Exact asymptotics and universality for gradient flows and other first order algorithms

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January 25, 2022



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Chen Cheng



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# Toy problem

Find  $\boldsymbol{\theta} \in \mathbb{R}^d$ , such that  $\|\boldsymbol{\theta}\|_2 = 1$ , and

$$egin{pmatrix} \langle x_1, oldsymbol{ heta} 
angle \geq \kappa\,, \ dots \ \langle x_n, oldsymbol{ heta} 
angle \geq \kappa\,. \end{aligned}$$

 $(\kappa < 0)$ 

# Toy problem ('Negative perceptron')



$$egin{aligned} &(x_i)_{i\leq n}\sim \mathsf{N}(0,oldsymbol{I}_d)\,, \ &\mathcal{E}_{n,d}(\kappa):=\left\{oldsymbol{ heta}\in\mathbb{S}^{d-1}:\langle x_i,oldsymbol{ heta}
ight\}\geq\kappa\;\;orall i\leq n
ight\}. \end{aligned}$$

Franz, Parisi 2016 (Physics); El Alaoui, Sellke, 2020; Baldi, Vershynin, 2021 (Math)

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ight\}\geq \kappa \ orall i\leq n
ight\}. \end{aligned}$$

Questions

- ▶ is  $\mathcal{E}_{n,d}(\kappa)$  non-empty?
- ▶ What is its geometry?
- ▶ Can we find  $\theta \in \mathcal{E}_{n,d}(\kappa)$  in polynomial time?

## Gradient flow

$$egin{cases} ext{find} & heta \in \mathbb{S}^{d-1} \,, \ ext{such that} & \langle oldsymbol{x}_i, oldsymbol{ heta} 
angle \geq \kappa \;\; orall i \leq n \ \end{cases}$$

$$egin{aligned} \dot{oldsymbol{ heta}}^t &= \sum_{i=1}^n 
hoig(\langle x_i, oldsymbol{ heta}^t 
angle - \kappa \|oldsymbol{ heta}^t\|_2ig) \left(x_i - \kappa oldsymbol{ heta}^tig) \ , \ \hat{oldsymbol{ heta}}^t &= rac{oldsymbol{ heta}^t}{\|oldsymbol{ heta}^t\|_2} \,, \quad 
ho(x) := rac{1}{1+e^x} \,. \end{aligned}$$

$$\text{If } \boldsymbol{\theta}^t \to \infty \text{, then } \boldsymbol{\hat{\theta}}^t \to \mathcal{E}_{n,d}(\kappa).$$

An experiment ( $\kappa = -3$ )



## ... and a theorem



Theorem (Zhong, Zhou, M, 2021) Assume  $n, d \to \infty$  with  $n, d \to \infty$  and define  $\delta_{s}(\kappa)$  via

$$\delta < \delta_{ ext{s}}(\kappa) \hspace{2mm} \Leftrightarrow \hspace{2mm} \liminf_{n o \infty} \mathbb{P}_{n,n/\delta}ig(\mathcal{E}_{n,d}(\kappa) 
eq \emptysetig) > 0$$

Then

$$\begin{array}{l} \bullet \ \ \delta_{\mathrm{l}}(\kappa) \leq \delta_{\mathrm{s}}(\kappa) \leq \delta_{\mathrm{u}}(\kappa), \ with \ \ \delta_{\mathrm{l}}(\kappa), \delta_{\mathrm{u}}(\kappa) = \Phi(\kappa)^{-1} \log |\kappa|(1+o_{\kappa}(1)). \\ \\ \bullet \ \ Linear \ \ prog. \ \ succeeds \ \ whp \ \ if \ \ \delta < \delta_{\mathrm{lin}}(\kappa) = \Phi(\kappa)^{-1}(1+o_{\kappa}(1)). \end{array}$$

# Questions



Does gradient flow have a sharp threshold δ<sub>GF</sub>(κ)?
 Is δ<sub>GF</sub>(κ) < δ<sub>s</sub>(κ)?

