A consensus-based global optimization method for high dimensional machine learning problems

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Motivations

The Model and algorithm

Numerical experiments

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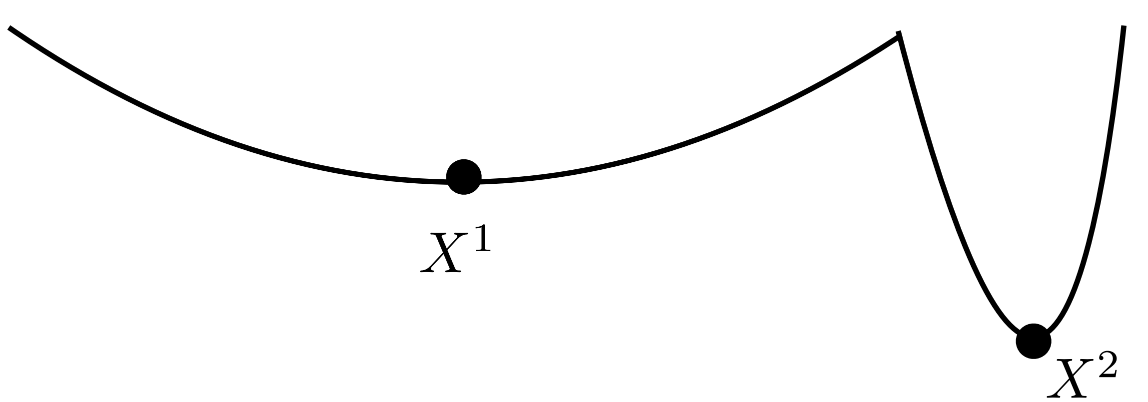
Numerical experiments

Goal: find $x^* = \text{argmin}_x \ L(x)$, $L(x)$ is a non-convex function.

For example: $L(x) = \frac{1}{n}\sum_i l_i(x)$

Why non-gradient method?

- Gradient is hard to calculate
- Objective function is non-smooth
- Flat local minimum



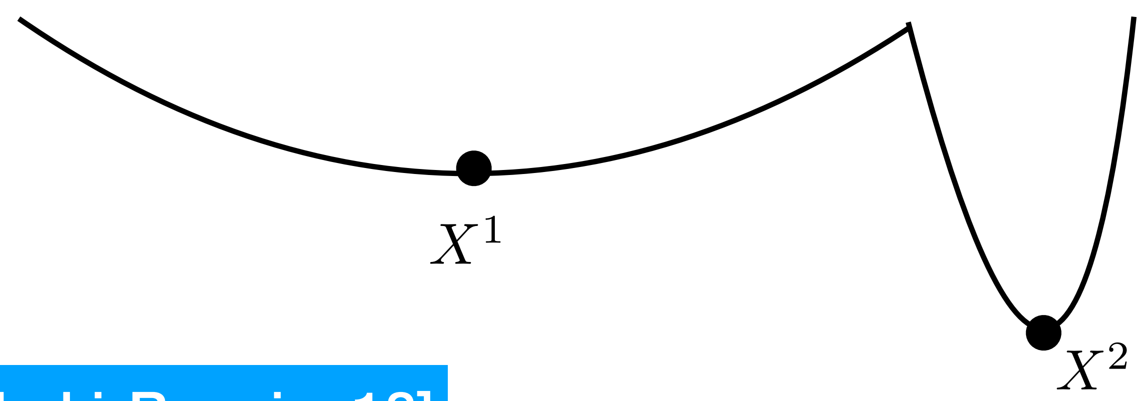
It is hard for gradient based method to escape from flat local minimum

$$\text{GD: } X'(t) = -\nabla L(X(t))$$

$$\text{SGD: } dX_t = -\nabla L(X_t) + \sqrt{\tfrac{1}{\beta}} dB_t$$

$$\text{p.d.f of SGD: } \partial_t p(t,x) = \nabla \cdot \left[\nabla L(x) p + \frac{2}{\beta} \nabla p \right]$$

$$p^{\infty}(x) = \tfrac{1}{Z} e^{-\frac{\beta}{2} L(x)}$$



[Z-Dai, 18], [Jastrzebski-Bengio, 18]

$$\frac{\mathbb{P}(\text{converge to } X^1)}{\mathbb{P}(\text{converge to } X^2)} = \sqrt{\frac{\det H_2}{\det H_1}} e^{\frac{\beta}{2}(L_2 - L_1)}$$

