A Dynamic Approach to Variable Selection and Sparse Recovery: Differential Inclusions

Yuan Yao

School of Mathematical Sciences
Peking University

May 1, 2014

with Stanley Osher (UCLA), Feng Ruan (PKU & Stanford), Jiechao Xiong (PKU), and Wotao Yin (UCLA), et al.

1. Inverse Scale Space (ISS) Dynamics
   - ISS
   - Bias of LASSO
   - Dynamics of Bregman Inverse Scale Space
   - Discrete Algorithm: Linearized Bregman Iteration

2. Path Consistency Theory
   - Sign-consistency
   - l_2-consistency

3. Discussion

Background

Assume that $\beta^* \in \mathbb{R}^p$ is sparse and unknown. Consider recovering β^* from

$$y = X\beta^* + \epsilon,$$

where ϵ is **noise**.

Note

- $S := \mathrm{supp}(\beta^*)$ and T be its complement.
- X_S (X_T) be the columns of X with indices restricted on S (T)
- $\epsilon \sim \mathcal{N}(0, \sigma^2)$ (sub-Gaussian in general)
- X is n-by-p, with $p \gg n$.

Algorithms and Statistical Consistency

- Orthogonal Matching Pursuit (OMP, Mallat-Zhang'93)
    - noise-free: Tropp'04
    - noise: Cai-Wang'11
- LASSO (Tibshirani'96), also Basis Pursuit (Chen-Donoho-Saunders'96), Dantzig Selector (Candes-Tao'07)
    - sign-consistency: Yuan-Lin'06, Zhao-Yu'06, Zou'07, Wainwright'09
    - l_2-consistency: Bickel-Ritov-Tsybakov'09 (also Dantzig)
- Anything else do you wanna hear?

"Optimization + Noise" in H.D. Statistics?

- $p >> n$: impossible to be *strongly convex*

$$\min_{\beta} L(\beta) := \frac{1}{n}\sum_{i=1}^{n} \rho(y_i - x_i^T\beta), \quad \text{convex } \rho \text{ (Huber'73)}$$

- in presence of noise, not every optimizer $\arg\min L(\beta)$ is desired: mostly overfitting
- convex constraint/penalization: avoid overfiting, tractable but lead to bias $\Rightarrow$ non-convex? (hard to find global optimizer)
- dynamics: every algorithm is dynamics (Turing), not necessarily optimizing an objective function

Oracle Estimator

If S is disclosed by an oracle, the *oracle estimator* is the subset least square solution with $\tilde{\beta}^*_T = 0$ and for $\Sigma_n = \frac{1}{n} X_S^T X_S \to \Sigma_S$,

$$\tilde{\beta}^*_S = \Sigma_n^{-1} \left(\frac{1}{n} X_S^T y \right) = \beta^*_S + \frac{1}{n} \Sigma_n^{-1} X_S^T \epsilon, \qquad (1)$$

$\frac{1}{2n}\|X\tilde{\beta}^*_S - y\|^2$

"Oracle properties"

- **Model selection consistency**: $\mathrm{supp}(\tilde{\beta}^*) = S$;
- **Normality**: $\tilde{\beta}^*_S \sim \mathcal{N}(\beta^*, \frac{\sigma^2}{n} \Sigma_n^{-1})$.

So $\tilde{\beta}^*$ is unbiased, i.e. $E[\tilde{\beta}^*] = \beta^*$.

Recall LASSO

LASSO:

$$\min_{\beta} \|\beta\|_1 + \frac{t}{2n}\|y - X\beta\|_2^2. \qquad t = \frac{1}{\lambda}$$

optimality condition:

$$\frac{\rho_t}{t} = \frac{1}{n} X^T (y - X\beta_t), \tag{2a}$$

$$\rho_t \in \partial \|\beta_t\|_1, \tag{2b}$$

where $\lambda = 1/t$ is often used in literature.

