Beyond i.i.d. Gaussian Models : Exact Asymptotics with Realistic Data

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Stat. Phys./High-Dimensional Approach

- typical case
- benchmark, random design problems
- exact solutions
- strong assumptions

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- benchmark, random design problems
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How realistic are the stat. phys. benchmarks ?
What can we do to make them more realistic ?

Teacher Student Generalized Linear Model

Observe "*teacher*" generative model

$$\boldsymbol{y} = f_0(\boldsymbol{X}\boldsymbol{w}_0) \in \mathbb{R}^n, \quad \boldsymbol{w}_0 \in \mathbb{R}^d \quad \boldsymbol{X} \in \mathbb{R}^{n\times d} \text{ i.i.d. } \mathcal{N}(0,1)$$

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Learn with "*student*"

$$\boldsymbol{w}^\star \in \underset{\boldsymbol{w} \in \mathbb{R}^d}{\operatorname{argmin}} \, L\left(\boldsymbol{y}, \boldsymbol{X}\boldsymbol{w}\right) + r(\boldsymbol{w})$$

- L, r are a convex loss and penalty
- $n, d \to \infty$ with fixed ratio

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Beyond i.i.d. assumption : introduce correlation

Introducing Correlation : a Block Covariance Model

Teacher and student with different feature spaces

Block covariate model proposed in

[B. Loureiro, **CG**, H. Cui, S. Goldt, M. Mézard, F. Krzakala, L. Zdeborova '21]

$$\begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{v} \end{bmatrix} \in \mathbb{R}^{p+d} \sim \mathcal{N}\left(0, \begin{bmatrix} \Psi & \Phi \\ \Phi^\top & \Omega \end{bmatrix}\right) \qquad y^\mu = f_0\left(\frac{1}{\sqrt{p}} \boldsymbol{w}_0^\top \boldsymbol{u}^\mu\right),$$

$$\boldsymbol{w}^\star = \mathrm{argmin}_{\boldsymbol{w}\in\mathbb{R}^d} \left[\sum_{\mu=1}^{n} l\left(\frac{\boldsymbol{w}^\top \boldsymbol{v}^\mu}{\sqrt{d}}, y^\mu\right) + r(\boldsymbol{w})\right]$$

Many works: [E. Dobriban, S. Wager '15][PL. Bartlett, PM. Long, G. Lugosi, A. Tsigler '19][T. Hastie, A. Montanari, S. Rosset, RJ. Tibshirani '19][M. Celentano, A. Montanari, Y. Wei '20]

Solution to Block Covariance model

Theorem (informal)[B. Loureiro, CG, H. Cui, S. Goldt, M. Mézard, F. Krzakala, L. Zdeborova '21]

Unique fixed point of self-consistent equations

$$\begin{cases} V = \mathbb{E}_{(\omega,\bar{\theta})\sim\mu}\left[\frac{\omega}{\lambda+\hat{V}\omega}\right] \\ m = \frac{\hat{m}}{\sqrt{\gamma}}\mathbb{E}_{(\omega,\bar{\theta})\sim\mu}\left[\frac{\bar{\theta}^2}{\lambda+\hat{V}\omega}\right] \\ q = \mathbb{E}_{(\omega,\bar{\theta})\sim\mu}\left[\frac{\hat{m}^2\bar{\theta}^2\omega+\hat{q}\omega^2}{(\lambda+\hat{V}\omega)^2}\right] \end{cases}, \quad \begin{cases} \hat{V} = \frac{\alpha}{V}(1-\mathbb{E}_{s,h\sim\mathcal{N}(0,1)}[z'(V,m,q)]) \\ \hat{m} = \frac{1}{\sqrt{\rho\gamma}}\frac{\alpha}{V}\mathbb{E}_{s,h\sim\mathcal{N}(0,1)}\left[sz(V,m,q)-\frac{m}{\sqrt{\rho}}z'(V,m,q)\right] \\ \hat{q} = \frac{\alpha}{V^2}\mathbb{E}_{s,h\sim\mathcal{N}(0,1)}\left[\left(\frac{m}{\sqrt{\rho}}s+\sqrt{q-\frac{m^2}{\rho}}h-z(V,m,q)\right)^2\right] \end{cases}$$

where $z(V,m,q) = \mathrm{prox}_{Vl(.,f_0(\sqrt{\rho}s))}(\rho^{-1/2}ms + \sqrt{q-\rho^{-1}m^2}h)$

