Guarantees for the Langevin Monte Carlo sampling algorithm in terms of Wasserstein distance

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Applications in

- Bayesian statistics
- Volume computation
- ...

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Problem: good approximation $\Rightarrow$ small h $\Rightarrow$ many iterations to approximate X_t up to time T.
How to choose h? How many iterations do we need to achieve a given accuracy ϵ.

Total variation distance and log-concave μ

Let μ, ν be two measures. The total variation distance between them is given by

$$TV(\nu, \mu) = \max_{\mathcal{B}} |P_\mu(\mathcal{B}) - P_\nu(\mathcal{B})|,$$

where $\mathcal{B}$ is a Borel set.

μ is log-concave if it has density e^{-u} with u convex. This property traditionaly ensures exponential convergence for many quantities quantifying the distance between X_t and μ (Entropy, Fisher information, total variation, Wasserstein distance, ...).

Total variation distance and log-concave μ

Theorem [Dalalyan 2015, fixed h]
Suppose μ is log-concave and ∇u is bounded. Then, one can choose h and T in order to reach an ϵ accuracy in total variation in no more than $O(\epsilon^{-2} p(p^2 + \log^2(1/\epsilon))$ steps.

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$$TV(M^n, \mu) \leq TV(M^n, X_{nh}) + TV(X_{nh}, \mu).$$

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Approximation term.

$$\leq (CpTh)^{1/2}$$

Exponential convergence from log-concavity.

$$\leq \frac{1}{2} e^{C_1 p - C_2 T}$$

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Problems:

- In this analysis, taking too large of a T is harmful.
- In practice, by the discrete nature of the computation, the total variation distance between μ and our approximation is infinite.
- Better rates for diffusion approximation are known for other distances. [Alfonsi, Jourdain, Kohatsu-Higa 2015]

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Disappears if one has access to a *warm start*.

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Wasserstein Distance

Let μ and ν be two measures over a metric space (E, d). The Wasserstein disance between these two measures is given by :

$$W_p^p(\mu, \nu) = \inf_{\pi \in \Pi(\mu,\nu)} \int_{E \times E} d(x, y)^p d\pi(x, y)$$

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Theorem [Durmus and Moulines 2015]
Suppose μ is log-concave and ∇u is bounded. Then, one can choose $h(n)$ in order to reach an ϵ accuracy in total variation/W_2 distance in no more than $O(\epsilon^{-2} p)$ steps.

Our assumptions

- μ has a finite second moment.
- The first 2 derivatives of u are Lipschitz continuous with respective Lipschitz constants L_1, L_2, i.e.

$$\forall 1 \leq k \leq 2, \forall x, y \in \mathbb{R}^p, \|\nabla^k u(x) - \nabla^k u(y)\| \leq L_k \|x - y\|.$$

- For any n, $\mathbb{E}[\|M^n\|^2] \leq Cp$.
- There exists $\rho > 0$ such that, if X_0 has finite second moment,

$$W_2(X_t, \mu) \leq e^{-\rho t} W_2(X_0, \mu).$$

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Last assumption is true if μ is strictly log-concave, but also holds in more general cases, for instance it holds if μ is strictly log-concave outside of a bounded set **Theorem**[Bolley, Gentil, Guilli, 2012].

Main Result

Theorem
For any $n \geq 0$,

$$W_2(M^{n+1}, \mu) \leq Ch(n)^{3/2}\sqrt{p} + e^{-\rho h(n)} W_2(M^n, \mu).$$

For any n sufficiently large,

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Sketch of proof Let X_t continuous process started in M^n.

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Approximation

Exponential convergence to μ

$\leq max(C_1 h(n)^{3/2}\sqrt{p}, C_2(h)h(n)^2 p).$

$\leq e^{-\rho h(n)} W_2(M^n, \mu).$

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No more than $O(\epsilon^{-1}p)$ steps required to reach an ϵ accuracy.

Sketch of proof

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For $t < h(n)$, $\bar{X}$ is the continuous Euler's scheme associated to M.

$$\frac{dW_2(X_t, \bar{X}_t)}{dt} \leq L_1 W_2(X_t, \bar{X}_t) + \mathbb{E}[|b(\bar{X}_s) - \mathbb{E}[b(\bar{X}_0)|\bar{X}_s]|^2]^{1/2}$$

Taylor expansion:

$$\begin{aligned} b(\bar{X}_s) - b(\bar{X}_0) &= \nabla b(\bar{X}_s).(\bar{X}_s - \bar{X}_0) \\ &\quad + \left[\int_0^1 \nabla b(v\bar{X}_s + (1-v)\bar{X}_0) - \nabla b(\bar{X}_s) dv\right](\bar{X}_s - \bar{X}_0) \end{aligned}$$

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Strong error: $\mathbb{E}[|b(\bar{X}(s)) - b(\bar{X}_0)|^2]$.

