Finite-sample Analysis of *M*-estimators using Self-concordance

Dmitrii M. Ostrovskii, Francis Bach

INRIA-CWI Workshop 2018
INRIA, Paris

Problem setup

Statistical learning problem

Given some **loss** $\ell : \mathcal{Y} \times \mathbb{R} \to \mathbb{R}$, find a minimizer $\theta_* \in \mathbb{R}^d$ of **expected risk**:

$$\theta_* \in \operatorname*{Argmin}_{\theta \in \mathbb{R}^d} L(\theta) := \mathbf{E}[\ell(Y, X^\top \theta)],$$

where expectation $\mathbf{E}[\cdot]$ is w.r.t. the unknown distribution $\mathcal{P}$ of $(X, Y) \in \mathbb{R}^d \times \mathcal{Y}$. Since $\mathcal{P}$ is unknown, θ_* can't be found; instead, it is estimated from **i.i.d. sample**:

$$(X_1, Y_1), ..., (X_n, Y_n) \sim \mathcal{P} \quad \text{(i.i.d.)}$$

- Y only depends (non-linearly) on $\eta = X^\top \theta$, a linear combination of inputs.
- Random-design **classification**, $\mathcal{Y} = \{0, 1\}$, and **regression**, $\mathcal{Y} = \mathbb{R}$.
- Performance of an estimate $\widehat{\theta}$ measured by **excess risk** $L(\widehat{\theta}) - L(\theta_*)$.

Goal

- **Empirical risk minimization:** replace $L(\theta)$ with **empirical risk**:

$$\widehat{\theta}_n \in \operatorname*{Argmin}_{\theta \in \mathbb{R}^d} \left\{ L_n(\theta) := \frac{1}{n} \sum_{i=1}^{n} \ell(Y_i, X_i^\top \theta) \right\}.$$

  Also called M-**estimation** in statistics.

- Special case: conditional **quasi maximum likelihood estimator** (qMLE):

$$\ell(y, \eta) = -\log p_\eta(y)$$

  for some density $p_\eta(y)$ parametrized by η.

  - "Quasi": the true distribution $\mathcal{P}$ might **not** belong to this model.

Goal

Extend classical theory of qMLE, holding in the limit $n \to \infty$ with fixed d, to **finite-sample** setup.

- Encompass model **misspecification** and non-likelihood M-estimators.

Motivation 1: Classical asymptotic theory*

- **Local regularity assumptions**: $L(\theta)$ sufficiently smooth at θ_*, and

$$\mathbf{H} := \nabla^2 L(\theta_*) \succ 0.$$

- Gradient covariance $\mathbf{G} := \mathbf{E}[\nabla_\theta \ell(Y, X^\top \theta_*) \nabla_\theta \ell(Y, X^\top \theta_*)^\top]$, and let

$$\mathbf{M} := \mathbf{H}^{-1/2} \mathbf{G} \mathbf{H}^{-1/2}.$$

  $d_{\text{eff}} := \text{tr}(\mathbf{M})$ is the **effective dimension**. In well-specified models:

$$\mathbf{G} = \mathbf{H} \;\Rightarrow\; \mathbf{M} = \mathbf{I}_d \;\Rightarrow\; d_{\text{eff}} = d.$$

- In the limit $n \to \infty$, Central Limit Theorem & Taylor Expansion give:

$$\sqrt{n}\mathbf{H}^{-1/2}(\widehat{\theta}_n - \theta_*) \rightsquigarrow \mathcal{N}(0, \mathbf{M}),$$

$$n\|\mathbf{H}^{1/2}(\widehat{\theta}_n - \theta_*)\|^2 \rightsquigarrow \mathcal{N}(0, \mathbf{M})^2, \quad 2n(L(\widehat{\theta}_n) - L(\theta_*)) \rightsquigarrow \mathcal{N}(0, \mathbf{M})^2.$$

$$\left\{ L(\widehat{\theta}_n) - L(\theta_*), \; \|\mathbf{H}^{-1/2}(\theta_n - \theta_*)\|^2 \right\} = O\left(\frac{d_{\text{eff}} \log(1/\delta)}{n} \right).$$

*[Borovkov, 1998; van der Vaart, 1998; Lehmann and Casella, 2006].