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$n, p, d \to \infty$, training and generalization error :

$$\mathcal{E}_{\mathrm{train.}}(\hat{w}) \xrightarrow[d\to\infty]{P} \mathbb{E}_{s,h\sim\mathcal{N}(0,1)}\left[l\left(\mathrm{prox}_{V^\star l(.,f_0(\sqrt{\rho}s))}\left(\frac{m^\star}{\sqrt{\rho}}s+\sqrt{q^\star-\frac{m^{\star 2}}{\rho}}h\right), f_0(\sqrt{\rho}s)\right)\right]$$

$$\mathcal{E}_{\mathrm{gen.}}(\hat{w}) \xrightarrow[d\to\infty]{P} \mathbb{E}_{(\nu,\lambda)}\left[\hat{g}\left(\hat{f}(\lambda), f_0(\nu)\right)\right]$$

Proof uses **convex Gaussian comparison inequalities**

[M. Stojnic, '13][C. Thrampoulidis, E. Abbasi, B. Hassibi '18]

How well does is work ?

Ridge regression works well ...

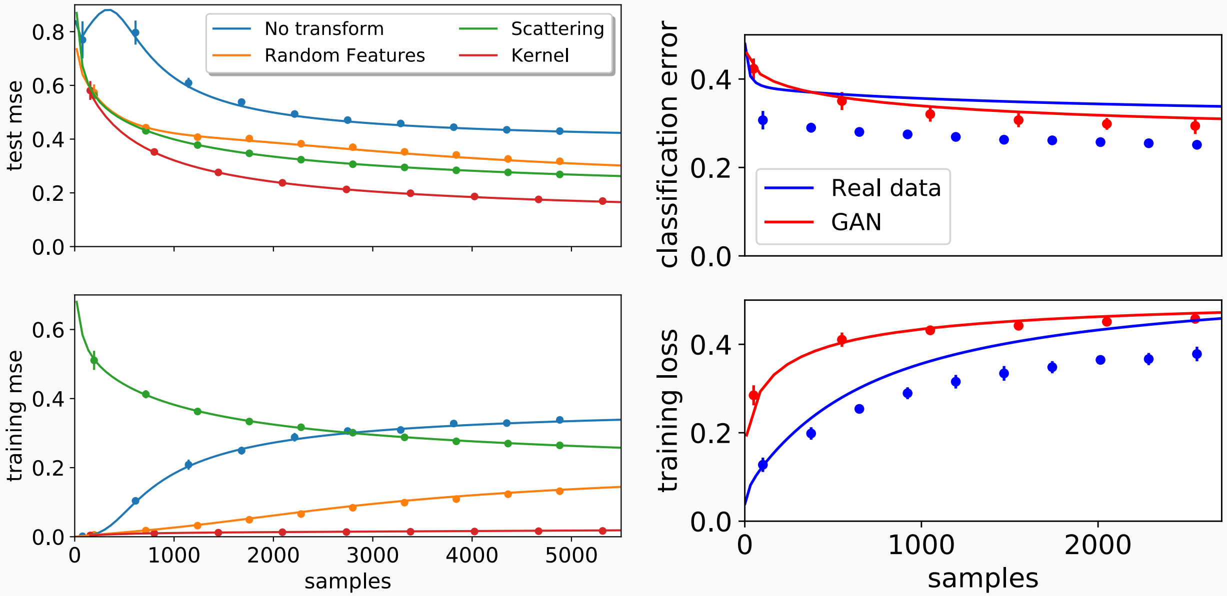

Figure 1: (Left) Ridge regression on real data. (Right) Logistic regression with real and synthetic (GAN) data