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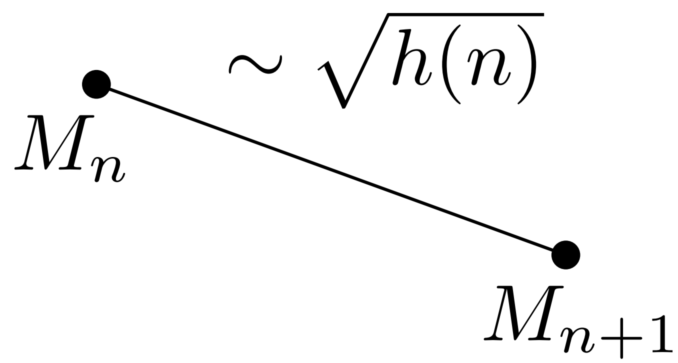

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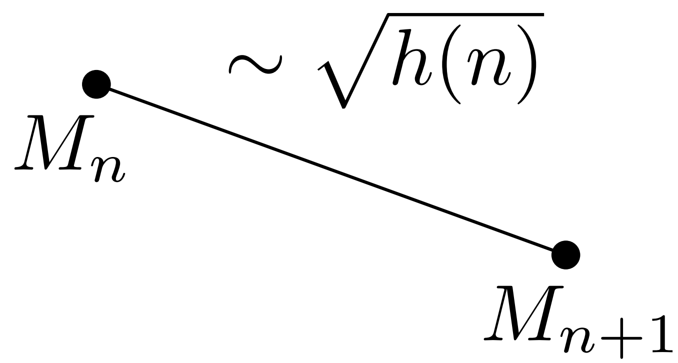

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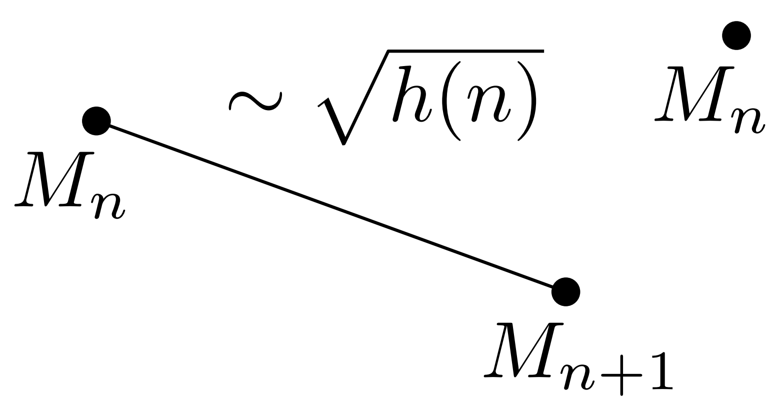

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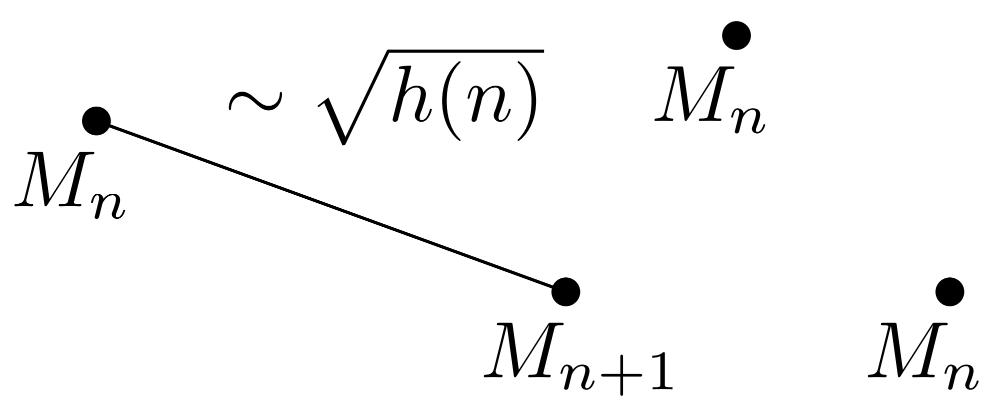