>1 **<1**

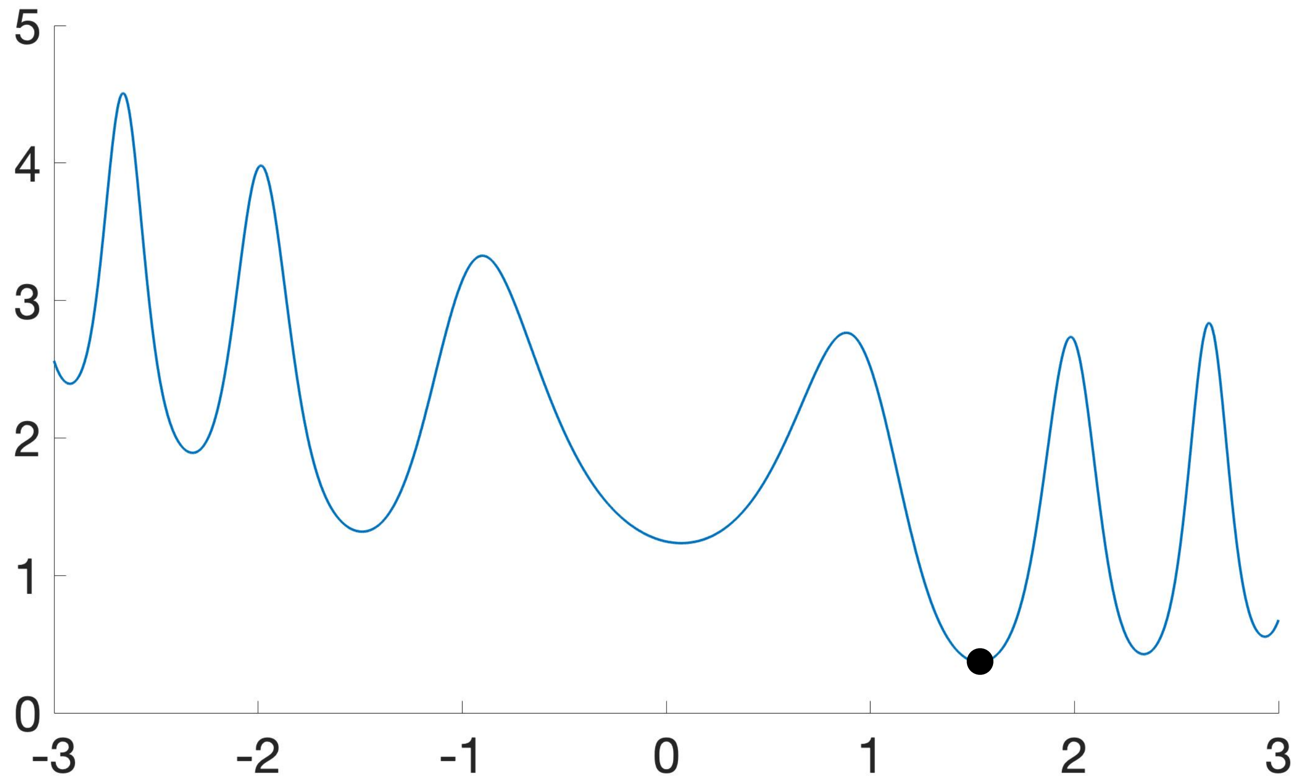
When $\dfrac{\sqrt{\det H_1}}{\sqrt{\det H_2}} < \dfrac{e^{\frac{\beta}{2} L_1}}{e^{\frac{\beta}{2} L_2}}$, SGD is more likely to converge to the flat local minimum.