... but classification is more problematic

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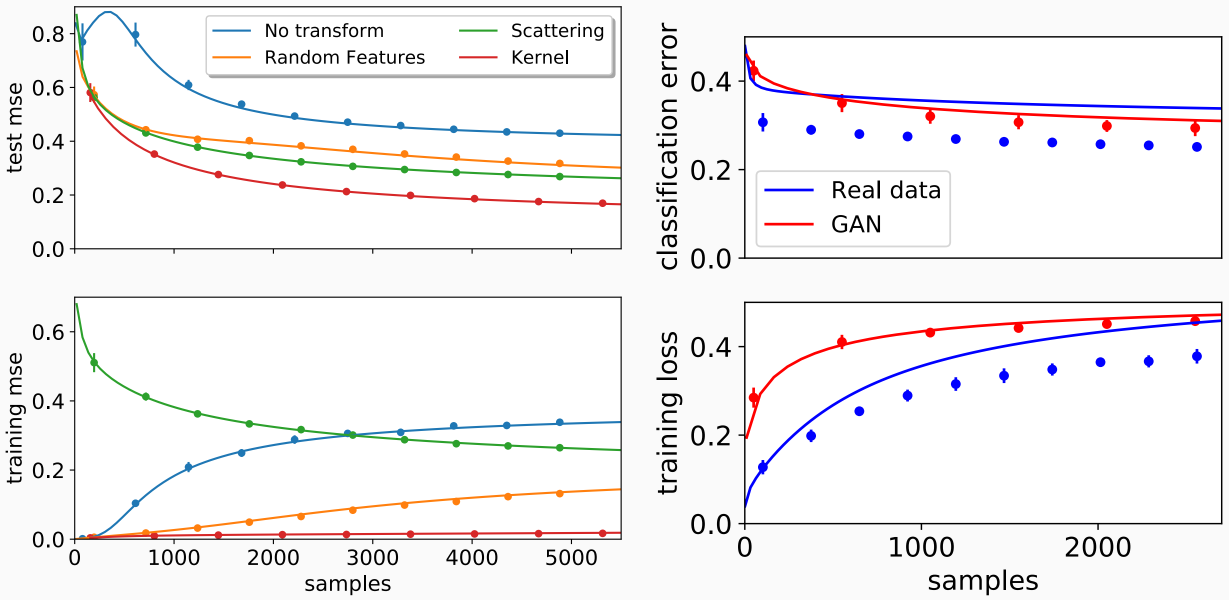

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Need for another realistic benchmark problem

Gaussian mixtures are meaningful

Study classification of k-Gaussian mixture with convex GLM

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- Benchmark problem in ML, universal approximation, ...
- many scenarios described by Gaussian mixtures (GANs, 'Neural collapse', ...)

[M. Seddik, C. Louart, M. Tamaazousti, R. Couillet, '20][V. Papyan, X. Han, D.Donoho, '20]

Classifying Gaussian Mixtures with Convex GLM

Data and teacher

$$\boldsymbol{x} \in \mathbb{R}^d, \boldsymbol{y} \in \mathbb{R}^K \quad P(\boldsymbol{x}, \boldsymbol{y}) = \sum_{k=1}^{K} y_k \rho_k \mathcal{N}\left(\boldsymbol{x} \,|\, \boldsymbol{\mu}_k, \Sigma_k\right),$$