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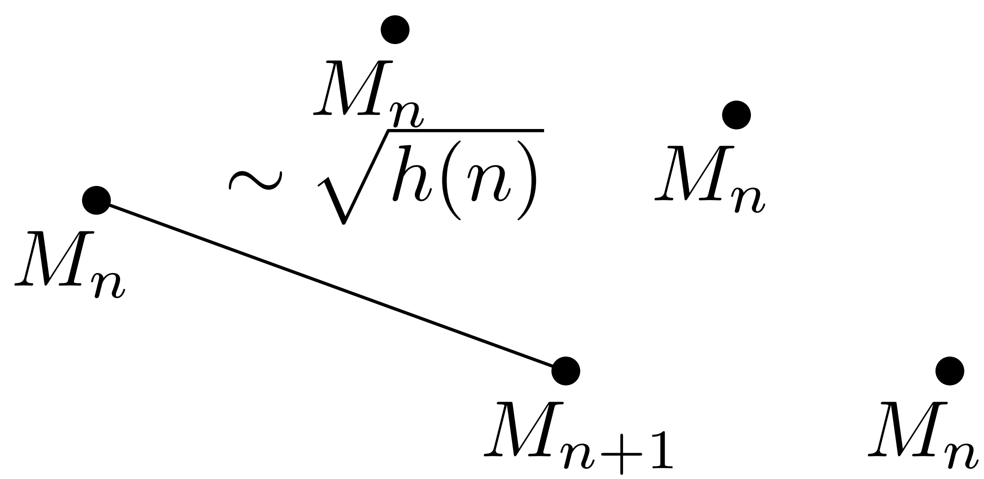

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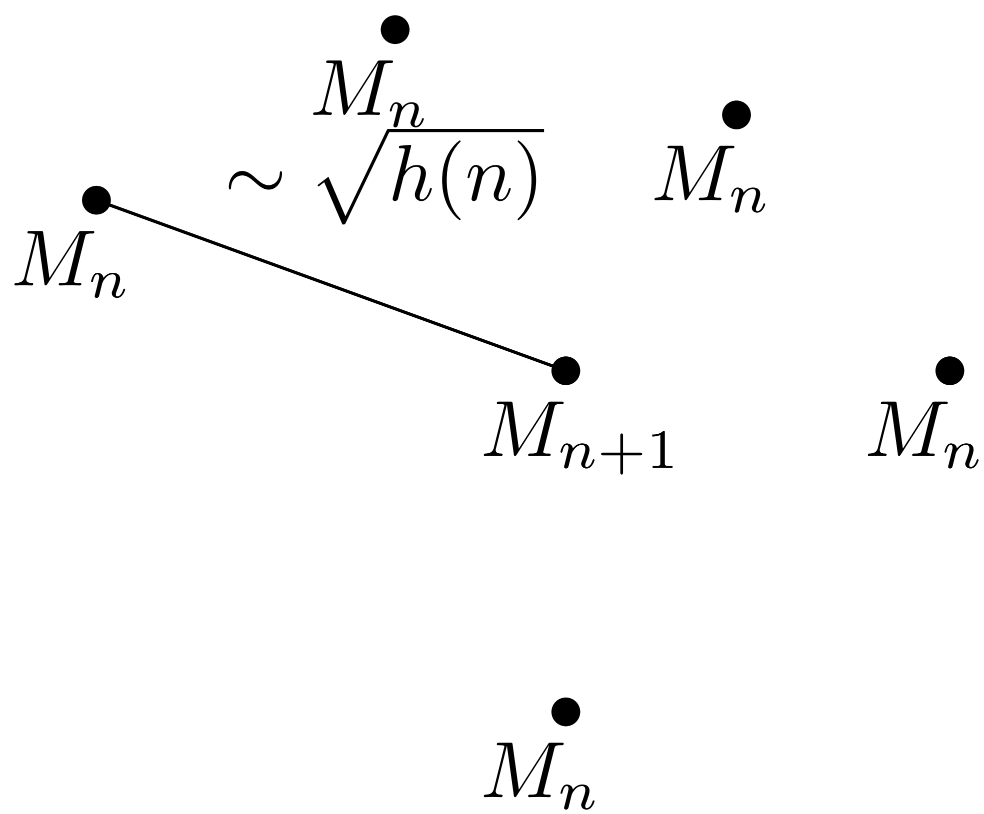

