4th year Review - Statistical Physics Perspectives on Learning in High Dimensions

Advisor: Surya Ganguli

Madhu Advani

Stanford University

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Outline

Current Research: High Dimensional M-estimation

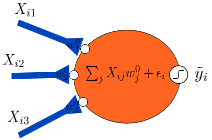
1. Optimal Unregularized M-estimation
2. Optimal Regularized M-estimation

Future Directions

1. Extensions of High Dimensional M-estimation
2. Network Implementation of Compressed Sensing
3. Network Implementation of Reinforcement Learning (credit assignment)

Problem Setup

$$y_i = \mathbf{X_i} \cdot \mathbf{w^0} + \epsilon_i \qquad i \in [1, \ldots N]$$



- Noise $\epsilon_i \sim f$ not necessarily gaussian
- (Easy) Classical Regime: $\kappa = P/N \to 0$
- (Hard) High Dimensional Regime: $\kappa = P/N \neq 0$

We want to find $\mathbf{w^0}$

Section 1

Unregularized Theory

M-estimation and Maximum Likelihood

M-estimation

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \left[\sum_i \rho \left(y_i - \mathbf{X}_i \cdot \mathbf{w} \right) \right]$$

E.g. $\rho(x) = x^2, |x|, -\log f(x)$

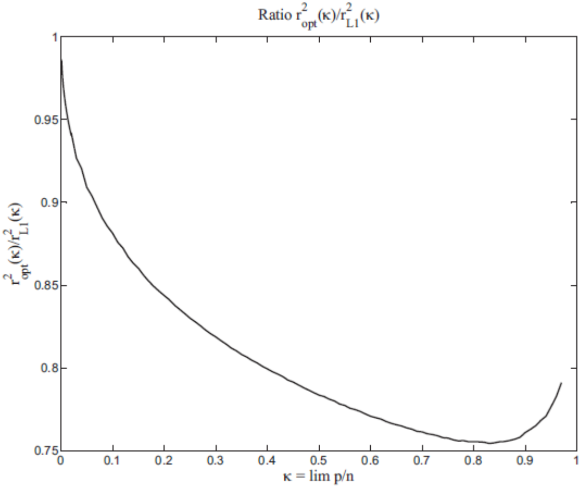
P fixed, $N \to \infty$

$$||\hat{w} - w^0||^2 = \frac{\left(\int \psi(x) f(x) dx \right)^2}{\int \psi^2 f(x) dx} \qquad \psi = \frac{\partial}{\partial w} \rho$$

$\psi_{\text{opt}} = \frac{f'}{f}$, $\rho_{\text{opt}} = -\log f$

$$\hat{\mathbf{w}}_{\text{ML}} = \arg\max_{\mathbf{w^0}} P \left(\mathbf{y}, \mathbf{X} | \mathbf{w^0} \right) = \arg\min_{\mathbf{w}} \left[\sum_i -\log f \left(y_i - \mathbf{X}_i \cdot \mathbf{w} \right) \right]$$

Sub-optimality of Maximum Likelihood in High Dimensions



El Karoui, et. al. PNAS 2013

Statistical Physics Formulation

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \sum_i \rho\left(y_i - \mathbf{X}_i \cdot \mathbf{w}\right)$$

Spin Glass System

Define spins $\mathbf{u} = \mathbf{w^0} - \mathbf{w}$ and Energy of system of spins:

$$E_{\mathbf{\Lambda}}(\mathbf{u}) = \sum_i \rho\left(\mathbf{X}_i \cdot \mathbf{u} + \epsilon_i\right)$$

Energy and temperature induce an equilibrium Gibbs distribution

$$P_G(\mathbf{u}) = \frac{e^{-\beta E_{\mathbf{\Lambda}}(\mathbf{u})}}{Z_{\mathbf{\Lambda}}} \qquad Z_{\mathbf{\Lambda}} = \int e^{-\beta E_{\mathbf{\Lambda}}(\mathbf{u})} du$$

$$\lim_{\beta \to \infty} P_G(\mathbf{u}) = \delta\left(\mathbf{u} - \mathbf{w^0} + \hat{\mathbf{w}}\right)$$

The Unregularized Case

$$q = \frac{1}{P}\sum_{j=1}^{P} \langle\, u_j \,\rangle_{\mathrm{G}}^2$$

Coupled Equations Relating Order Parameters q, c

$$\left\langle\left\langle \left(\mathrm{prox}_{c\rho}\left(\sqrt{q}z+\epsilon\right) - \sqrt{q}z - \epsilon\right)^2 \right\rangle\right\rangle_{z,\epsilon} = \kappa q$$

$$\left\langle\left\langle\, \mathrm{prox}'_{c\rho}(\sqrt{q}z+\epsilon) \,\right\rangle\right\rangle_{z,\epsilon} = 1-\kappa$$