- Tibshirani'1996 (LASSO)
- Chen-Donoho-Saunders'1996 (BPDN)

The Bias of LASSO

- Path consistency: $\exists \tau_n \in (0,\infty)$, $\mathrm{supp}(\hat\beta_{\tau_n}) = S$ (e.g. , Zhao-Yu'06, Zou'06, Yuan-Lin'07, Wainwright'09)
- LASSO is biased, i.e. $\mathbb{E}(\hat\beta) \neq \beta^*$,

$$\mathbb{E}(\hat\beta_{\tau_n})_S = \tilde\beta^*_S - \frac{1}{\tau_n}\Sigma_n^{-1}\rho_{\tau_n}, \quad \tau_n > 0$$

$\approx \mathrm{sign}(\beta^*_S)$; $\tilde\beta^*_S = \beta^*$

- e.g. $X = Id$, $n = p = 1$,

$y > 0$

$$\hat\beta_\tau = \begin{cases} 0, & \text{if } \tau < 1/y; \\ y - 1/\tau, & \text{otherwise,} \end{cases} \qquad y = \beta^* + \epsilon$$

- (Fan-Li'2001) non-convex penalty is necessary (SCAD, Zhang's PLUS, Zou's Adaptive LASSO, etc.)
- Any other simple scheme?

$\frac{\rho_t}{t} = \frac{1}{n}X^T(y - X\beta)$

$= \frac{1}{n}X^T(X\beta^* + \epsilon - X\beta)$

$t.$ $\mathrm{sign}(\beta_t) = \mathrm{sign}(\beta^*)$

$\frac{\rho_t}{t}\Big|_S = \left(\frac{1}{n}X_S^T X_S\right)(\beta^* - \beta_t) + \frac{1}{n}X_S^T\epsilon$

$\Sigma_n = \frac{1}{n}X_S^T X_S$

Differentiation of LASSO's KKT Equation

Taking derivative (assuming differentiability) w.r.t. t

$$\rho_t = \frac{1}{n} X^T (y - X\beta_t) t$$

ρ_t

$$\Rightarrow \underset{0}{\dot{\rho}_t} = \frac{1}{n} X^T (y - X(\dot{\beta}_t t + \beta_t)), \quad \rho_t \in \partial \|\beta_t\|_1$$

- Debias: sign-consistency $(\mathrm{sign}(\beta_\tau) = \mathrm{sign}(\beta^*)) \Rightarrow$ $\dot{\rho}_{\tau,S} = 0 \Rightarrow$ oracle estimator $\tilde{\beta}^* = \dot{\beta}_\tau \tau + \beta_\tau =: \beta'_\tau$
- e.g. $X = Id$, $n = p = 1$,

$$\mathbb{E}[\beta'_t] = \begin{cases} 0, & \text{if } t < 1/y; \\ \mathbb{E}(y) = \beta^* + \varepsilon, & \text{otherwise}, \end{cases}$$

$y > 0$

Inverse scale space (ISS)

Nonlinear ODE (differential inclusion)

$$\dot{\rho}_t = \frac{1}{n} X^T (y - X\beta_t), \tag{3a}$$

$$\rho_t \in \partial \|\beta_t\|_1. \tag{3b}$$

starting at $t = 0$ and $\rho(0) = \beta(0) = \mathbf{0}$.

- Replace ρ/t in LASSO by $\mathrm{d}\rho/\mathrm{d}t$
- Burger-Gilboa-Osher-Xu'06 (image recovery and recovers the objects in an image in an inverse-scale order as t increases (larger objects appear in β_t first))

Solution Path

- β_t is piece-wise constant in t:

$$\begin{aligned} \beta_{t_{k+1}} = \arg\min_\beta \quad & \|y - X\beta\|_2^2 & & \\ \text{subject to} \quad & (\rho_{t_{k+1}})_i \beta_i \geq 0 & \forall\ i \in S_{k+1}, & \\ & \beta_j = 0 & \forall\ j \in T_{k+1}. & \end{aligned} \qquad (4)$$

- $t_{k+1} = \sup\{t > t_k : \rho_{t_k} + \frac{t - t_k}{n} X^T (y - X\beta_{t_k}) \in \partial \|\beta_{t_k}\|_1\}$
- ρ_t is piece-wise linear in t,

$$\begin{cases} \rho_t = \rho_{t_k} + \frac{t - t_k}{t_{k+1} - t_k} \rho_{t_{k+1}}, \\ \beta_t = \beta_{t_k}, \end{cases} \qquad t \in [t_k, t_{k+1}),$$