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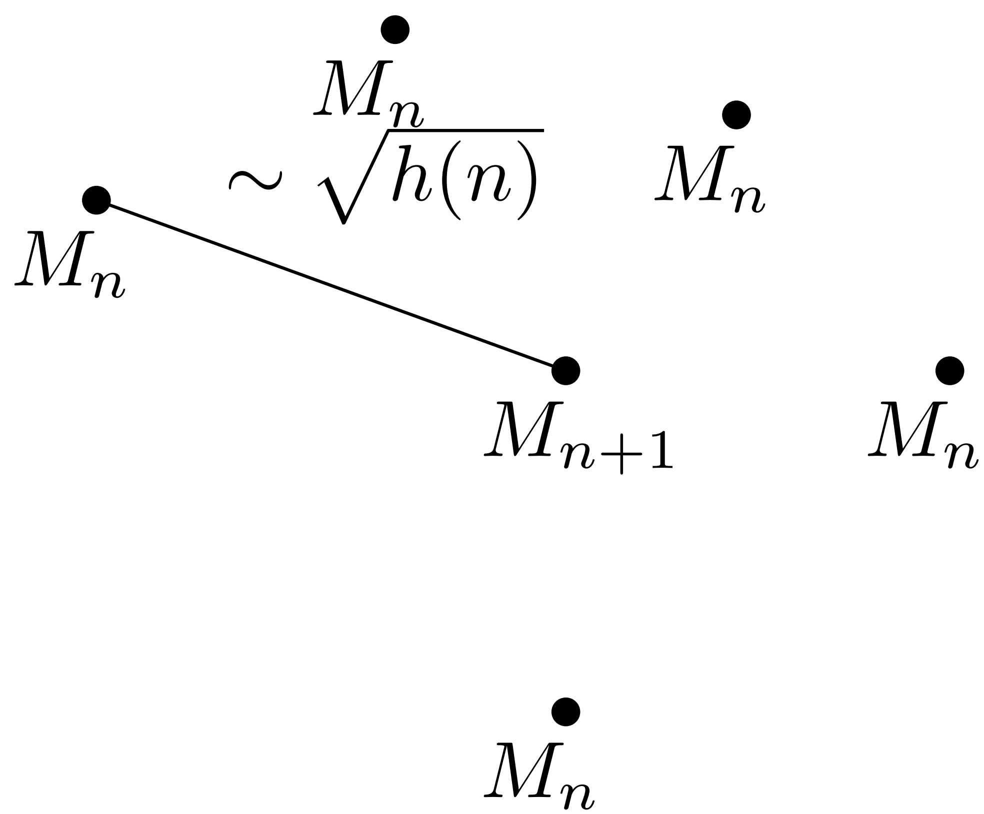

If the measure of M^n is *smooth enough*, the first term of the Taylor expansion is of order h.

Other Schemes

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Ozaki's discretization scheme: approximates X_t by $\bar{X}_t$ with drift a diffusion process $\bar{X}_t$ with drift

$$b_t(\bar{X}_t) = -\nabla u(\bar{X}_{\tau_t}) - \nabla^2 u(\bar{X}_{\tau_t})(\bar{X}_t - \bar{X}_{\tau_t}),$$

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Closed form solution: let $B = (I - e^{-h(n)\nabla b})(\nabla b)^{-1} b$ and $\Sigma = (I - e^{-2h(n)\nabla b})(\nabla b)^{-1}$ then $\bar{X}_{X_{\sum_{i=0}^{n-1} h(i)}} = M^n$ with

$$M^{n+1} = M^n + B + \Sigma^{1/2}\mathcal{N}_n.$$

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Theorem
For any $n \geq 0$,

$$W_2(M^{n+1}, \mu) \leq e^{h(n)L_1} \frac{L_2}{\sqrt{2}} \left[\frac{h(n)^3 \mathbb{E}[\|M^n\|_2^2]}{3} + \frac{h(n)^2 p}{2} \right] + e^{-\rho h(n)} W_2(M^n, \mu).$$

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$\Rightarrow$ No major improvement on the rate, each iteration is more costly (computing Hessian matrix of u).

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Rough idea (maybe works?): use Central Limit Theorem for W_2 distance (Bobkov 2013, B. 2015) $\Rightarrow$ the addition of multiple noise converges to a Gaussian $\Rightarrow$ fallback to the Euler's scheme.

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- $\mathbb{E}_\pi[\|X\|^2] < \infty$.
- μ is strictly ρ log-concave

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Theorem[B. 2015] If μ is log-concave then, for any $T > 0$

