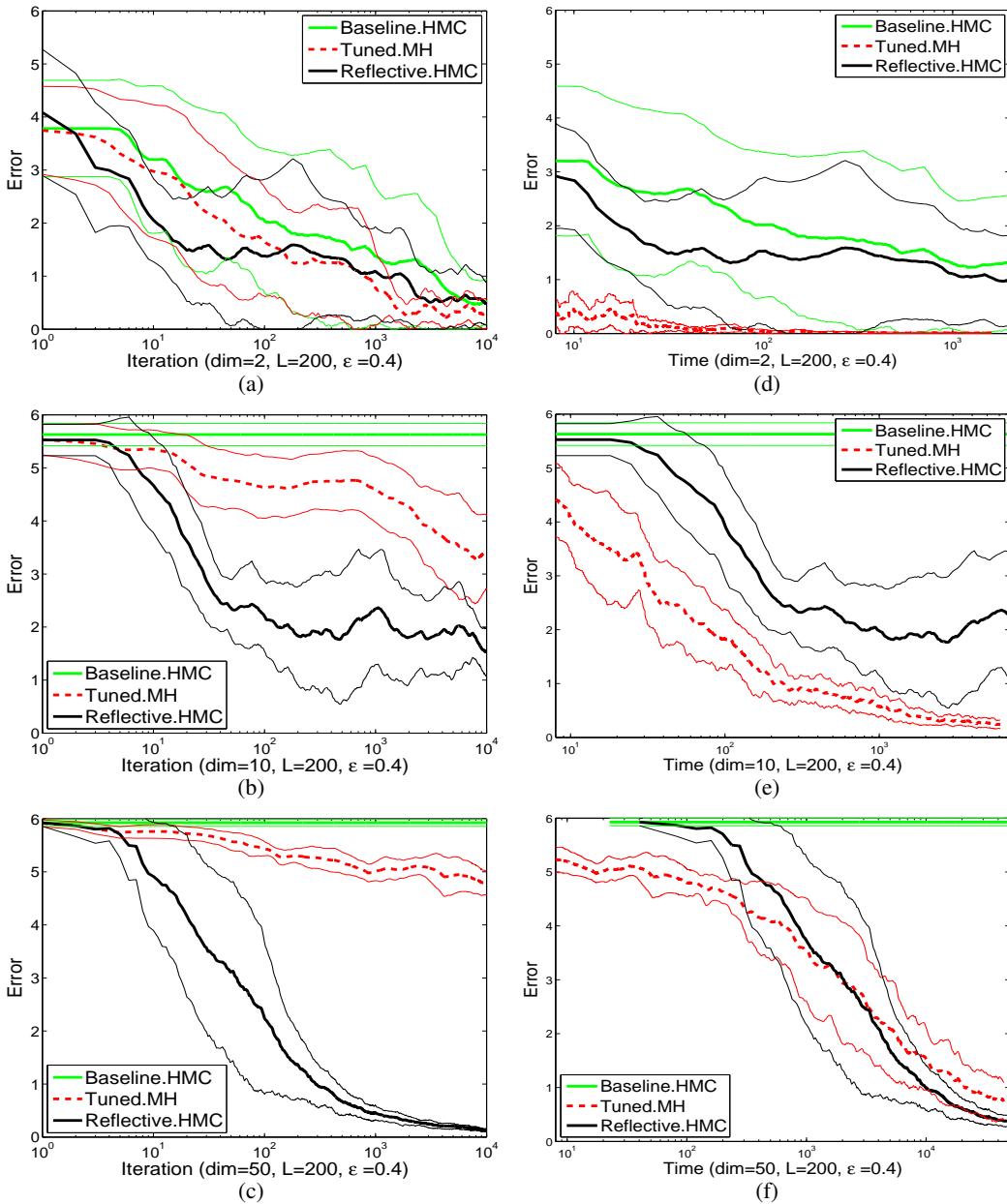


Figure 16: Error (worst mean absolute error per dimension) versus iterations (left) and time (ms) (right). Results correspond leapfrog parameters $L = 200$, $\epsilon = 0.4$.