It is hard for gradient based method to escape from flat local minimum

Example:

$$\ell(x, \hat{x}_i) = e^{\sin(2x^2)} + \frac{1}{10}(x - \hat{x}_i - \frac{\pi}{2})^2, \quad \hat{x}_i \sim N(0, 0.1)$$

$$L(x) = \frac{1}{n}\sum_i \ell(x, \hat{x}_i)$$



Success rate for SGD to find the correct global minimum is 18%

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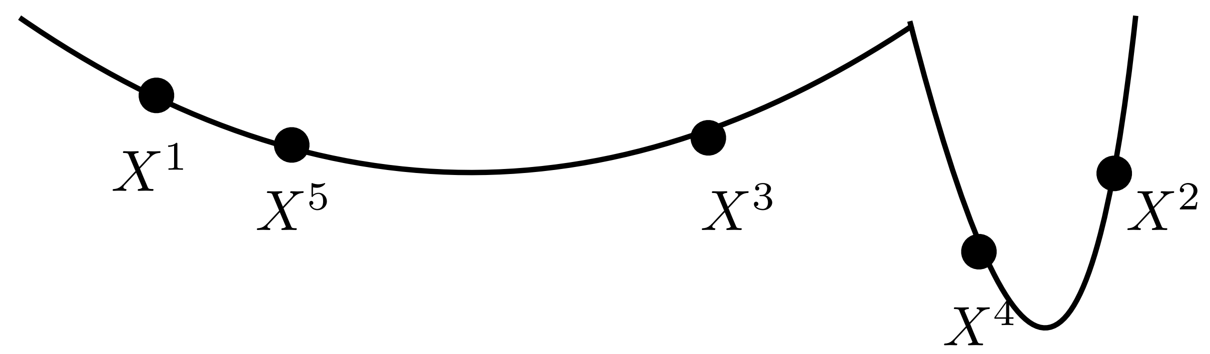
Related Work [Pinnau-Totzeck-Tse-Martin, 17]



For $j = 1, \cdots, N$

$$dX^j = -\lambda(X^j - \bar{x}^*)H^\epsilon(L(X^j) - L(\bar{x}^*))\,dt + \sigma|X^j - \bar{x}^*|dW^j$$

$$\text{where } \bar{x}^* = \frac{1}{\sum_{j=1}^N e^{-\beta L(X^j)}} \sum_{j=1}^N X^j e^{-\beta L(X^j)}.$$

Relax to their weighted average, in the meantime, explore their surrounding environment.

Require $\lambda \sim O(d)$ to guarantee the convergence of the method

Bad for high-dimensional problems

First improvement

$$dX^j = -\lambda(X^j - \bar{x}^*)\,dt + \boxed{\sigma \sum_{k=1}^{d} (X^j - \bar{x}^*)_k dW_k^j \vec{e}_k}$$

component-wise geometric Brownian motion

— Intuitively, now the diffusivity allows the particles to explore each dimension with different rate, so more possible to find the global minimum.

Previous model

Assume $x^* = a$ is a constant.

$$dX = -\lambda(X-a)\,dt + \sigma|X-a|dW^j$$

For each dimension i

$$d[(X)_i - (a)_i] = -\lambda[(X)_i - (a)_i]\,dt + \sigma|X-a|d(W^j)_i$$

By Ito's formula and then take expectation

$$d\mathbb{E}[(X)_i - (a)_i]^2 = -2\lambda\mathbb{E}[(X)_i - (a)_i]^2\,dt + \sigma^2\mathbb{E}|X-a|^2 dt$$

Sum over all dimension

$$\frac{d}{dt}\mathbb{E}|X-a|^2 = -2\lambda\mathbb{E}|X-a|^2 + \sigma^2\sum_{i=1}^{d}\mathbb{E}|X-a|^2 = \boxed{(-2\lambda+\sigma^2 d)\mathbb{E}|X-a|^2}.$$

$$\boxed{2\lambda > d\sigma^2}$$

[Carrillo-Choi-Totzeck-Tse, 18]