Motivation 2: Random-design linear regression, I

- Gaussian model $Y = \mathcal{N}(X^\top\theta, \sigma^2)$ leads to quadratic loss and risk:

$$\ell(Y, X^\top\theta) = \frac{1}{2\sigma^2}(Y - X^\top\theta)^2,$$
$$L(\theta) - L(\theta_*) = \frac{1}{2}\|\mathbf{H}^{1/2}(\theta - \theta_*)\|^2,$$
$$L_n(\theta) - L_n(\theta_*) = \frac{1}{2}\|\mathbf{H}_n{}^{1/2}(\theta - \theta_*)\|^2 + \underbrace{\langle \nabla L_n(\theta_*), \theta - \theta_* \rangle}_{\text{zero-mean}}$$

- In particular, at any θ we have $\nabla^2 L(\theta) \equiv \mathbf{H}$ and $\nabla^2 L_n(\theta) \equiv \mathbf{H}_n$ with

$$\mathbf{H} = \mathbf{E}[XX^\top], \quad \mathbf{H}_n = \frac{1}{n}\sum_{i=1}^n X_i X_i^\top.$$

Theorem T: Estimation of a sample covariance matrix [Vershynin, 2010]

Assume $\mathbf{H}^{-1/2}X$ is subgaussian, i.e., has tails lighter than $\mathcal{N}(\mu, \mathbf{I}_d)$, and

$$n \gtrsim d + \log(1/\delta).$$

Then, with probability at least $1 - \delta$ it holds:

$$0.5\mathbf{H} \preccurlyeq \mathbf{H}_n \preccurlyeq 2\mathbf{H}.$$

Motivation 2: Random-design linear regression, II

Theorem 0: Finite-sample risk bound for linear regression [Hsu et al., 2012]

Assume that $\mathbf{H}^{-1/2}X$ and $\mathbf{G}^{-1/2}\nabla\ell_\theta(Y, X^\top\theta_*)$ are subgaussian, and

$$n \gtrsim d + \log(1/\delta).$$

Then w.p. at least $\geq 1-\delta$,

$$L(\widehat{\theta}_n) - L(\theta_*) \lesssim \|\mathbf{H}^{1/2}(\widehat{\theta}_n - \theta_*)\|^2 \lesssim \|\mathbf{H}^{-1/2}\nabla L_n(\theta_*)\|^2 \lesssim \frac{d_{\text{eff}}\log(1/\delta)}{n}.$$

Proof sketch:

1. Since $\nabla L_n(\widehat{\theta}_n) = 0$, we have $\|\mathbf{H}_n^{1/2}(\widehat{\theta}_n - \theta_*)\|^2 = \|\mathbf{H}_n^{-1/2}\nabla L_n(\theta_*)\|^2$.
2. Combining with **Theorem T**,

$$L(\widehat{\theta}_n) - L(\theta_*) = \tfrac{1}{2}\|\mathbf{H}^{1/2}(\widehat{\theta}_n - \theta_*)\|^2 \leq 2\|\mathbf{H}^{-1/2}\nabla L_n(\theta_*)\|^2;$$

3. Since $\mathbf{G}^{-1/2}\nabla L_n(\theta_*)$ is the average of n i.i.d. subgaussian vectors,

$$\|\mathbf{H}^{-1/2}\nabla L_n(\theta_*)\|^2 \lesssim \frac{d_{\text{eff}}\log(1/\delta)}{n}. \quad \blacksquare$$

Towards the general case

- Generally, risk is not quadratic, and Hessians are not constant:

$$\nabla^2 L(\theta) = \mathbf{H}(\theta), \quad \nabla^2 L_n(\theta) = \mathbf{H}_n(\theta).$$

- To extend the previous argument, we must control the precision of **local quadratic approximation** of $L_n(\theta)$ and $L(\theta)$ around θ_*.
- We exploit **self-concordance**, a concept introduced in [Nesterov and Nemirovski, 1994] in the theory of interior-point methods, and brought to the statistical learning context in [Bach, 2010] to study logistic regression.