- Sign consistency $\rho_t = \mathrm{sign}(\beta^*) \Rightarrow \beta_t = \tilde{\beta}^*$

Discretized Algorithm

Damped Dynamics: continuous solution path

β_t

$$\dot{\rho}_t + \frac{1}{\kappa}\dot{\beta}_t = \frac{1}{n}X^T(y - X\beta_t), \quad \rho_t \in \partial\|\beta_t\|_1. \tag{5}$$

$k \to \infty$

Linearized Bregman Iteration as forward Euler discretization (Osher-Burger-Goldfarb-Xu-Yin'05, Yin-Osher-Goldfarb-Darbon'08): for $\rho_k \in \partial\|\beta_k\|_1$,

$$\rho_{k+1} + \frac{1}{\kappa}\beta_{k+1} = \rho_k + \frac{1}{\kappa}\beta_k + \frac{\alpha_k}{n}X^T(y - X\beta_k),$$

- Damping factor: $\kappa > 0$
- Step size: α_k

Comparisons

Linearized Bregman Iteration:

$$z_{t+1} = z_t - \alpha_t X^T(\kappa X Shrink(z_t, 1) - y)$$

- This is not **ISTA**:

$$z_{t+1} = Shrink(z_t - \alpha_t X^T(Xz_t - y), \lambda)$$

  - ISTA solves **LASSO** for fixed λ
- This is not **OMP** which only adds in variables.
- This is not Donoho-Maleki-Montanari's **AMP**

Matrix Completion

The **Linearized Bregman Iteration** can be generalized to Matrix completions (Cai-Candes-Shen'10)

$$z_{t+1} = z_t - \alpha_t X^T \cdot (\kappa X \cdot \mathit{Shrink}(z_t, 1) - y)$$

where

- Shrink is an Singular Value Shrinkage operator
- X, y, z are matrices with matrix inner products

ISS/LBI often beats LASSO

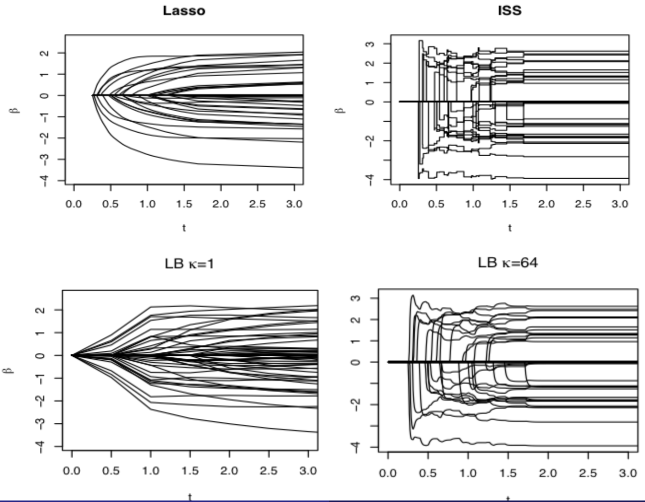
$n = 200$, $p = 100$, $S = \{1, \ldots, 30\}$, $x_i \sim N(0, \Sigma_p)$ ($\sigma_{ij} = 1/(3p)$ for $i \neq j$ and 1 otherwise)

σ	LB($\kappa = 4$)	LB($\kappa = 64$)	LB($\kappa = 1024$)	ISS	LASSO
1	0.9771(0.0124)	0.994(0.0069)	0.9947(0.0065)	0.9948(0.0064)	0.9945(0.0068)
3	0.9604(0.0169)	0.9867(0.009)	0.9882(0.0083)	0.9884(0.0082)	0.9879(0.0086)
5	0.9393(0.0226)	0.9659(0.0188)	0.9673(0.0188)	0.9676(0.0187)	0.9671(0.0187)

TABLE 1

Mean AUC (standard deviation) for three methods at different noise levels (σ): ISS has a slightly better performance than LASSO in terms of AUC and as κ increases, the performance of LB approaches that of ISS. As noise level σ increases, the performance of all the methods drops.