New model

$$dX = -\lambda(X-a)\,dt + \sigma\sum_{k=1}^{d}(X^j-a)_k dW_k^j\vec{e}_k$$

$$d[(X)_i - (a)_i] = -\lambda[(X)_i - (a)_i]\,dt + \sigma[(X)_i - (a)_i]d(W^j)_i$$

$$d\mathbb{E}[(X)_i - (a)_i]^2 = -2\lambda\mathbb{E}[(X)_i - (a)_i]^2\,dt + \sigma^2[(X)_i - (a)_i]^2 dt$$

$$\frac{d}{dt}\mathbb{E}|X-a|^2 = -2\lambda\mathbb{E}|X-a|^2 + \sigma^2\sum_{i=1}^{d}\mathbb{E}(X-a)_i^2 = \boxed{(-2\lambda+\sigma^2)\mathbb{E}|X-a|^2}.$$

$$\boxed{2\lambda > \sigma^2}$$

Mean field limit of the continuous model

$$dX^j = -\lambda(X^j - \bar{x}^*)\,dt + \sigma \sum_{k=1}^{d} (X^j - \bar{x}^*)_k dW_k^j \vec{e}_k$$

$$\Big\downarrow \; N \to \infty$$

$$dX = -\lambda(X - X^*)dt + \sigma \sum_{i=1}^{d} \vec{e}_i (X - X^*)_i dW_i$$

$$\text{with } X^* = \frac{\mathbb{E}(X e^{-\beta L(X)})}{\mathbb{E}(e^{-\beta L(X)})}.$$

Theorem: [Carrilo-Jin-Li-Z, 19]

Under some condition on the initial distribution of X and λ, σ, $X(t) \to \tilde{x}$ exponentially fast and,

$$L(\tilde{x}) \le -\frac{1}{\beta} \log \mathbb{E} e^{-\beta L(X(0))} + \frac{\log 2}{\beta} \le L(x^*) + O(\beta^{-1})$$

The initial law of X

The largeness of β

Numerical method

A gradient-free optimization method

$$\text{Goal: find } x^* = \text{argmin}_x \; L(x) = \text{argmin}_x \; \frac{1}{n}\sum_i l_i(x)$$

Algorithm [Carrillo-Jin-Li-Z-19]

Initially, randomly generate N particles X^j, at each step we randomly update M particles.

O(nN)

- Calculate $\boxed{\cancel{L(X^j)}}$, $\boxed{\cancel{j = 1, \cdots, N.}}$

O(N)

$$\hat{L}(X^j) = \frac{1}{m}\sum_{i\in b} l_i(x), \; b \subset \{1. \cdots, n\}.$$

O(n)

only for $j \in B \subset \{1, \cdots, N\}, |B| = M$

O(M)

O(m)

O(1)

- Find a weighted average: $\bar{X}^* = \frac{1}{\boxed{\sum_{j=1}^N} \mu^j} \boxed{\sum_{j=1}^N} X^j \mu^j, \quad \mu^j = e^{-\beta \boxed{\cancel{L(X^j)}}}$

- Let X^j move towards X^* and and explore their neighbor at the same time.

$$X^j \leftarrow X^j - \lambda\gamma(X^j - \bar{X}^*) + \sigma\sqrt{\gamma}\sum_{i=1}^d \vec{e}_i \left(X^j - \bar{X}^*\right)_i z_i, \quad z_i \sim \mathcal{N}(0,1)$$