Self-concordant losses

We always assume that $\ell(y, \eta)$ is convex in the second argument.

Definition. $\ell(y, \eta)$ is **self-concordant (SC)** if $\forall (y, \eta) \in \mathcal{Y} \times \mathbb{R}$ it holds

$$|\ell'''_\eta(y, \eta)| \le C[\ell''_\eta(y, \eta)]^{3/2}.$$

- While the above definition is homogeneous in η, the next one is not:

Definition. $\ell(y, \eta)$ is **pseudo self-concordant (PSC)** if instead it holds

$$|\ell'''_\eta(y, \eta)| \le C\ell''_\eta(y, \eta).$$

- **PSC** losses are somewhat more common than **SC** ones.
- However, we will see that obtaining optimal rate for **PSC** losses requires somewhat larger sample size.

Example 1: Generalized linear models

Conditional negative log-likelihood of Y given $\eta = X^\top \theta$ in the form

$$\ell(y, \eta) = -y\eta + a(\eta) - b(y),$$

where $a(\eta)$ is called the **cumulant**, and is given by

$$a(\eta) = \log \int_{\mathcal{Y}} e^{y\eta + b(y)} \mathrm{d}y.$$

This defines the density $p_\eta(y) \propto e^{y\eta + b(y)}$ such that $a(\eta) = \mathbf{E}_{p_\eta}[Y]$, and

$$\ell_\eta^{(s)}(y, \eta) = a^{(s)}(\eta) = \mathbf{E}_{p_\eta}[(Y - \mathbf{E}_{p_\eta} Y)^s], \quad s \geq 2.$$

SC/**PSC** specify a relation between 2nd and 3rd central moments of $p_\eta(\cdot)$

PSC: **Logistic regression** and any GLM for classification ($\mathcal{Y} = \{0, 1\}$) since

$$|a'''(\eta)| \leq \mathbf{E}_{p_\eta}|(Y - \mathbf{E}_{p_\eta}[Y])^3| \leq \mathbf{E}_{p_\eta}[(Y - \mathbf{E}_{p_\eta}[Y])^2] = a''(\eta).$$

PSC: **Poisson regression:** $Y \sim \text{Poisson}(e^\eta)$, then $a(\eta) = \exp(\eta)$.

SC: **Exponential-response model:** $Y \sim \text{Exp}(\eta)$, $\eta > 0$, $a(\eta) = -\log(\eta)$.

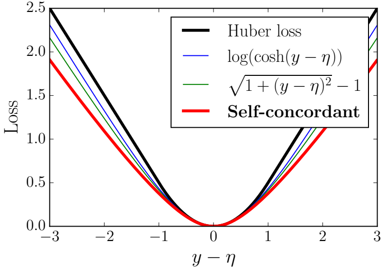
Example 2: Robust estimation

Loss $\ell(y,\eta) = \varphi(y-\eta)$ with $\varphi(t)$ convex, even, 1-Lipschitz, and $\varphi''(0) = 1$.

- **Huber loss**

$$\varphi(t) = \begin{cases} t^2/2, & |t| \le 1, \\ \tau t - 1/2, & |t| > 1. \end{cases}$$

$\varphi''(t)$ discontinuous at ± 1.



PSC: **Pseudo-Huber losses:** $\varphi(t) = \log\cosh(t)$, $\varphi(t) = \sqrt{1+t^2} - 1$.

SC: **Fenchel dual of the log-barrier** $\phi(u) = -\log(1-u^2)/2$ on $[-1,1]$:

$$\varphi(t) = \frac{1}{2}\left[\sqrt{1+4t^2} - 1 + \log\left(\frac{\sqrt{1+4t^2}-1}{2t^2}\right)\right].$$

Basic result

Recall that in the general case, we have the Hessian process $\mathbf{H}(\theta)$, given by

$$\mathbf{H}(\theta) := \mathbf{E}[\ell''(Y, X^\top\theta)XX^\top] = \mathbf{E}[\widetilde{X}(\theta)\widetilde{X}(\theta)^\top],$$

where $\widetilde{X}(\theta) := [\ell''(Y, X^\top\theta)]^{1/2}X$ is the *curvature-scaled design*.