# More ambitious (2-layer neural nets)

$$x_i \sim N(0, I_d), \ y_i \sim Unif(\{+1, -1\}), \ a_\ell \in \{+1, -1\}:$$

$$egin{cases} & ext{find} & heta_1,\ldots, heta_k\in\mathbb{S}^{d-1}\,, \ & ext{such that} & y_i\sum_{\ell=1}^k a_\ell\sigma(\langle heta_\ell,x_i
angle)\geq\kappa \ \ orall i\leq n \end{cases}$$

- What is the interpolation threshold  $\delta_s(k, \kappa)$ ?
- ▶ Does gradient flow have a sharp threshold  $\delta_{GF}(k, \kappa)$ ?
- $\blacktriangleright \ \text{Is} \ \delta_{\rm GF}(k,\kappa) < \delta_{\rm s}(k,\kappa)?$

...

Franz, Hwang, Urbani,2019

### General first order flows

#### Data



Variable:  $\boldsymbol{\theta} \in \mathbb{R}^{d \times k}$ 

Flow

$$rac{\mathrm{d}oldsymbol{ heta}^t}{\mathrm{d}t} = -oldsymbol{ heta}^t \Lambda^t - oldsymbol{X}^{\mathsf{T}}oldsymbol{\ell}_t(oldsymbol{X}oldsymbol{ heta}^t;oldsymbol{y}),$$

Data

$$oldsymbol{X} = \left[egin{array}{cccc} \cdots & x_1^{\mathsf{T}} & \cdots & \ \cdots & x_2^{\mathsf{T}} & \cdots & \ dots & dots & dots & \ \dots &$$

Variable:  $\boldsymbol{\theta} \in \mathbb{R}^{d \times k}$ 

Flow

$$rac{\mathrm{d} oldsymbol{ heta}^t}{\mathrm{d} t} = - oldsymbol{ heta}^t \Lambda^t - X^{\mathsf{T}} oldsymbol{\ell}_t(X oldsymbol{ heta}^t;y) \, ,$$

•

Data

$$oldsymbol{X} = \left[egin{array}{cccc} \cdots & x_1^{ op} & \cdots & \ \cdots & x_2^{ op} & \cdots & \ dots & dots & \ \dots & \ \$$

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More general than gradient flow!Could add white noise term.

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- Could add white noise term.

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 .

#### Example #1: Negative perceptron

$$\dot{oldsymbol{ heta}}^t = \sum_{i=1}^n \left( oldsymbol{x}_i - \kappa \hat{oldsymbol{ heta}}^t 
ight) 
ho(\langle oldsymbol{x}_i, oldsymbol{ heta}^t 
angle - \kappa \|oldsymbol{ heta}^t\|_2)\,, \qquad \hat{oldsymbol{ heta}}^t := rac{oldsymbol{ heta}^t}{\|oldsymbol{ heta}^t\|_2}\,,$$

 $\dot{oldsymbol{ heta}}^t = oldsymbol{X}^{\mathsf{T}} 
ho(oldsymbol{X}oldsymbol{ heta}^t - u_t oldsymbol{1}) - \lambda_t oldsymbol{ heta}_t \,, \ u_t, \lambda_t \in \mathbb{R} \quad ext{concentrate.}$ 

$$rac{\mathrm{d}oldsymbol{ heta}^t}{\mathrm{d}t} = -oldsymbol{ heta}^t \Lambda^t - oldsymbol{X}^{\mathsf{T}}oldsymbol{\ell}_t(oldsymbol{X}oldsymbol{ heta}^t;oldsymbol{y})$$
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Example #2: 2-layer neural network

$$\dot{oldsymbol{ heta}}_j^t = -\lambda_t oldsymbol{ heta}_j^t - 
abla_{oldsymbol{ heta}_j} \widehat{R}_n(oldsymbol{ heta}^t) \qquad j \leq k \ \widehat{R}_n(oldsymbol{ heta}^t) = rac{1}{n} \sum_{i=1}^n ig(y_i - \sum_{j \leq k} a_j \sigma(oldsymbol{ heta}_j^t)ig)^2.$$