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Table 1: Rate of rejections/reflections and refractions for sampling 10,000 particles using baseline
931 HMC (HMC) and reflective HMC (RHMC) where model dimension = 2. (The rates are averaged
932 over 10 Markov chains.)
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L	Alg.	ϵ			
		0.05	0.1	0.2	0.4
10	HMC	no. reject: 1492.7	no. reject: 3479.9	no. reject: 6087.2	no. reject: 8358.4
	RHMC	no. reject: 1280.6	no. reject: 2892.8	no. reject: 4904.6	no. reject: 6880.9
		no. reflect: 298.5	no. reflect: 839.1	no. reflect: 2007.2	no. reflect: 2972.2
		no. refract: 217.1	no. refract: 585.3	no. refract: 1365.1	no. refract: 10152.1
20	HMC	no. reject: 1966.8	no. reject: 5120.1	no. reject: 7673.1	no. reject: 9564.6
	RHMC	no. reject: 1307.7	no. reject: 4791.3	no. reject: 6055.1	no. reject: 8866.2
		no. reflect: 785.1	no. reflect: 931.9	no. reflect: 3758.6	no. reflect: 13977.5
		no. refract: 556.4	no. refract: 734.3	no. refract: 2603.7	no. refract: 36627.5
50	HMC	no. reject: 3587.7	no. reject: 6696.4	no. reject: 9195.2	no. reject: 9510.6
	RHMC	no. reject: 2012.2	no. reject: 4510.8	no. reject: 8175.9	no. reject: 7958.5
		no. reflect: 2129.6	no. reflect: 4685.6	no. reflect: 8018.5	no. reflect: 59906.3
		no. refract: 1567.7	no. refract: 3165.8	no. refract: 16627.1	no. refract: 121706.7
100	HMC	no. reject: 5288.0	no. reject: 8264.3	no. reject: 8904.9	no. reject: 9416.3
	RHMC	no. reject: 3152.5	no. reject: 5495.8	no. reject: 6510.4	no. reject: 6998.3
		no. reflect: 4029.0	no. reflect: 10549.3	no. reflect: 20825.6	no. reflect: 172305.0
		no. refract: 2920.2	no. refract: 7266.3	no. refract: 51209.3	no. refract: 261964.0
200	HMC	no. reject: 7100.1	no. reject: 8421.4	no. reject: 9221.1	no. reject: 9426.0
	RHMC	no. reject: 2366.9	no. reject: 6450.9	no. reject: 6679.2	no. reject: 7047.6
		no. reflect: 11509.1	no. reflect: 18628.0	no. reflect: 66031.6	no. reflect: 498257.6
		no. refract: 7693.9	no. refract: 22783.0	no. refract: 143159.7	no. refract: 645459.2

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 984 Table 2: Rate of rejections/reflections and refractions for sampling 10,000 particles using baseline
 985 HMC (HMC) and reflective HMC (RHMC) where model dimension = 10. (The rates are averaged
 986 over 10 Markov chains.)