Theorem 1: Finite-sample excess risk bound for self-concordant losses

Assume that the loss is **SC**, and $\mathbf{G}^{-1/2}\nabla\ell_\theta(Y, X^\top\theta_*)$ and $\mathbf{H}(\theta_*)^{-1/2}\widetilde{X}(\theta_*)$ are subgaussian. Whenever

$$n \gtrsim d + \log(1/\delta) \vee d_{\text{eff}}\, d \log(1/\delta),$$

with probability $1-\delta$ it holds

$$L(\widehat{\theta}_n) - L(\theta_*) \lesssim \|\mathbf{H}^{1/2}(\widehat{\theta}_n - \theta_*)\|^2 \lesssim \frac{d_{\text{eff}}\log(1/\delta)}{n}. \qquad (\star)$$

- ☺ Distribution conditions are local (only at θ_*);
- ☹ Large sample complexity – scaling as the product $O(d_{\text{eff}}\, d)$.

Analysis: Key observation

Given $\mathbf{H}(\theta) = \nabla^2 L(\theta)$, consider **Dikin ellipsoids** of $L(\theta)$ at θ_0:

$$\Theta(\theta_0, r) := \{\theta : \|\mathbf{H}(\theta_0)^{1/2}(\theta - \theta_0)\|^2 \leq r^2\}.$$

Key Observation. Suppose that $\mathbf{H}_n(\theta) \approx \mathbf{H}_n(\theta_*)$ w.h.p. for any $\theta \in \Theta(\theta_*, r)$. Then, $\widehat{\theta}_n \in \mathrm{Argmin}\, L_n(\theta)$ can be localized to $\Theta(\theta_*, r)$ once

$$\|\mathbf{H}(\theta_*)^{-1/2}\nabla L_n(\theta_*)\|^2 \lesssim r^2,$$

Proof sketch:

- Indeed, by definition of $\widehat{\theta}_n$, $L_n(\widehat{\theta}_n) \leq L_n(\theta_*)$. Assume $\widehat{\theta}_n \notin \Theta_n(\theta_*, r)$.
- Pick $\bar{\theta}_n \in [\theta_*, \widehat{\theta}_n]$ **on the border of** $\Theta_n(\theta_*, r)$. Still, $L_n(\bar{\theta}_n) \leq L_n(\theta_*)$.

$$0 \geq L_n(\bar{\theta}_n) - L_n(\theta_*) \approx \langle \nabla L_n(\theta_*), \bar{\theta}_n - \theta_* \rangle + \underbrace{\|\mathbf{H}_n(\theta_*)^{1/2}(\bar{\theta}_n - \theta_*)\|^2}_{\approx r^2 \text{ (by Theorem T)}}.$$

- By Cauchy-Schwarz, we arrive at $\|\mathbf{H}(\theta_*)^{-1/2}\nabla L_n(\theta_*)\|^2 \gtrsim r^2$.

Contradiction! ∎

Analysis: Recap

- Once $\widehat{\theta}_n$ has been localized to the neighborhood of θ_* where $L_n(\theta)$ is quadratic, we can mimick the argument for linear regression.
- Localization is guaranteed once

$$\|\mathbf{H}(\theta_*)^{-1/2}\nabla L_n(\theta_*)\|^2 \lesssim r^2,$$

which leads to the second threshold for n:

$$n \gtrsim \frac{1}{r^2} d_{\text{eff}} \log(1/\delta).$$

- **Now the question is:**

What is the radius r of the Dikin ellipsoid in which $\mathbf{H}_n(\theta) \approx \mathbf{H}_n(\theta_*)$?

  - **Short answer:** we can afford $r^2 \approx 1/d$ using self-concordance.