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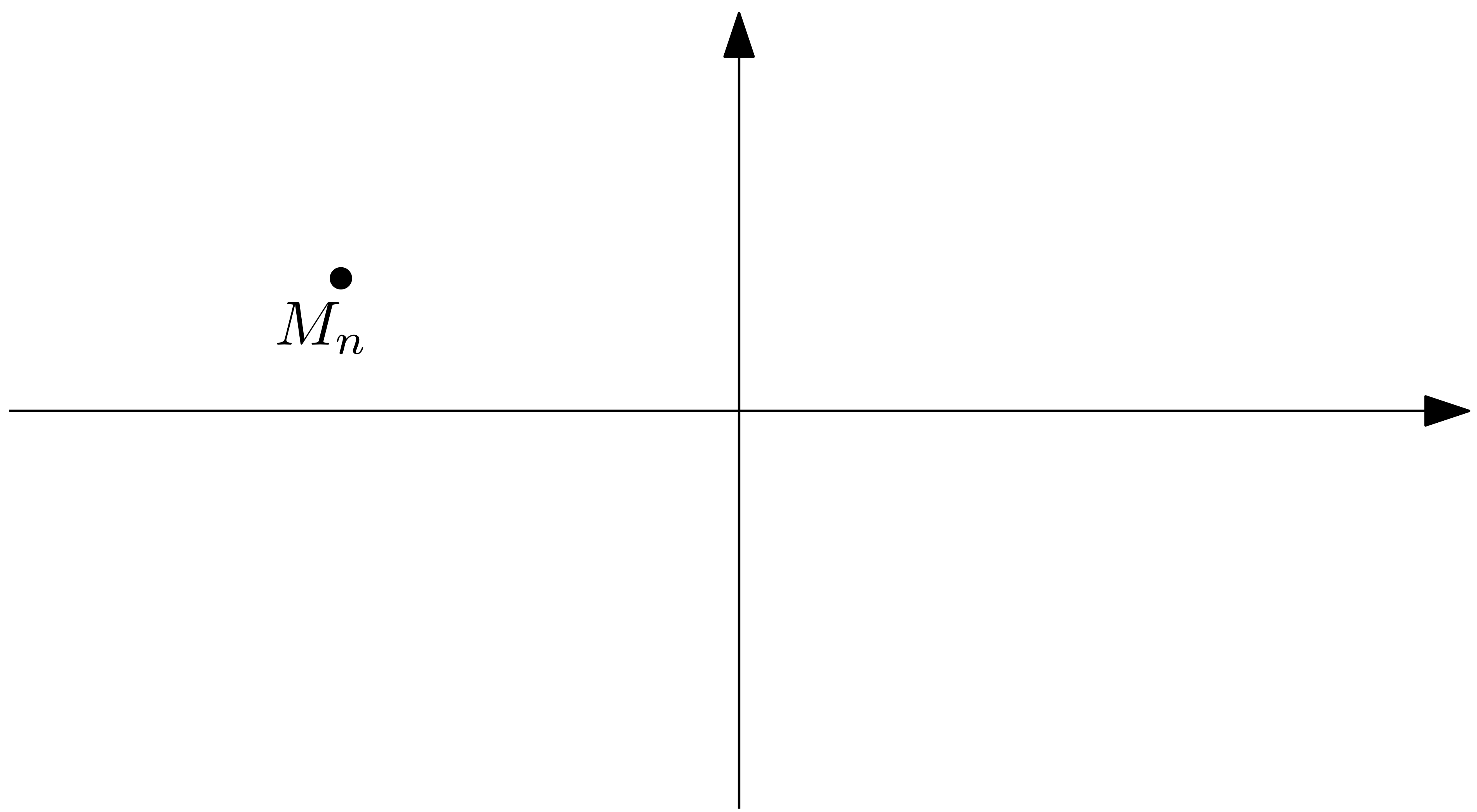

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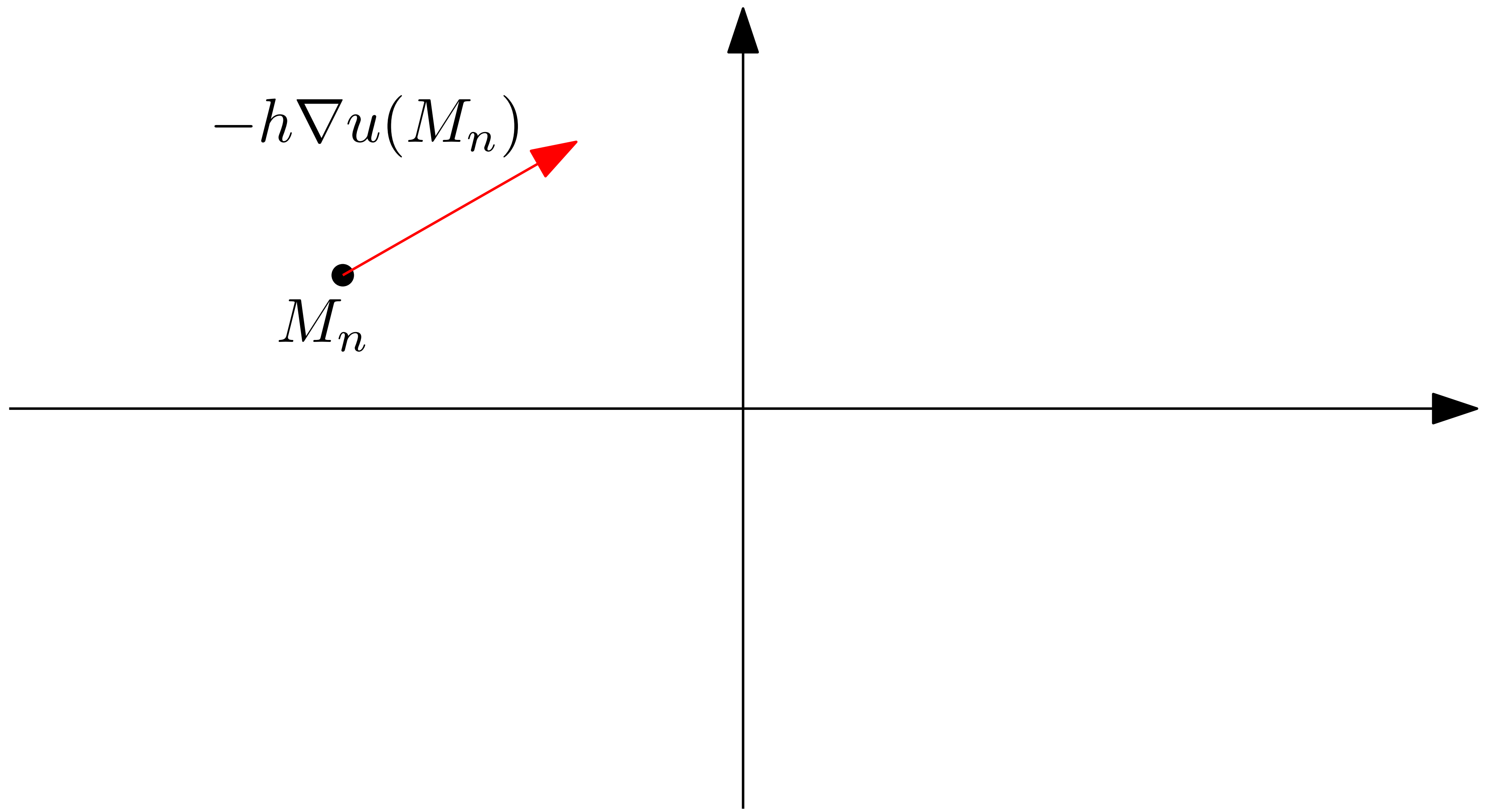