- $X_{ij} \in \mathcal{N}(0, 1/P)$
- ρ convex
- $\epsilon_i \sim f$ iid

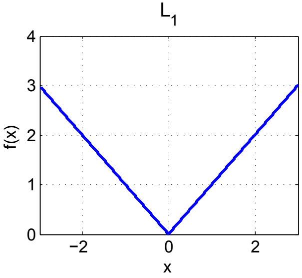
Proximal Map

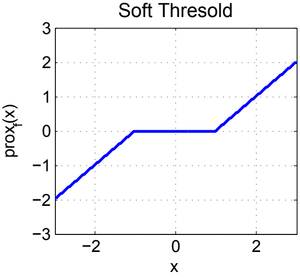
Definition

$$prox_f(x) = \arg\min_y \left[\frac{(x-y)^2}{2} + f(y) \right]$$

$$= [I + \partial f]^{-1}(x)$$

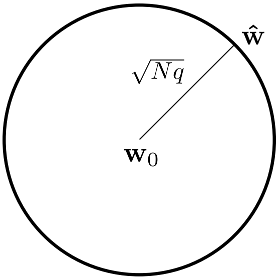
Example:





Analytic Estimator Error

How to choose ρ to minimize q?



$$\left\langle\left\langle \left(\mathrm{prox}_{c\rho}(\sqrt{q}z+\epsilon)-\sqrt{q}z-\epsilon\right)^2 \right\rangle\right\rangle_{z,\epsilon} = \kappa q$$

$$\left\langle\left\langle \mathrm{prox}'_{c\rho}(\sqrt{q}z+\epsilon) \right\rangle\right\rangle_{z,\epsilon} = 1-\kappa$$

Optimal Unregularized M-estimator

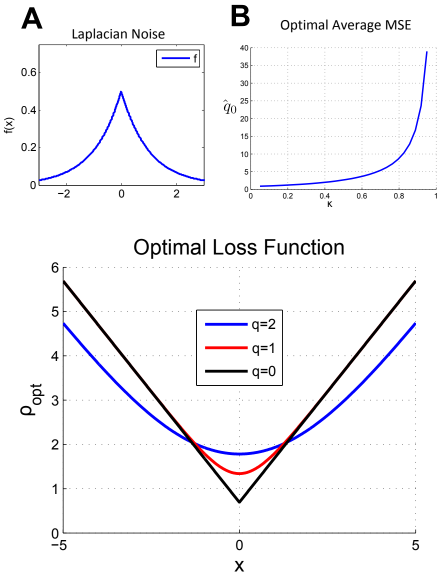
Optimal M-estimator

$$\rho_{\text{opt}}(x) = -\inf_y \left[\ln(\zeta_{\hat{q}}(y)) + \frac{(x-y)^2}{2\hat{q}} \right] \qquad \zeta_{\hat{q}} = f * \phi_{\hat{q}}$$

$$\hat{q} = \min q \qquad \text{s.t.} \quad qI_q = \kappa \qquad I_q = \int_{-\infty}^{\infty} \frac{\zeta_q'^2(y)}{\zeta_q(y)} dy$$

- $\hat{q}$ - best possible asymptotic MSE for a convex M-estimator
- ρ_{opt} is the optimal loss function (assuming log-concave noise)
- Note: Not maximum likelihood, and ρ varies with dimensionality κ

Optimal Unregularized M-estimator



Section 2

Regularized Theory

Adding a Regularizer

$$P(\mathbf{w^0}|\mathbf{X},\mathbf{y}) = \frac{P(\mathbf{X},\mathbf{y}|\mathbf{w^0})P(\mathbf{w^0})}{P(\mathbf{X},\mathbf{y})} \propto \prod_i f(y_i - \mathbf{X_i}\cdot\mathbf{w^0}) \prod_j g(w_j^0)$$

Maximum a Priori

$$\hat{\mathbf{w}}_{\mathrm{MAP}} = \arg\min_{\mathbf{w}} \left[\sum_i -\log f(y_i - \mathbf{X}_i\cdot\mathbf{w}) + \sum_j -\log g(w_j) \right]$$

Regularized M-estimation

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \left[\sum_i \rho(y_i - \mathbf{X}_i\cdot\mathbf{w}) + \sum_j \sigma(w_j) \right]$$