But regularization paths are different



Convergence theory does not explain

- Bregman ISS

$$\dot{\rho}(t) = \frac{1}{n} X^T (y - X\beta(t)),$$
$$\rho(t) \in \partial \|\beta(t)\|_1.$$

Limit is solution to $\min_\beta \|\beta\|_1$, s.t. $X^T y = X^T X \beta$, possibly overfitted under noise.

- Linearized Bregman ISS

$$\dot{\rho}(t) + \frac{1}{\kappa}\dot{\beta}(t) = \frac{1}{n} X^T (y - X\beta(t)),$$
$$\rho(t) \in \partial \|\beta(t)\|_1.$$

Limit is solution to $\min_\beta \|\beta\|_1 + \frac{1}{2\kappa}\|\beta\|_2^2$, s.t. $X^T y = X^T X \beta$.

Early Stopping Regularization!

Our aim is to show that there exists points on their paths $(\beta(t), \rho(t))_{t\geq 0}$, which are

- sparse
- sign-consistent (the same sparsity pattern of nonzeros as true signal)
- unbiased (or less bias) than LASSO path
- decidable in a data-dependent way (adaptive)

Path Consistency Theory

Precisely

- Under what conditions one can achieve
  - sign consistency (model selection consistency)
  - l_2-consistency ($\|\beta(t) - \tilde{\beta}^*\|_2 \leq O(\sqrt{s \log p/n})$)
- When sign-consistency holds, Bregman ISS path returns the oracle estimator without bias
- Early stopping regularization against overfitting noise

Assumptions

(A1) Restricted Strongly Convex: $\exists \gamma \in (0, 1]$,

Cov $$\frac{1}{n} X_S^T X_S \geq \gamma I$$

(A2) Incoherence/Irrepresentable Condition: $\exists \eta \in (0, 1)$,

$$\left\| \frac{1}{n} X_T^T X_S^{\dagger} \right\|_{\infty} = \left\| \frac{1}{n} X_T^T X_S \left(\frac{1}{n} X_S^T X_S \right)^{-1} \right\|_{\infty} \leq 1 - \eta$$

- The incoherence condition is used independently in Tropp'04, Yuan-Lin'05, Zhao-Yu'06, and Zou'06, Wainwright'09,etc.

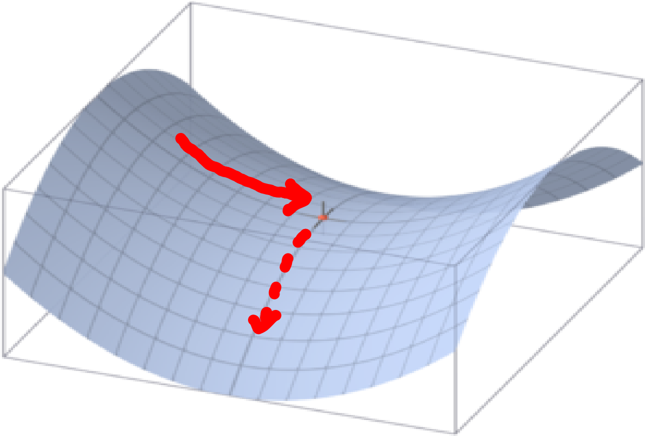
Understanding the Dynamics

Bregman ISS as gradient descent in dual space:

$$\dot{\rho}_t = -\nabla L(\beta_t) = \frac{1}{n} X^T (y - X(\dot{\beta}_t t + \beta_t)), \quad \rho_t \in \partial \|\beta_t\|_1$$

- incoherence condition and strong signals ensure it firstly evolves on index set S to reduce the loss
- strongly convex in subspace restricted on index set $S \Rightarrow$ fast decay in loss
- early stopping after all strong signals are detected, before picking up the noise

Early stop around the saddle point



Path Consistency

Theorem (Path Consistency of Bregman ISS)

Assume (A1) and (A2). Define

$$\bar{\tau} := \frac{\eta}{2\sigma}\sqrt{\frac{n}{\log p}}\left(\max_{j\in T}\|X_j\|\right)^{-1},$$

and the smallest magnitude $\beta^*_{\min} = \min(|\beta^*_i| : i \in S)$. *Then*