## General First Order Flows: Assumptions

$$rac{\mathrm{d}oldsymbol{ heta}^t}{\mathrm{d}t} = -oldsymbol{ heta}^t \Lambda^t - oldsymbol{X}^{\mathsf{T}}oldsymbol{\ell}_t(oldsymbol{X}oldsymbol{ heta}^t;oldsymbol{y})\,.$$

$$\blacktriangleright \ n, d \to \infty, \ n/d \to \delta, \ k \ \text{fixed}, \ t = O(1)$$

- ▶  ${X_{ij}}$  iid  $\mathbb{E}{X_{ij}} = 0$ ,  $\mathbb{E}{X_{ij}^2} = 1/d$ , subgaussian.
- $\triangleright$   $\ell$  differentiable, with bounded Lipschitz Jacobian.
- $\blacktriangleright \ y_i = f(\boldsymbol{\theta}_*^{\mathsf{T}} \boldsymbol{x}_i; \boldsymbol{z}_i), \, \boldsymbol{\theta}_* \in \mathbb{R}^{d \times k_0}, \, \boldsymbol{z}_i \text{ independent of } \boldsymbol{x}_i.$
- Empirical distribution of rows of  $\theta^0$ ,  $\theta_*$  converges.

## Our approach

Discretize time (first order methods)

Reduction to Approximate Message Passing<sup>1</sup>
 (AMP)

- S Apply existing asymptotic characterizations of AMP<sup>2</sup>
- 4 Take the continuous time limit.

<sup>&</sup>lt;sup>1</sup>Celentano, M, Wu, 2021 <sup>2</sup>Bayati, M, 2011; Chen, Lam, 2021

## Our approach

- I Discretize time (first order methods)
- Reduction to Approximate Message Passing<sup>3</sup> (AMP)
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- Take the continuous time limit.

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## Time discretization

$$rac{\mathrm{d}oldsymbol{ heta}^t}{\mathrm{d}t} = -oldsymbol{ heta}^t \Lambda^t - oldsymbol{X}^{\mathsf{T}}oldsymbol{\ell}_t(oldsymbol{X}oldsymbol{ heta}^t;oldsymbol{y}).$$

Euler scheme

$$oldsymbol{ heta}_arepsilon^{t+arepsilon} = oldsymbol{ heta}_arepsilon^t - arepsilon oldsymbol{X}^{\mathsf{T}} oldsymbol{\ell}_t(oldsymbol{X}oldsymbol{ heta}_arepsilon^t;oldsymbol{y}).$$

Claim

$$\lim_{\varepsilon \to 0} \limsup_{n, d \to \infty} \sup_{t \leq T} \frac{1}{n} \| \boldsymbol{\theta}^t - \boldsymbol{\theta}_{\varepsilon}^t \|_2^2 = 0$$

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$$oldsymbol{ heta}_{arepsilon}^{t+arepsilon} = oldsymbol{ heta}_{arepsilon}^t - arepsilon oldsymbol{X}^{ oldsymbol{ heta}} oldsymbol{ heta}_{arepsilon}^t; oldsymbol{y} oldsymbol{ heta}_{arepsilon}^t; oldsymbol{ heta}_{arepsilon}^t; oldsymbol{y} oldsymbol{ heta}_{arepsilon}^t; oldsymbol{y} oldsymbol{ heta}_{arepsilon}^t; oldsymbol{y} oldsymbol{ heta}_{arepsilon}^t; oldsymbol{ heta}_{ar$$

#### Will drop y hereafter

## General First Order Methods

$$egin{aligned} & u^{t+1} = X f_t(v^1, \dots, v^t)\,, \ & v^t = X^{\mathsf{T}} g_t(u^1, \dots, u^t)\,, \ & \hat{ heta}^t = h_t(u^1, \dots, u^t)\,. \end{aligned}$$

$$\blacktriangleright \quad u^t \in \mathbb{R}^{d \times k}, \ v^t \in \mathbb{R}^{n \times k}.$$

- Each iteration multiplication by X or  $X^{\mathsf{T}}$ .
- $f_t, g_t, h_t$  Lipschitz, act entry-wise<sup>5</sup>.

Claim:

Euler scheme is a GFOM.