Other Schemes: an example

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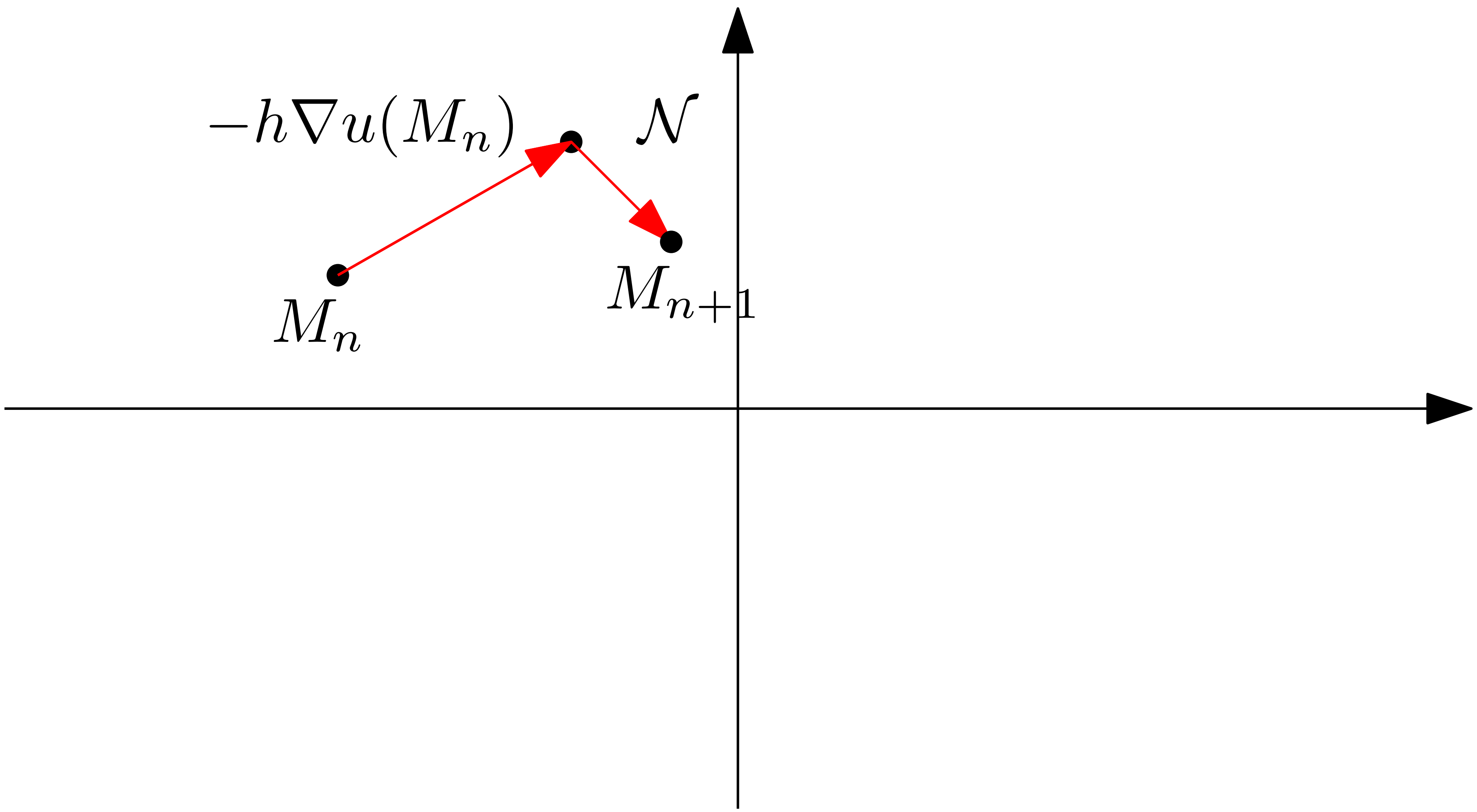