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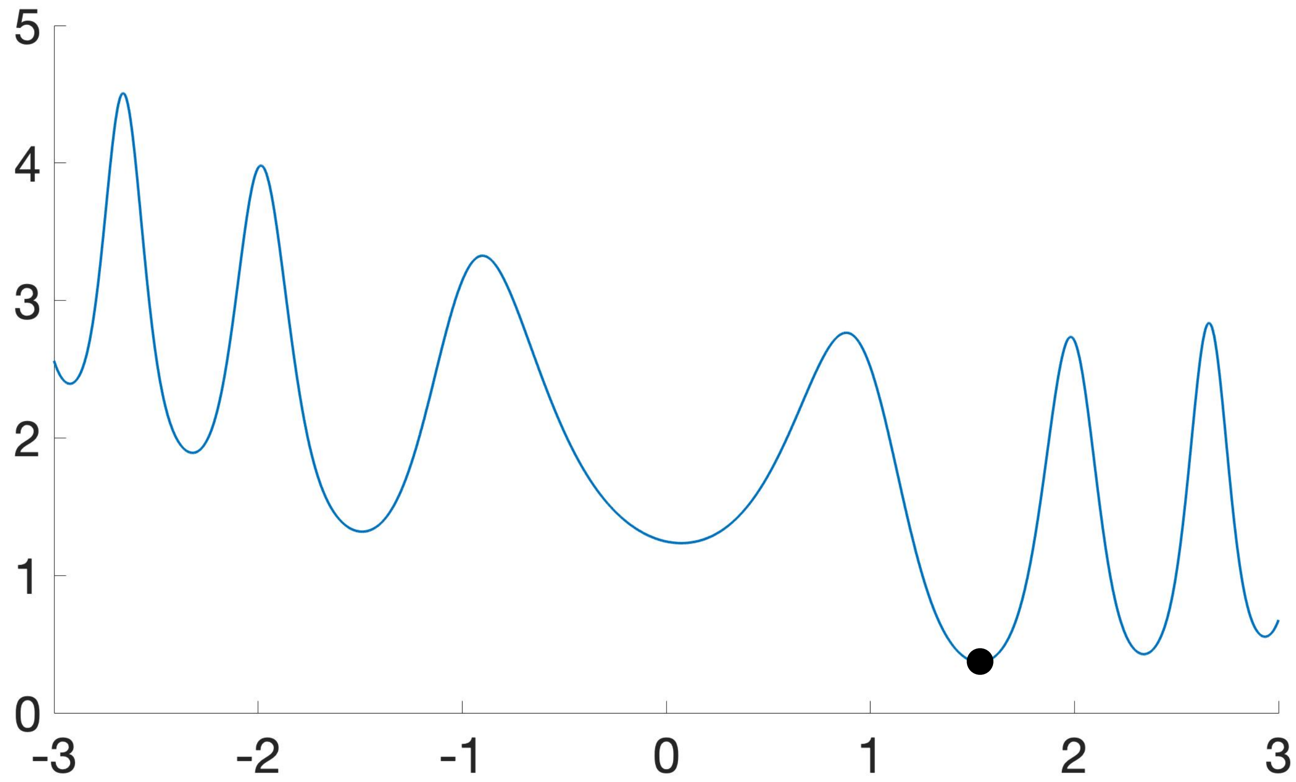
$$L(x) = \frac{1}{n}\sum_i \ell(x, \hat{x}_i)$$



Success rate of our method is 98%!
(with N = 100, M = 20)

$$L(x) = \frac{1}{d}\sum_{i=1}^{d}\left[(x_i - B)^2 - 10\cos\left(2\pi(x_i - B)\right) + 10\right] + C$$