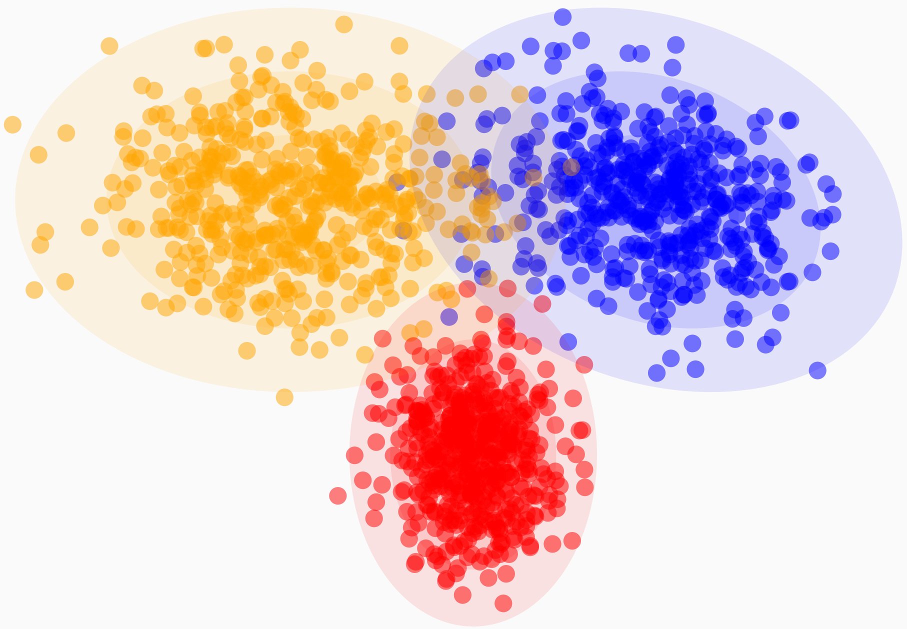

Figure 2: K=3, d=2

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Student

$$\boldsymbol{W}^\star \in \min_{\boldsymbol{W} \in \mathbb{R}^{d \times K}} L\left(\boldsymbol{Y}, \boldsymbol{X}\boldsymbol{W}\right) + r(\boldsymbol{W})$$

Learn K separating hyperplanes, i.e. a matrix $\boldsymbol{W} \in \mathbb{R}^{d \times K}$

Examples : ridge regression, softmax with cross-entropy, ...

Main result (informal)

Theorem [B. Loureiro, G. Sicuro, CG, A. Pacco, F. Krzakala, L. Zdeborova '21]

Fixed-point of self-consistent equations

$$\begin{cases} \boldsymbol{Q}_k = \frac{1}{d}\mathbb{E}_{\Xi}[\boldsymbol{G}\Sigma_k\boldsymbol{G}^\top] \\ \boldsymbol{m}_k = \frac{1}{\sqrt{d}}\mathbb{E}_{\Xi}[\boldsymbol{G}\boldsymbol{\mu}_k] \\ \boldsymbol{V}_k = \frac{1}{d}\mathbb{E}_{\Xi}\left[\left(\boldsymbol{G}\odot\left(\hat{\boldsymbol{Q}}_k\otimes\Sigma_k\right)^{-\frac{1}{2}}\odot(\boldsymbol{I}_K\otimes\Sigma_k)\right)\Xi_k^\top\right] \end{cases} \qquad \begin{cases} \hat{\boldsymbol{Q}}_k = \alpha\rho_k\mathbb{E}_{\boldsymbol{\xi}}\left[\boldsymbol{f}_k\boldsymbol{f}_k^\top\right] \\ \hat{\boldsymbol{V}}_k = -\alpha\rho_k\boldsymbol{Q}_k^{-\frac{1}{2}}\mathbb{E}_{\boldsymbol{\xi}}\left[\boldsymbol{f}_k\boldsymbol{\xi}^\top\right] \\ \hat{\boldsymbol{m}}_k = \alpha\rho_k\mathbb{E}_{\boldsymbol{\xi}}\left[\boldsymbol{f}_k\right] \end{cases}$$

$$\text{where } \boldsymbol{G} = \mathrm{A}^{\frac{1}{2}}\odot\mathrm{Prox}_{r(\mathrm{A}^{\frac{1}{2}}\odot\bullet)}(\mathrm{A}^{\frac{1}{2}}\odot\boldsymbol{B}),\ \mathrm{A}^{-1}\equiv\textstyle\sum_k\hat{\boldsymbol{V}}_k\otimes\Sigma_k,\ \boldsymbol{B}\equiv\sum_k\left(\boldsymbol{\mu}_k\hat{\boldsymbol{m}}_k^\top+\Xi_k\odot\sqrt{\hat{\boldsymbol{Q}}_k\otimes\Sigma_k}\right)$$