Note separability. Solvable for convex σ, ρ

Motivation

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \sum_a \rho(y_a - \mathbf{X_a} \cdot \mathbf{w}) + \sum_i \sigma(w_i)$$

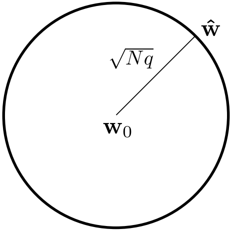
Applications

- Maximum Likelihood (ML) and MAP commonly applied to High Dimensional Bio-informatics problems, where we should expect poor performance
- Deriving/Understanding the Optimal M-estimator has potential applications for statistical inference and signal processing.
- Tractability of this form of optimization popular: Compressed Sensing, LASSO, Elastic Net

Regularized M-estimation

$$y_i = \mathbf{X}_i \cdot \mathbf{w^0} + \epsilon_i \qquad\qquad w_j^0 \sim g, \epsilon_i \sim f$$

$$E_{\mathbf{\Lambda}}(\mathbf{u}) = \sum_i \rho\left(\mathbf{X}_i \cdot \mathbf{u} + \epsilon_i\right) + \sum_a \sigma\left(w_a^0 - u_a\right)$$



Regularized M-estimation

Optimal Inference

$$\rho^R_{\text{opt}}(x) = -\inf_y \left[\ln(\zeta_{\tilde{q}_0}(y)) + \frac{(x-y)^2}{2\tilde{q}_0} \right]$$

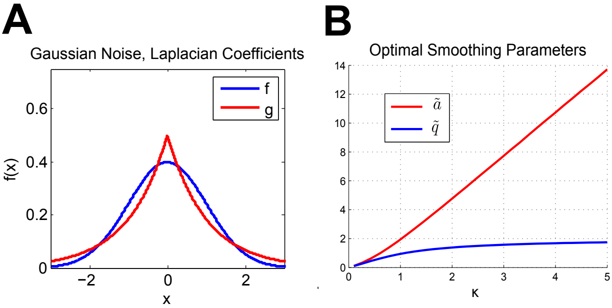
$$\sigma^R_{\text{opt}}(x) = -\frac{\tilde{q}_0}{\tilde{a}} \inf_y \left[\ln(\xi_{\tilde{a}}(y)) + \frac{(x-y)^2}{2\tilde{a}} \right]$$

$$\tilde{q}_0, \tilde{a} = \arg\min_{q_0, a} q_0$$

$$\text{s.t.} \quad aI_{q_0} = \kappa, \quad a^2 J_a = a - q_0 \qquad I_q = \int \frac{\zeta_q'^2}{\zeta_q}, \quad J_a = \int \frac{\xi_a'^2}{\xi_a}$$

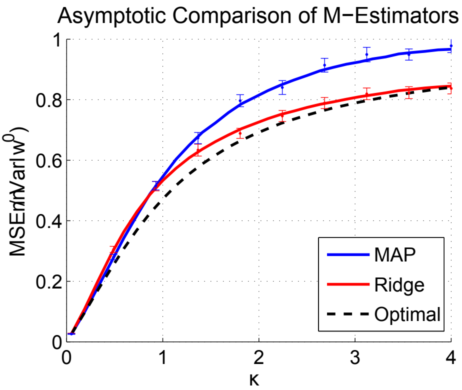
- $\rho_{\text{opt}}, \sigma_{\text{opt}}$ are optimal M-estimator (log concave f, g)
- $\tilde{q}_0$ is the asymptotic MSE
- $\tilde{q}_0, \tilde{a}$ are smoothing parameters

Unregularized M-estimator



M-estimator Comparison

$$\rho_{\text{MAP}}(x) = \frac{x^2}{2} \qquad \sigma_{\text{MAP}}(x) = |x|$$
$$\rho_{\text{Ridge}}(x) = \frac{x^2}{2} \qquad \sigma_{\text{Ridge}}(x) = \frac{x^2}{2}$$



Section 3

Future Extensions of High Dimensional M-estimation

Generalized Models

$$y_i = \eta(\mathbf{X_i} \cdot \mathbf{w^0}) + \epsilon_i$$

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \left[\sum_i \rho(y_i - \eta\left(\mathbf{X_i} \cdot \mathbf{w}\right)) + \sum_j \sigma(w_j) \right]$$

$$E(\mathbf{w}) = \sum_i \rho\left(\eta\left(\mathbf{X_i} \cdot \mathbf{w^0}\right) - \eta\left(\mathbf{X_i} \cdot (\mathbf{w^0} - \mathbf{u}) + \epsilon_i\right)\right) + \sum_j \sigma(w_j^0 - u_j)$$

Future Directions - Phase Transitions in Clustering

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