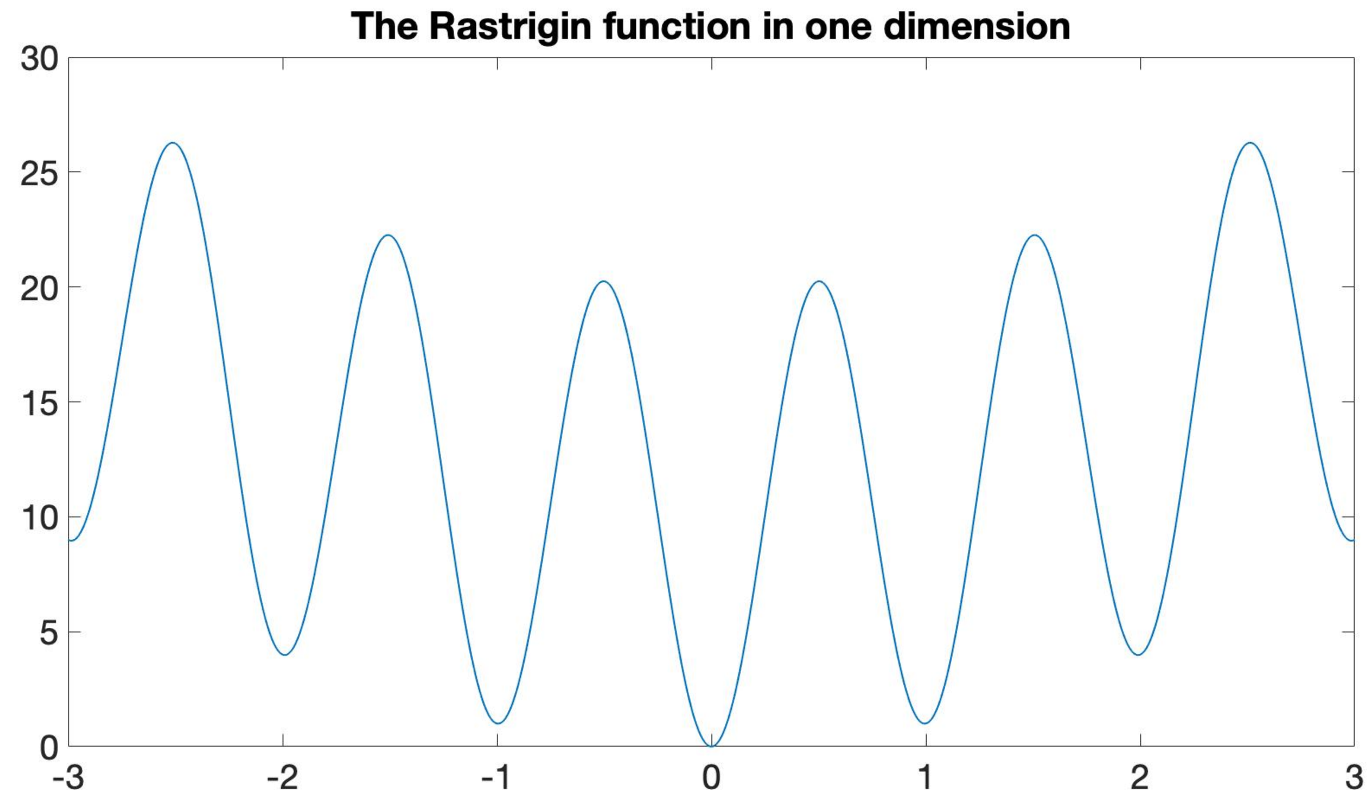


TABLE 2. Rastrigin function in $d = 20$ with $\alpha = 30$.

x_*		N 50	100	200
0	success rate	34.%	61.1%	62.2%
	$\frac{1}{d}\mathbb{E}[\|v_f(T) - x_*\|^2]$	$3.12e^{-1}$	$2.47e^{-1}$	$2.42e^{-1}$
1	success rate	34.5%	57.1%	61.6%
	$\frac{1}{d}\mathbb{E}[\|v_f(T) - x_*\|^2]$	$3.09e^{-1}$	$2.52e^{-1}$	$0.244e^{-1}$
2	success rate	35.5%	54.8%	62.4%
	$\frac{1}{d}\mathbb{E}[\|v_f(T) - x_*\|^2]$	$3.06e^{-1}$	$2.51e^{-1}$	$2.44e^{-1}$

[Pinnau-Totzeck-Tse-Martin, 17]