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L	Alg.	ϵ			
		0.05	0.1	0.2	0.4
10	HMC	no. reject: 1492.2	no. reject: 3677.1	no. reject: 7284.7	no. reject: 9664.6
	RHMC	no. reject: 143.3	no. reject: 897.7	no. reject: 4175.4	no. reject: 9076.4
		no. reflect: 1437.1	no. reflect: 3642.0	no. reflect: 7713.7	no. reflect: 13378.9
		no. refract: 235.6	no. refract: 433.9	no. refract: 660.9	no. refract: 2301.4
20	HMC	no. reject: 2754.0	no. reject: 5472.9	no. reject: 8873.8	no. reject: 9946.3
	RHMC	no. reject: 130.7	no. reject: 799.7	no. reject: 4260.2	no. reject: 9365.8
		no. reflect: 3089.3	no. reflect: 6864.7	no. reflect: 15013.6	no. reflect: 32340.3
		no. refract: 554.4	no. refract: 878.3	no. refract: 1348.5	no. refract: 5057.8
50	HMC	no. reject: 5738.4	no. reject: 8337.8	no. reject: 9629.4	no. reject: 9987.0
	RHMC	no. reject: 141.9	no. reject: 680.2	no. reject: 4921.8	no. reject: 9497.0
		no. reflect: 8035.2	no. reflect: 15536.1	no. reflect: 36844.7	no. reflect: 113852.2
		no. refract: 1315.6	no. refract: 2731.2	no. refract: 3553.6	no. refract: 14880.1
100	HMC	no. reject: 8139.5	no. reject: 9771.6	no. reject: 9968.1	no. reject: 9999.7
	RHMC	no. reject: 157.2	no. reject: 960.0	no. reject: 4359.8	no. reject: 9640.1
		no. reflect: 16291.1	no. reflect: 36164.2	no. reflect: 67230.7	no. reflect: 321873.9
		no. refract: 2307.4	no. refract: 4260.1	no. refract: 11126.0	no. refract: 24149.7
200	HMC	no. reject: 9600.1	no. reject: 9987.0	no. reject: 9999.9	no. reject: 10000.0
	RHMC	no. reject: 156.7	no. reject: 744.1	no. reject: 5399.3	no. reject: 9662.6
		no. reflect: 32738.1	no. reflect: 64447.1	no. reflect: 168753.9	no. reflect: 1022839.6
		no. refract: 5022.2	no. refract: 9978.9	no. refract: 14639.0	no. refract: 36450.5

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 1039 Table 3: Rate of rejections/reflections and refractions for sampling 10,000 particles using baseline
 1040 HMC (HMC) and reflective HMC (RHMC) where model dimension = 50. (The rates are averaged
 1041 over 10 Markov chains.)
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L	Alg.	ϵ			
		0.05	0.1	0.2	0.4
10	HMC	no. reject: 5455.4	no. reject: 8267.9	no. reject: 9618.1	no. reject: 9997.5
	RHMC	no. reject: 69.1	no. reject: 271.3	no. reject: 1074.3	no. reject: 4157.0
		no. reflect: 7609.2	no. reflect: 17121.9	no. reflect: 31497.3	no. reflect: 66778.1
		no. refract: 0.0	no. refract: 0.0	no. refract: 0.0	no. refract: 0.0
20	HMC	no. reject: 8301.4	no. reject: 9719.0	no. reject: 9999.5	no. reject: 10000.0
	RHMC	no. reject: 64.2	no. reject: 289.8	no. reject: 988.0	no. reject: 4197.3
		no. reflect: 17257.4	no. reflect: 33841.4	no. reflect: 66524.4	no. reflect: 141453.9
		no. refract: 0.0	no. refract: 0.0	no. refract: 0.2	no. refract: 0.0
50	HMC	no. reject: 9869.9	no. reject: 10000.0	no. reject: 10000.0	no. reject: 10000.0
	RHMC	no. reject: 59.9	no. reject: 233.8	no. reject: 878.4	no. reject: 3921.5
		no. reflect: 40732.3	no. reflect: 82537.0	no. reflect: 160209.2	no. reflect: 331565.0
		no. refract: 0.0	no. refract: 0.0	no. refract: 0.0	no. refract: 0.0
100	HMC	no. reject: 9998.8	no. reject: 10000.0	no. reject: 10000.0	no. reject: 10000.0
	RHMC	no. reject: 56.9	no. reject: 215.1	no. reject: 960.5	no. reject: 3899.6
		no. reflect: 85937.0	no. reflect: 157553.7	no. reflect: 356408.4	no. reflect: 665330.2
		no. refract: 0.4	no. refract: 0.2	no. refract: 0.0	no. refract: 0.0
200	HMC	no. reject: 10000.0	no. reject: 10000.0	no. reject: 10000.0	no. reject: 10000.0
	RHMC	no. reject: 60.2	no. reject: 229.8	no. reject: 888.9	no. reject: 3911.3
		no. reflect: 157838.8	no. reflect: 335667.9	no. reflect: 667757.6	no. reflect: 1325778.9
		no. refract: 0.2	no. refract: 0.0	no. refract: 0.2	no. refract: 1.6