Analysis: Self-concordance at play

What is the radius r of the Dikin ellipsoid in which $\mathbf{H}_n(\theta) \approx \mathbf{H}_n(\theta_*)$?

1. Recall that

$$\mathbf{H}_n(\theta) = \frac{1}{n}\sum_{i=1}^{n} \ell''(Y_i, X_i^\top \theta) X_i X_i.$$

2. Integrating $|\ell'''(y,\eta)| \le [\ell''(y,\eta)]^{\frac{3}{2}}$ from $\eta_* = X^\top \theta_*$ to $\eta = X^\top \theta$,

$$\frac{1}{(1+[\ell''(y,\eta_*)]^{\frac{1}{2}}|\eta-\eta_*|)^2} \le \frac{\ell''(y,\eta)}{\ell''(y,\eta_*)} \le \frac{1}{(1-[\ell''(y,\eta_*)]^{\frac{1}{2}}|\eta-\eta_*|)^2},$$

$$\frac{1}{(1+|\langle \widetilde{X}(\theta_*), \theta-\theta_*\rangle|)^2} \le \frac{\ell''(Y, X^\top\theta)}{\ell''(Y, X^\top\theta_*)} \le \frac{1}{(1-|\langle \widetilde{X}(\theta_*), \theta-\theta_*\rangle|)^2}.$$

3. The ratio is bounded if $|\langle \widetilde{X}(\theta_*), \theta-\theta_*\rangle| \le c < 1$, i.e., by Cauchy-Schwarz,

$$\underbrace{\|\mathbf{H}(\theta_*)^{-1/2}\widetilde{X}(\theta_*)\|}_{\approx\sqrt{d}} \cdot \underbrace{\|\mathbf{H}(\theta_*)^{1/2}(\theta-\theta_*)\|}_{r} \le c \;\Rightarrow\; \boxed{r \gtrsim \frac{1}{\sqrt{d}}}. \quad \blacksquare$$

Improved result

Theorem 2: Improved sample complexity for self-concordant losses

Assume the loss is **SC**, $\mathbf{G}^{-1/2}\nabla \ell_\theta(Y, X^\top \theta_*)$ is subgaussian, and $\mathbf{H}(\theta)^{-1/2}\widetilde{X}(\theta)$ is subgaussian in the unit Dikin ellipsoid of $L(\theta)$ at θ_*:

$$\Theta(\theta_*, 1) = \{\theta : \|\mathbf{H}(\theta_*)^{1/2}(\theta - \theta_*)\| \le 1\}.$$

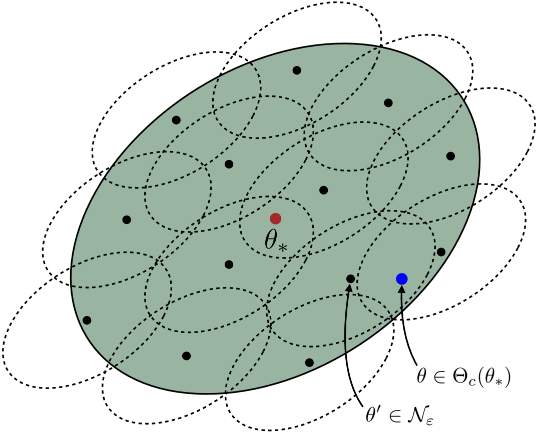
Then for $(\star)$ it is sufficient that

$$n \gtrsim d \log(d/\delta) \vee d_{\text{eff}} \log(1/\delta),$$

Main idea:

- Sample complexity $n \gtrsim d_{\text{eff}}\, d$ in Theorem 1 is due to Hessian approximation in the small Dikin ellipsoid with $r = O(1/\sqrt{d})$ rather than $r = O(1)$.
- We need to prove that $\mathbf{H}_n(\theta) \approx \mathbf{H}_n(\theta_*)$ for $\theta \in \Theta(\theta_*, 1)$. To do this, we combine self-concordance with a **covering argument**.