$$\boldsymbol{f}_k\equiv\boldsymbol{V}_k^{-1}(\boldsymbol{h}_k-\boldsymbol{\omega}_k),\ \boldsymbol{h}_k=\boldsymbol{V}_k^{1/2}\mathrm{Prox}_{\ell(\boldsymbol{e}_k,\boldsymbol{V}_k^{1/2}\bullet)}(\boldsymbol{V}_k^{-1/2}\boldsymbol{\omega}_k),\ \boldsymbol{\omega}_k\equiv\boldsymbol{m}_k+\boldsymbol{b}+\boldsymbol{Q}_k^{1/2}\boldsymbol{\xi}_k$$

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Training and generalization for $n, d\to\infty$:

$$\epsilon_t = 1-\sum_{k=1}^{K}\rho_k\mathbb{E}_{\boldsymbol{\xi}}\left[\hat{y}_k(\boldsymbol{h}_k)\right], \quad \epsilon_g = 1-\sum_{k=1}^{K}\rho_k\mathbb{E}_{\boldsymbol{\xi}}\left[\hat{y}_k(\boldsymbol{\omega}_k)\right].$$

Main result : important points

- very generic statement
- greatly simplifies with assumptions on covariances, separability of functions, ...
- in most cases reduces to low dimensional statement

Examples : synthetic random design problems

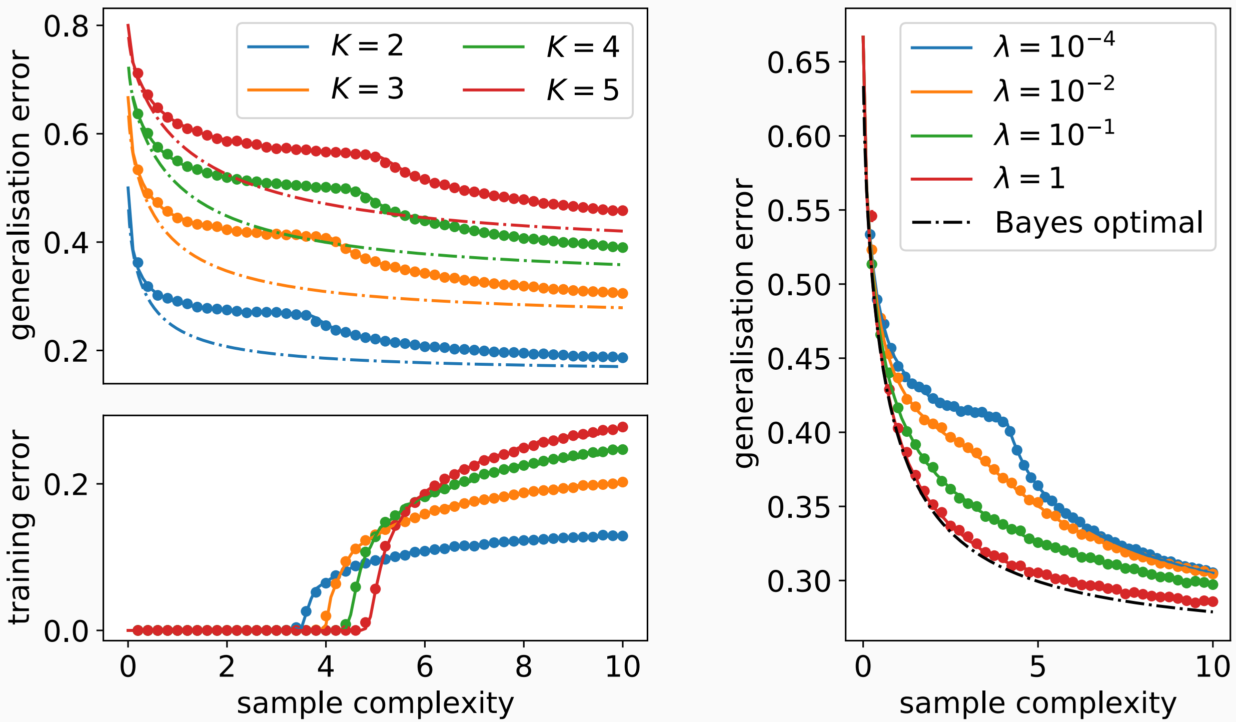

Figure 3: Ridge penalized logistic regression on K Gaussian clusters, $\Sigma_k = \Delta Id$. (Left) Sample complexity (Right) Regularization