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# Approximate Message Passing (AMP)

$$egin{aligned} & u^{t+1} = X\psi_t(v^1,\ldots,v^t) - \sum\limits_{s=1}^t \phi_s(u^1,\ldots,u^s)\cdot a_{t,s}\,, \ & v^t = X^\mathsf{T}\phi_t(u^1,\ldots,u^t) - \sum\limits_{s=1}^{t-1}\psi_s(v^1,\ldots,v^s)\cdot b_{t,s}\,, \ & \hat{ heta}^t = artheta_t(u^1,\ldots,u^t)\,. \end{aligned}$$

• 
$$\psi_t, \phi_t, \vartheta_t$$
 Lipschitz, act entry-wise<sup>6</sup>.

- ▶  $a_{t,s}, b_{t,s} \in \mathbb{R}^{k \times k}$  deterministic, with explicit formulas.
- Key property (state evolution)

$$rac{1}{d}\sum_{i=1}^d \delta_{u^1_i,...u^t_i} \Rightarrow {\sf N}(0, {m \Sigma}_{\leq t})\,, \quad + ext{recursion for } {m \Sigma}\,.$$

<sup>6</sup>More general assumptions, see Berthier, M, Nguyen 2018; M, Wu, 2022

# Approximate Message Passing (AMP)

$$egin{aligned} & u^{t+1} = oldsymbol{X} \psi_t(v^1,\ldots,v^t) - \sum\limits_{s=1}^t \phi_s(u^1,\ldots,u^s) \cdot a_{t,s}\,, \ & v^t = oldsymbol{X}^ op \phi_t(u^1,\ldots,u^t) - \sum\limits_{s=1}^{t-1} \psi_s(v^1,\ldots,v^s) \cdot b_{t,s}\,, \ & \hat{oldsymbol{ heta}}^t = artheta_t(u^1,\ldots,u^t)\,. \end{aligned}$$

#### Remarks

- Any AMP algorithm is a GFOM
- ► Any GFOM is equivalent to an AMP algorithm<sup>7</sup> (With suitable post-processing ϑ<sub>t</sub>)

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### DMFT asymptotics

## Dynamical Mean Field Theory

$$rac{\mathrm{d}oldsymbol{ heta}^t}{\mathrm{d}t} = -oldsymbol{ heta}^t \Lambda^t - oldsymbol{X}^{\mathsf{T}}oldsymbol{\ell}_t(oldsymbol{X}oldsymbol{ heta}^t;oldsymbol{y}).$$

General form: As  $n, d \to \infty$ ,

$$( heta_i^t)_{t\leq T} \Rightarrow ( heta^t)_{t\leq T}$$

where  $(\theta^t)_{t < T}$  is a diffusion process with memory.

Dynamical Mean Field Theory: History

Physics

▶ ...

Sompolinskiy, Zippelius, 1981

(SK model)

 Crisanti, Horner, Sommers, 1993; Cugliandolo, Kurchan, 1993 (spherical spin glass)

#### Mathematics

Ben Arous and Guionnet, 1995

(SK model)

- Ben Arous, Dembo, Guionnet 2006
- ... (Gaussian disorder)

(spherical spin glass)

# Dynamical Mean Field Theory: Recent work

### (Heuristic) Applications in high-dimensional statistics

Agoritsas et al., 2018 (Perceptrons)
Mannelli et al. 2020 (Tensor PCA)
Mignacco et al. 2020 (Gaussian mixtures)
...

### Universality

- Dembo, Lubetzky, Zeitouni, 2019
- Dembo, Gheissari, 2021

(Asymmetric interactions)

(Interacting diffusions)

Present work yields universality

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## DMFT process

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**DMFT** process  $(\theta^t, r^t \in \mathbb{R}^k)$ 

$$egin{aligned} &rac{\mathrm{d}}{\mathrm{d}t} heta^t = -(\Lambda^t+\Gamma^t) heta^t - \int_0^t R_\ell(t,s) heta^s\mathrm{d}s + u^t\,, \quad u\sim \mathsf{GP}(0,\,C_\ell/\delta)\,, \ &r^t = -rac{1}{\delta}\int_0^t R_ heta(t,s)\ell_s(r^s)\mathrm{d}s + w^t\,, \qquad w\sim \mathsf{GP}(0,\,C_ heta)\,. \end{aligned}$$