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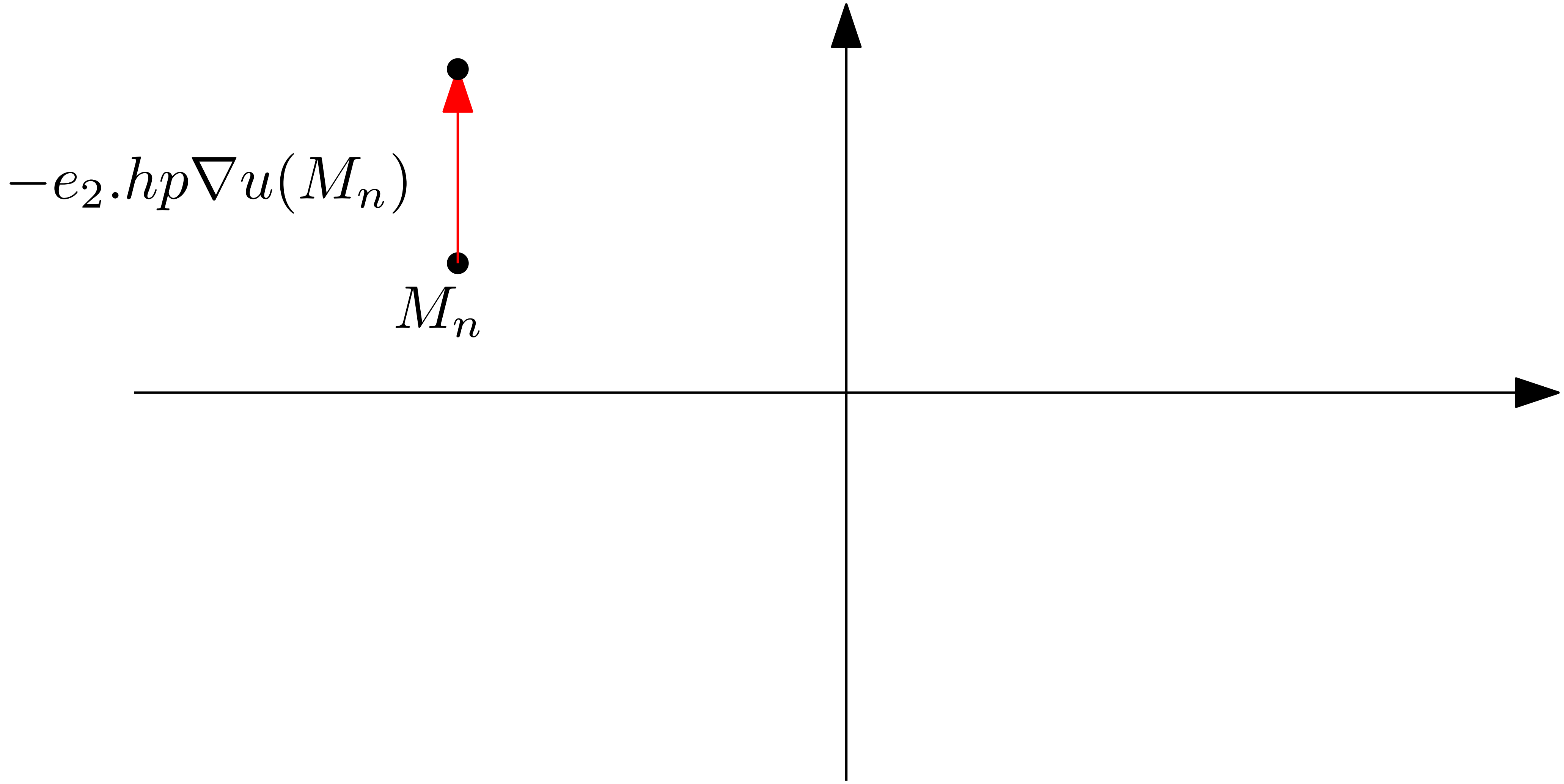