Related works :[T. Cover '69][E. Gardner, B. Derrida '89] [EJ. Candès, P. Sur '20] [F. Mignacco, F. Krzakala, Y. Lu, P. Urbani, L. Zdeborova '20][C. Thrampoulidis, S. Oymak, M. Soltanolkotabi '20]

Examples : real data

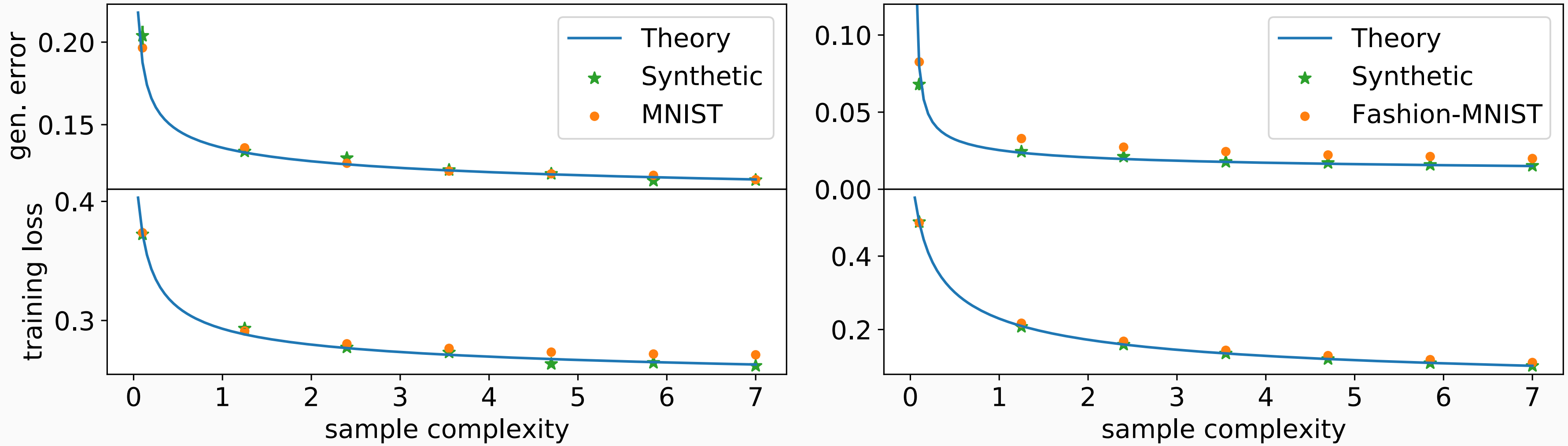

Figure 4: Binary classification on Mnist/Fashion-Mnist, odd vs even, Gaussian approximation and real data