DMFT: Fixed point conditions DMFT process  $(\theta^t, r^t \in \mathbb{R}^k)$ 

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Fixed point equations

$$egin{aligned} C_ heta(t,s) &= \mathbb{E}\left[ heta^t heta^{s\,\mathsf{T}}
ight], & R_ heta(t,s) \ C_\ell(t,s) &= \mathbb{E}\left[\ell_t(r^t)\ell_s(r^t)^\mathsf{T}
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## DMFT: Fixed point conditions

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abla_r\ell_t(r^t;z)
ight]\,. \end{aligned}$$

 $(C_ heta,R_ heta)=\mathcal{T}(C_\ell,R_\ell,\Gamma)\,,\quad (C_\ell,R_\ell,\Gamma)=\hat{\mathcal{T}}(C_ heta,R_ heta)$ 

## 1st theorem: Existence and uniqueness

#### Theorem (Celentano, Chen, M, 2021)

- The solution  $(C_{\theta}, R_{\theta}, C_{\ell}, R_{\ell}, \Gamma)$  of the fixed point conditions exists.
- It is unique among all tuples such that (C<sub>θ</sub>, R<sub>θ</sub>) are bounded in all compact sets in ℝ<sup>2</sup><sub>≥0</sub>.
- ► The DMFT processes  $(\theta^t)_{t\geq 0}$ ,  $(r^t)_{t\geq 0}$  are well defined with continuous sample paths.
- The map  $\mathcal{T} \circ \hat{\mathcal{T}}$  is a contraction.

## 2nd theorem: Convergence as $n, d ightarrow \infty$

### Theorem (Celentano, Chen, M, 2021)

Let  $d_W$  metrize weak convergence in  $C([0, T], \mathbb{R}^k)$ , and define  $r^t := X \theta^t \in \mathbb{R}^{n \times k}$ . Let  $P_{\theta_0^T}$ ,  $P_{r_0^T}$  be the laws of the DMFT processes. Then, we have

$$egin{aligned} & \operatorname{p-lim}_{n,d o\infty} \, d_{\mathrm{W}}\Big(rac{1}{d}\sum_{i=1}^d \delta_{( heta_i)_0^T}, \mathrm{P}_{ heta_0^T}\Big) = 0\,, \ & \operatorname{p-lim}_{n,d o\infty} \, d_{\mathrm{W}}\Big(rac{1}{n}\sum_{i=1}^n \delta_{(r_i)_0^T}, \mathrm{P}_{r_0^T}\Big) = 0\,. \end{aligned}$$

Convergence as  $n, d 
ightarrow \infty$ 

### Corollary

For any m, any  $\psi : \mathbb{R}^m \to \mathbb{R}$  bounded continuous, and any  $0 \le t_1 \le t_2 \le \cdots \le t_m$ , we have

$$\mathop{ ext{p-lim}}_{n,d o\infty}rac{1}{d}\sum_{i=1}^d\psi( heta_i^{t_1},\ldots, heta_i^{t_m})=\mathbb{E}\{\psi( heta^{t_1},\ldots, heta^{t_m})\}$$



### Epilogue: Statistically optimal methods

## Reduction

#### General First Order Methods $\longrightarrow$ Approximate Message Passing

#### Q: Can we determine the optimal GFOM?

Data

 $y_i = arphi(\langle {m x}_i, {m heta}_* 
angle, z_i), \quad {m x}_i \sim {\sf N}({\sf 0}, {m I}_d/d) \perp z_i \sim {\sf Unif}([{\sf 0}, 1]).$ 

General GFOM

$$egin{aligned} & u^{t+1} = X f_t(v^1, \dots, v^t)\,, \ & v^t = X^{ op} g_t(u^1, \dots, u^t)\,, \ & \hat{ heta}^t = h_t(u^1, \dots, u^t)\,. \end{aligned}$$

$$\lim_{n,d o\infty}rac{1}{d} \inf_{\{f_s,g_s,h_s\}\in\mathscr{F}}\mathbb{E}\{\|\hat{oldsymbol{ heta}}^t-oldsymbol{ heta}_*\|_2^2\}=???$$