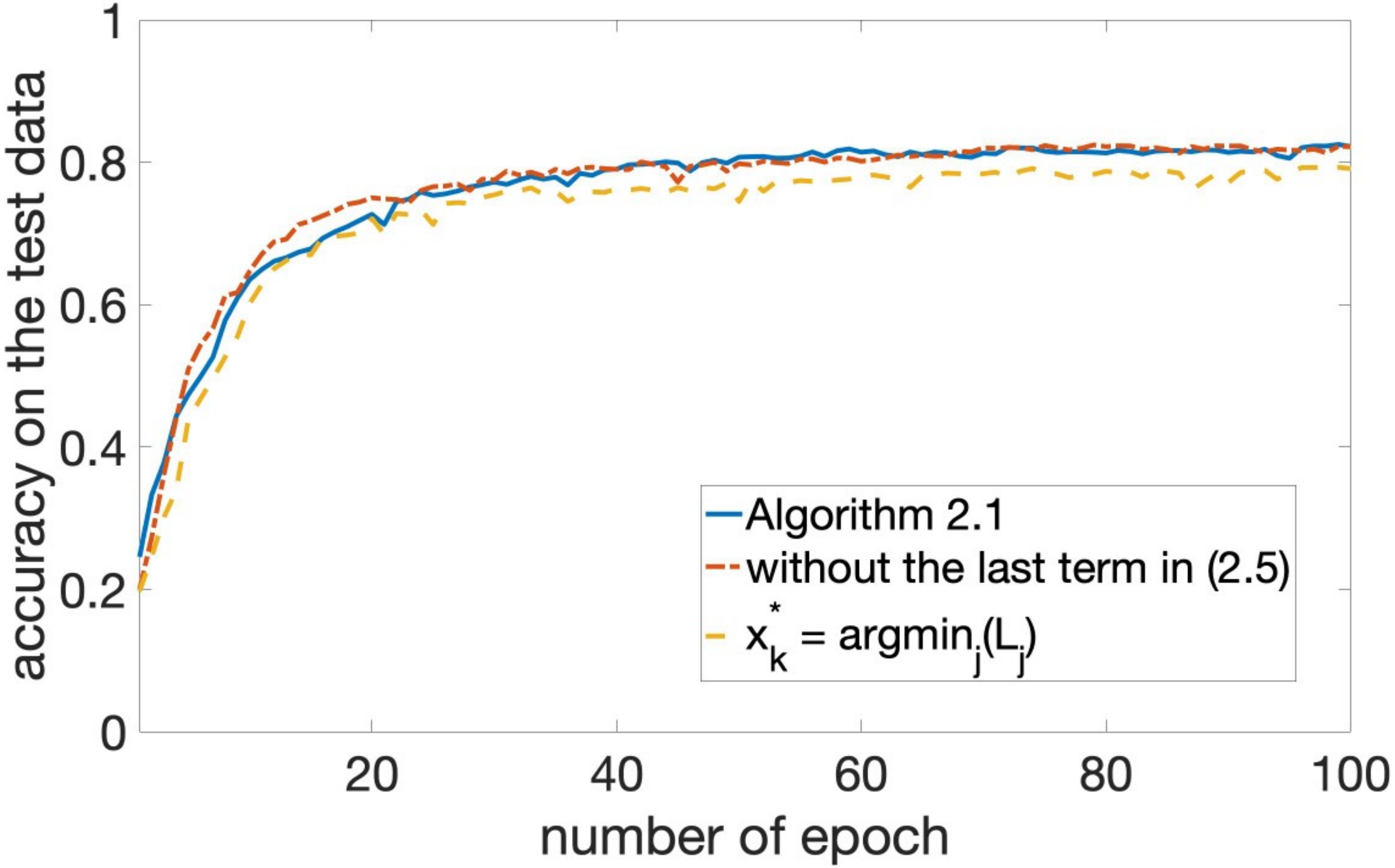
Rastrigin function in $d = 20$ with $\beta = 30$

	N = 50, M = 40 $\sigma = 5.1$	N = 100, M = 70 $\sigma = 5.1$	N = 200, M = 100 $\sigma = 5.1$
x* = 0, success rate	97%	99%	98%
x* = 0, $\frac{1}{d}\mathbb{E}\left[\|x_T^* - x^*\|^2\right]$	5.6E-03	5.03E-04	9.71E-04
x* = 1, success rate	94%	99%	95%
x* = 1, $\frac{1}{d}\mathbb{E}\left[\|x_T^* - x^*\|^2\right]$	3.9E-03	4.95E-04	3E-03
x* = 2, success rate	97%	100%	92%
x* = 2, $\frac{1}{d}\mathbb{E}\left[\|x_T^* - x^*\|^2\right]$	3.0E-03	8.06E-06	4E-03
Computing time saved	22.03%	30.11%	36.14%