Examples : real data

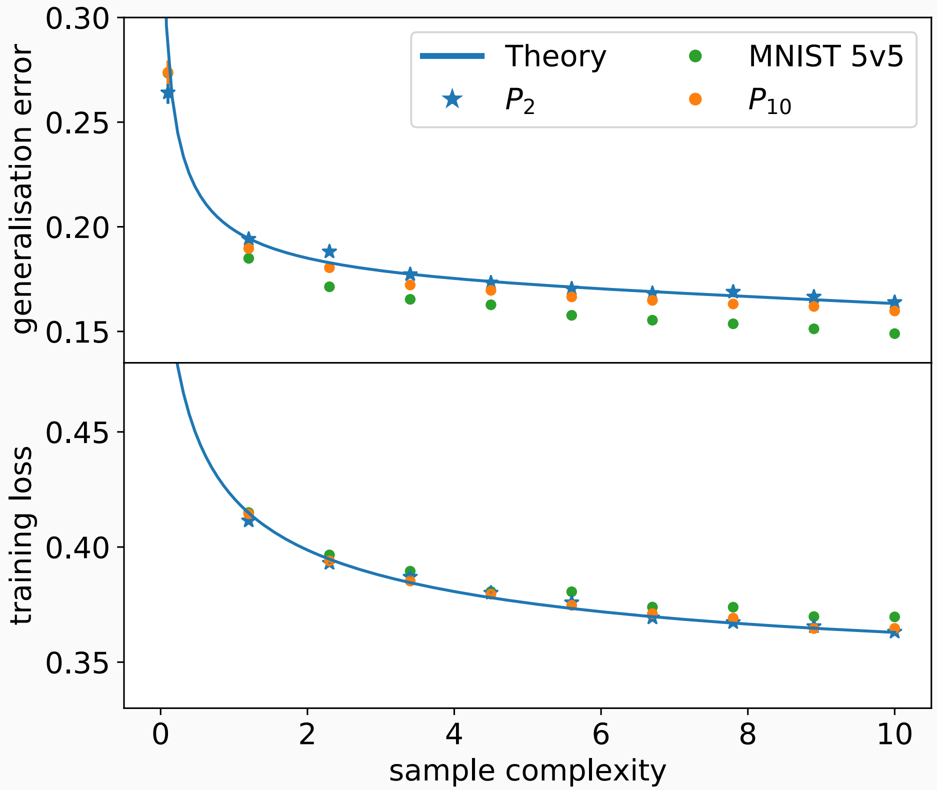

Figure 5: Adding more clusters to the Gaussian approximation

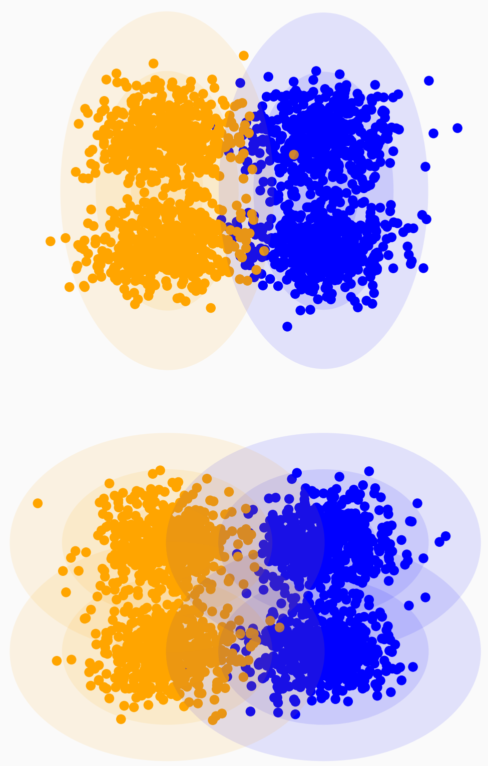

Figure 6: Idealized view

Sketch of proof

What are the difficulties ?

Learning a matrix : how are the different hyperplanes correlated/linked by the learning process ?

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Convex Gaussian Comparison Inequalities break down beyond least-squares

[C. Thrampoulidis, S. Oymak, M. Soltanolkotabi '20] (identity covariances)

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Family of iterations with closed form exact asymptotics : **state evolution (SE) equations**

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- handles block correlation structures (spatial coupling)
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First proof of SE equations due to E. Bolthausen (2009, math. phys.)
Then [M. Bayati, A. Montanari, '11]

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Sequence of matrices $\boldsymbol{u}, \boldsymbol{v}$:

$$\boldsymbol{u}^{t+1} = \boldsymbol{Z}^\top \boldsymbol{h}_t(\boldsymbol{v}^t) - \boldsymbol{e}_t(\boldsymbol{u}^t)\langle \boldsymbol{h}_t' \rangle^\top$$
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where $\boldsymbol{Z}$ (block-)Gaussian, $\boldsymbol{h}_t, \boldsymbol{e}_t$ are matrix valued functions.