Data

$$y_i = arphi(\langle x_i, oldsymbol{ heta}_* 
angle, z_i), \quad x_i \sim \mathsf{N}(\mathsf{0}, oldsymbol{I}_d/d) \perp z_i \sim \mathsf{Unif}([\mathsf{0}, \mathsf{1}]).$$

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 $\mathscr{F} :=$  separable Lipschitz functions

## Example: Noiseless phase retrieval

$$y_i = \langle x_i, oldsymbol{ heta}_* 
angle^2$$

Spectral initialization<sup>8</sup>

$$egin{aligned} oldsymbol{D}_n &:= \sum_{i=1}^n \mathcal{T}(y_i) x_i x_i^\mathsf{T}, \quad \mathcal{T}(y) = rac{y-1}{y+arepsilon}\,, \ oldsymbol{ heta}^0 &= c_{d,n} \cdot v_1(oldsymbol{D}_n)\,. \end{aligned}$$

<sup>8</sup>Mondelli, Montanari, 2018

# First order methods in phase retrieval

- Schniter, Rangan 2014
- Candés, Li, Soltanolkotabi, 2015
- Cai, Li, Ma, 2016
- ▶ Wang, Giannakis, Eldar, 2017
- Chen, Candés 2018
- Waldspurger, 2018
- Duchi, Ruan, 2019

▶ ...

- Maillard, Loureiro, Krzakala, Zdeborová, 2020
- Mondelli Venkatramanan, 2021
- Review: Fannjiang and Strohmer, 2020

## Experiment with a real image: d = 7560



Original image.



# A simulation: Reconstruction accuracy d = 400





- Truncated Amplitude Flow
- Prox-linear<sup>9</sup>
- Gradient descent.
- Bayes-optimal AMP.

<sup>9</sup>Not a GFOM.

(Wang, Giannakis, Eldar, 2017) (Duchi, Ruan, 2019)

## Minimal error

$$\blacktriangleright \ y = \varphi(X\theta_*,z)$$

- ▶ Side information v,  $d^{-1} \sum_{i \leq d} \delta_{\theta_{*,i},v_i} \Rightarrow P_{\Theta,V}$
- ►  $n, d \to \infty, n/d \to \delta$  { $X_{ij}$ } bounded 4-th moment.

Define

$$\mathsf{mmse}_{\Theta,\,V}(\pmb{lpha}) := \mathbb{E}[\Theta^2] - \mathbb{E}\{\mathbb{E}[\Theta \mid \pmb{lpha}\Theta + Z,\,V]^2\}.$$

and recursively:

$$egin{aligned} eta_s^2 &= rac{1}{\sigma_s^2} \mathbb{E}[\mathbb{E}[Z_0 \mid arphi(\sigma_s Z_0 + ilde{\sigma}_s Z_1, W), U, Z_1]^2], \qquad eta_s \geq 0, \ \sigma_{s+1}^2 &= rac{1}{\delta} \mathsf{mmse}_{\Theta, \, V}(eta_s), \qquad ilde{\sigma}_{s+1}^2 = rac{1}{\delta}(\mathbb{E}[\Theta^2] - \mathsf{mmse}_{\Theta, \, V}(eta_s)). \end{aligned}$$

# Minimal error

Theorem (Celentano, M, Wu, 2020; M, Wu, 2022)

For  $t \in NN_{>0}$ , let  $\hat{\theta}^t \in \mathbb{R}^d$  be the output of any GFOM after t iterations, the following holds:

$$ext{p-lim}_{n,d o\infty} rac{1}{d} \| \hat{oldsymbol{ heta}}^t - oldsymbol{ heta}_* \|_2^2 \geq \mathsf{mmse}_{\Theta,V}(oldsymbol{eta}_t).$$

Further, there exists a GFOM (Bayes AMP) which satisfies the above bound with equality.

### Conclusion

## Conclusion

First order methods comprise the most used algorithms in ML

- ▶ GFOMs as a useful abstraction/class.
- ▶ Reduction GFOM  $\rightarrow$  AMP
- ▶ Need to understand their behavior in high-dim/low SNR.
- New rigorous tool: DMFT (other avaiilable!)

### Thanks!

1