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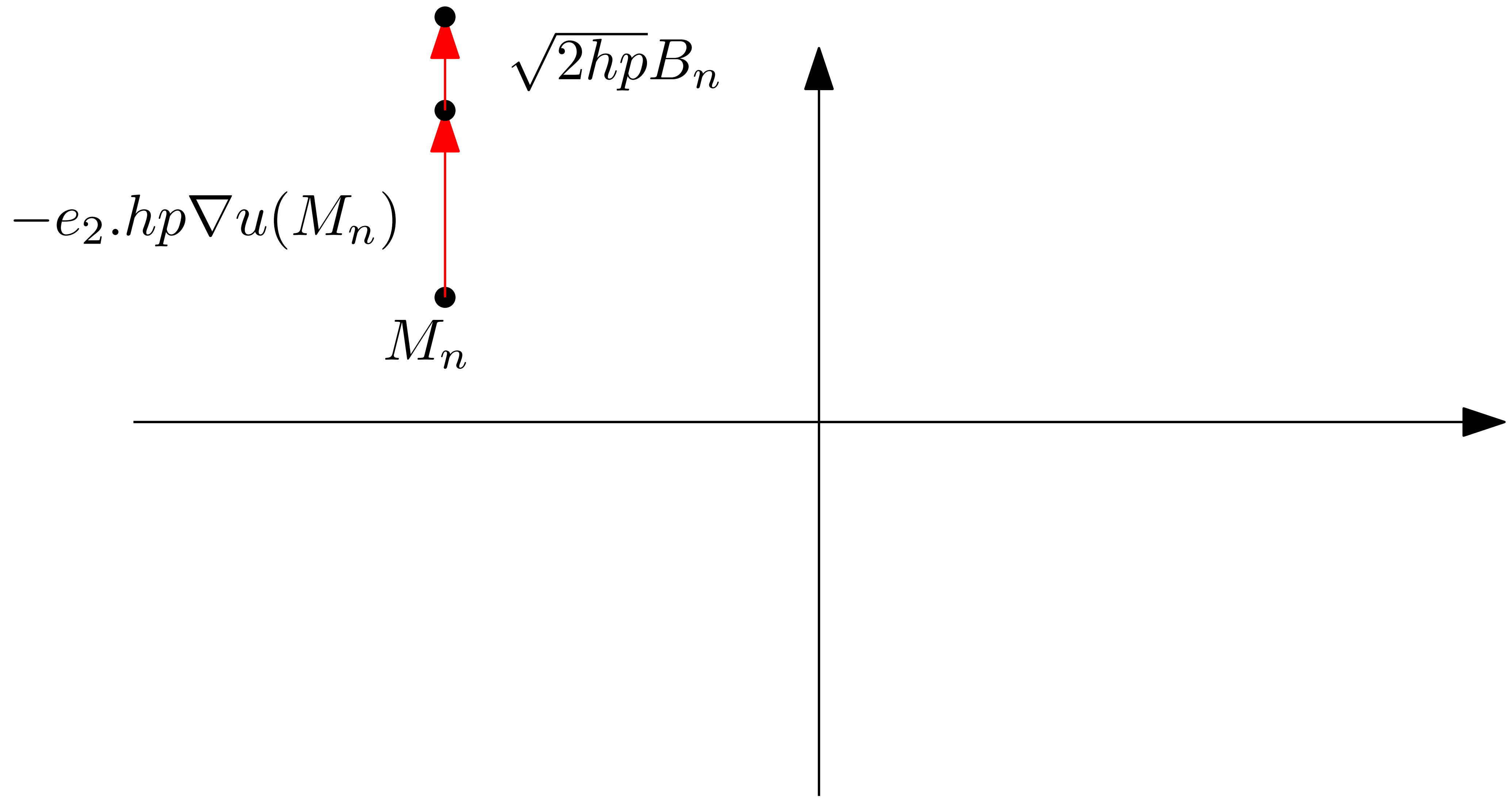

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Theorem Assume $h \leq \frac{\sqrt{\rho}}{\sqrt{p}L_1}$. Then, there exists a constant C such that

$$W_2(M^n,\mu) \leq (1-2h\rho+h^2L_1^2p)^{n/2}\frac{2hp}{2\rho h - pL_1^2h^2} + Ch^{1/2}p^{1+1/(4(i-2))}.$$

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$\Rightarrow$ needs no more than $O^*(\epsilon^{-2} p^{2+1/2(i-1)})$ (we conjecture $O^*(\epsilon^{-1} p^3)$) steps to reach an ϵ-accuracy. Still worse than Euler's Scheme.

Conclusion

- Linear rates (accuracy/dimension) for the LMC algorithm.
- Heuristic to choose h.
- Ozaki's discretization not interesting in higher dimension.
- Able to cope with general schemes.

- Sampling from a manifold.
- Dealing with measures on a convex set [Bubeck, Lehec, Eldan 2015].
- General schemes are not tight yet.
- Applications to Stochastic Gradient Descent.

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