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Brackets are Jacobian-like terms $\rightarrow$ **inherent to AMP**

Sketch of proof

Target :

$$\boldsymbol{W}^\star \in \min_{\boldsymbol{W} \in \mathbb{R}^{d \times K}} L(\boldsymbol{Y}, \boldsymbol{X}\boldsymbol{W}) + r(\boldsymbol{W}) \tag{1}$$

Tool :

$$\begin{aligned} \boldsymbol{u}^{t+1} &= \boldsymbol{Z}^\top \boldsymbol{h}_t(\boldsymbol{v}^t) - \boldsymbol{e}_t(\boldsymbol{u}^t)\langle \boldsymbol{h}'_t \rangle^\top \\ \boldsymbol{v}^t &= \boldsymbol{Z}\boldsymbol{e}_t(\boldsymbol{u}^t) - \boldsymbol{h}_{t-1}(\boldsymbol{v}^{t-1})\langle \boldsymbol{e}'_t \rangle^\top \end{aligned} \tag{2}$$

Sketch of proof

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Instructions:

- design $\boldsymbol{h}_t, \boldsymbol{e}_t$ s.t. fixed point of (2) matches opt. cond. of (1)
- find a converging trajectory (convexity helps)
- use state evolution equations (fixed point)

AMP for high-dim. stat : [M. Bayati, A. Montanari '11] [D. Donoho, A. Montanari '16]

Designing the AMP : a quick look

Often designed from a factor graph, see e.g. [L. Zdeborova, F. Krzakala '16]

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Reformulate the optimality condition

$$\boldsymbol{X}^\top \partial L(\boldsymbol{Y}, \boldsymbol{X}\boldsymbol{W}^\star) + \partial r(\boldsymbol{W}^\star) = 0$$

Match it with the fixed point

$$(Id + \boldsymbol{e}(\bullet)\langle \boldsymbol{h}' \rangle)(\boldsymbol{u}) = Z^\top \boldsymbol{h}(\boldsymbol{v})$$
$$(Id + \boldsymbol{h}(\bullet)\langle \boldsymbol{e}' \rangle)(\boldsymbol{v}) = Z\boldsymbol{e}(\boldsymbol{u})$$

[B. Loureiro, G. Sicuro, **CG**, A. Pacco, F. Krzakala, L. Zdeborova '21]

Validity of state evolution

Non-separable, block structure gradient

$$\boldsymbol{Z}^\top \begin{bmatrix} \partial\tilde{L}_1(\boldsymbol{Z}_1\tilde{\boldsymbol{W}}_1) & & & \\ & \partial\tilde{L}_2(\boldsymbol{Z}_2\tilde{\boldsymbol{W}}_2) & (0) & \\ & (0) & \ddots & \\ & & & \partial\tilde{L}_K(\boldsymbol{Z}_K\tilde{\boldsymbol{W}}_K) \end{bmatrix} + \begin{bmatrix} \partial\tilde{r}(\tilde{\boldsymbol{W}})_1 & & & \\ & \partial\tilde{r}(\tilde{\boldsymbol{W}})_2 & (0) & \\ & (0) & \ddots & \\ & & & \partial\tilde{r}(\tilde{\boldsymbol{W}})_K \end{bmatrix}$$

Spatially-coupled, matrix AMP : [A. Javanmard, A. Montanari '12]
Non-separable AMP : [R. Berthier, A. Montanari, P. Nguyen '18]

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Non-separable AMP : [R. Berthier, A. Montanari, P. Nguyen '18]

Combination included in [**CG**, R. Berthier '21]

Future directions

Relevance to realistic scenarios

- Gaussian models are relevant to a certain degree
- Gaussian density estimators are universal ...
- ... becomes more complicated than original problem !
- middle ground/parametrization relevant for given tasks ?

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Technical improvements

- more possibilities using AMP methods
- finite size analysis [C. Rush, R. Venkataramanan '18]
- universality properties [M. Bayati, M. Lelarge, A. Montanari '15]

Thank you

Collaborators : Bruno Loureiro, Gabriele Sicuro, Raphaël Berthier, Lenka Zdeborova and Florent Krzakala