Covering the Dikin ellipsoid



1. It is rather easy to prove first that $\mathbf{H}(\theta)$ is near-constant on $\Theta(\theta_*, 1)$.
2. By **SC**, $\mathbf{H}_n(\theta)$ is near-constant in smaller ellipsoids $\Theta(\theta, 1/\sqrt{d})$.
3. Now cover $\Theta(\theta_*, 1)$ by $\Theta(\theta, 1/\sqrt{d})$ with θ in the epsilon-net $\mathcal{N}_\varepsilon$, and control uniform deviations $\mathbf{H}_n(\theta)$ from $\mathbf{H}(\theta)$ on $\mathcal{N}_\varepsilon$. OK since $\log |\mathcal{N}_\varepsilon| = O(d \log d)$.

Pseudo self-concordant losses

- Because of the "incorrect" power of ℓ'' in **PSC**, we need an extra condition:

$$\mathbf{E}[XX^\top] \le \rho \mathbf{E}[\ell''(Y, X^\top \theta_*) XX^\top].$$

  for some $\rho > 0$. This condition is standard in logistic regression [Bach, 2010].
- We obtain similar results, but with ρ times worse sample complexity.
- Worst-case bounds on ρ can be exponentially bad [Hazan et al., 2014]. However, this is not the case in practice [Bach, 2010].

Conclusion and perspectives

We use **self-concordance** – a concept from optimization – to obtain statistical results – **near-optimal** rates in finite-sample regimes in some statistical models.

Perspectives:

- Regularized estimators.
- Iterative algorithms: stochastic approximation, Quasi-Newton, ...
- Other models: covariance matrix estimation with $\log\det$ loss, ...

Thank you!

References

Bach, F. (2010). Self-concordant analysis for logistic regression. *Electronic Journal of Statistics*, 4:384–414.

Borovkov, A. A. (1998). *Mathematical statistics*. Gordon and Breach Science Publishers.

Hazan, E., Koren, T., and Levy, K. Y. (2014). Logistic regression: tight bounds for stochastic and online optimization. In *Conference on Learning Theory*, pages 197–209.

Hsu, D., Kakade, S. M., and Zhang, T. (2012). Random design analysis of ridge regression. *The Journal of Machine Learning Research*, 23(9):1–24.

Lehmann, E. L. and Casella, G. (2006). *Theory of point estimation*. Springer Science & Business Media.

Nesterov, Y. and Nemirovski, A. S. (1994). *Interior-point polynomial algorithms in convex programming*. Society of Industrial and Applied Mathematics.

van der Vaart, A. W. (1998). *Asymptotic statistics*. Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge University Press.

Vershynin, R. (2010). Introduction to the non-asymptotic analysis of random matrices. *arXiv:1011.3027*.

Analysis: Recap (full)

- Once $\widehat{\theta}_n$ is in neighborhood of θ_* where $L_n(\theta)$ is quadratic, we're done:

$$L_n(\widehat{\theta}_n) - L_n(\theta_*) \lesssim \|\mathbf{H}_n(\theta_*)^{1/2}(\widehat{\theta}_n - \theta_*)\|^2 \lesssim \|\mathbf{H}_n^{-1/2}(\theta_*)\nabla L_n(\theta_*)\|^2;$$

  by Theorem T, as long as $n \geq d + \log(1/\delta)$,

$$\|\mathbf{H}_n^{-1/2}(\theta_*)\nabla L_n(\theta_*)\|^2 \approx \|\mathbf{H}^{-1/2}(\theta_*)\nabla L_n(\theta_*)\|^2 \lesssim \frac{d_{\text{eff}} \log(1/\delta)}{n}.$$

  Similarly for $L(\widehat{\theta}_n) - L(\theta_*)$.

- Localization is guaranteed once $\|\mathbf{H}_n^{-1/2}(\theta_*)\nabla L_n(\theta_*)\|^2 \lesssim r^2$, which leads to the second threshold for n:

$$n \gtrsim \frac{1}{r^2} d_{\text{eff}} \log(1/\delta).$$

- **Now the question is:**

What is the radius r of the Dikin ellipsoid in which $\mathbf{H}_n(\theta) \approx \mathbf{H}_n(\theta_*)$?