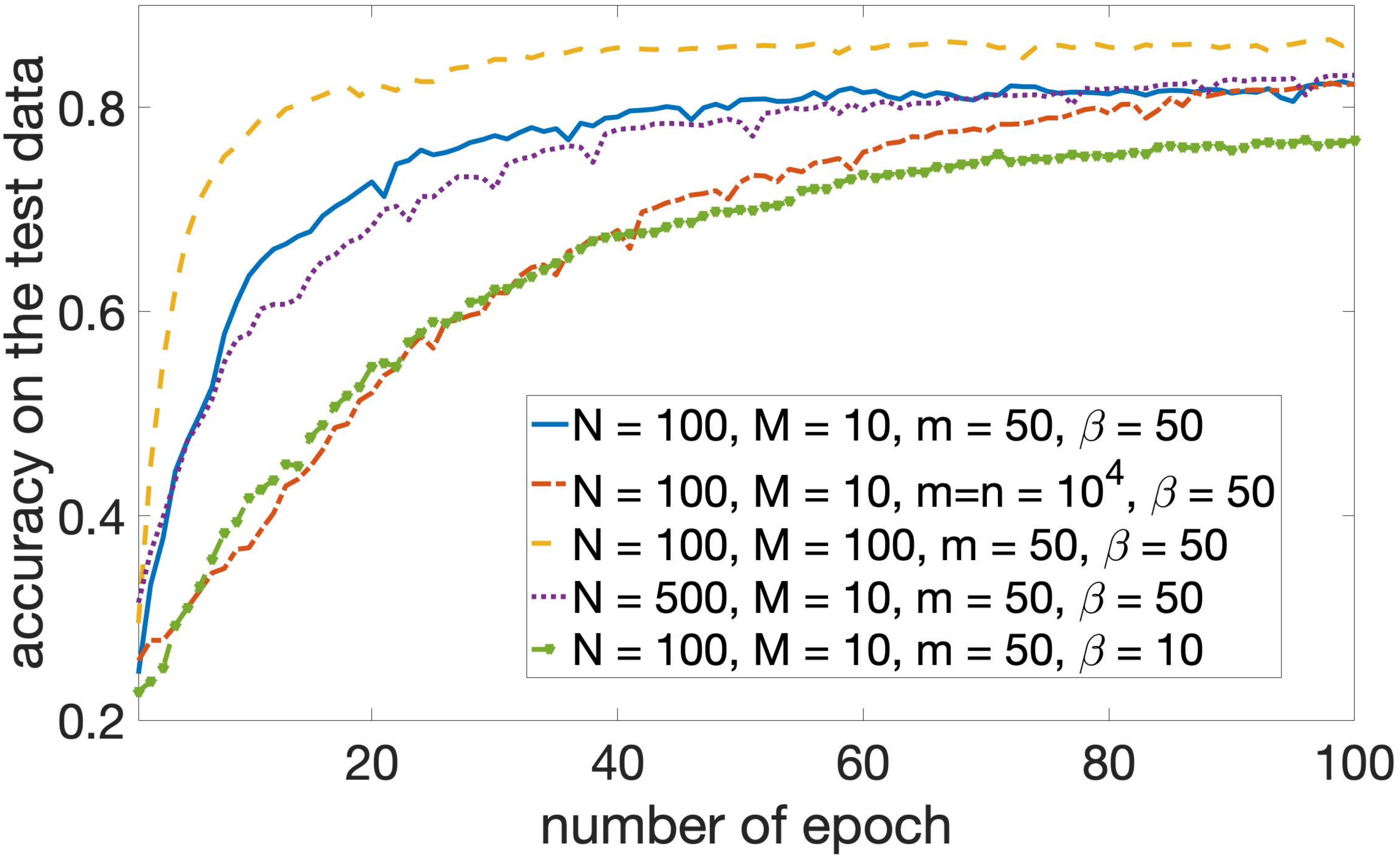
Learning MNIST data with two layer Neural Network

$$X \in \mathbb{R}^{7290}$$

$$\text{Only using } N = 100, M = 10$$



How parameters affect the performance



Future Directions

- Ongoing work: Constrained optimization problem
- How to choose all the parameters?
- Theory for the numerical method.

Thanks!