- **(No-false-positive)** *for all* $t \leq \bar{\tau}$, *the path has no-false-positive with high probability,* $\mathrm{supp}(\beta(t)) \subseteq S$*;*

Note: equivalent to LASSO with $\lambda^* = 1/\bar{\tau}$ (Wainwright'09)

Path Consistency, continued

Theorem (continued)

- **(Sign consistency for path)** *instead if the signal is strong enough such that*

$$\beta^*_{min} \geq \left(\frac{4\sigma}{\gamma^{1/2}} \vee \frac{8\sigma(2 + \log s)\left(\max_{j \in T} \|X_j\|\right)}{\gamma\eta} \right) \sqrt{\frac{\log d}{n}}$$

then there is $\tau \leq \bar{\tau}$ such that solution path $\beta(t)$ reaches sign consistency for every $t \in [\tau, \bar{\tau}]$.

Open: can we drop $\log s$ above? Nearly equivalent to LASSO (Wainwright'09)

Path Consistency, continued

Theorem (continued)

- **(l_2-consistency)** *Under (A1) and (A2), there is an early stopping $\tau_n \in [0, \overline{\tau}]$, such that with high probability $\|\beta(\tau_n) - \beta^*\|_2 \leq C_0\sqrt{\frac{s \log d}{n}}$, where*

$$C_0 = \frac{2\sigma}{\gamma^{1/2}} + \frac{8\sigma\left(\max_{j\in T}\|X_j\|\right)}{\eta\gamma}$$

Note: for $\bar{\gamma} I_s \geq \frac{1}{n} X_S^T X_S \geq \underline{\gamma} I_s$,

$$\|\beta(\overline{\tau}) - \beta^*\|_2 \leq \sqrt{\frac{\bar{\gamma}}{\underline{\gamma}}}\left(C_0 + \frac{2\sigma}{\sqrt{\underline{\gamma}}}\right)\sqrt{\frac{s \log p}{n}}$$

Remark

- Similar results for LASSO are established in Wainwright'09 with $\lambda^* = 1/\bar{\tau}$, where the lasso path are sign-consistent
- $\beta(\bar{\tau})$ is unbiased, β^* while LASSO estimator is biased
- The l_2-error bound is of minimax optimal rates
- The (temporal) mean path

$$\bar{\beta}(\tau) := \frac{1}{\tau}\int_0^\tau \beta(s)ds \tag{6}$$

is sign-consistent under precisely the same condition as LASSO, though they are different!

Generalization To Discrete Setting

Theorem (Linearized Bregman Iterations)

Assume that κ is large enough and α is small enough, with $\kappa\alpha\|X_S^* X_S\| < 2$,

$$\bar{\tau} := \frac{(1 - B/\kappa\eta)\eta}{2\sigma}\sqrt{\frac{n}{\log p}}\left(\max_{j\in T}\|X_j\|\right)^{-1}$$

$$\beta^*_{max} + 2\sigma\sqrt{\frac{\log p}{\gamma n}} + \frac{\|X\beta^*\|_2 + 2s\sqrt{\log n}}{n\sqrt{\gamma}} \triangleq B \leq \kappa\eta,$$

then all the results can be extended to discrete algorithm setting (Linearized Bregman Iterations).

Data-dependent Stopping Rules

- Residue $r(t) := y - X\beta(t)$
- Adaptive early stopping rules (Cai-Wang'11)
  - $\|r(t)\|_2 \leq \sigma\sqrt{n + 2\sqrt{n \log n}}$
  - $\|X^T r(t)\|_\infty \leq 2\sigma\sqrt{\max_i \|X_i\| \log p}$
- σ can be estimated through Huber's concomitant scale estimation
  - consistency: Sun-Zhang (scaled LASSO) and Belloni-Chernozhukov-Wang (square-root Lasso)

Idea of Proof: I

1. No-false-positive condition is the same as LASSO
2. For $t \leq \bar{\tau}$ consider *Oracle dynamcs*

$$\frac{d\rho'_S}{dt} = -\frac{1}{n} X_S^T X_S (\beta'_S - \tilde{\beta}^*_S), \quad \rho'_S(t) \in \partial \|\beta'_S(t)\|_1, \qquad (7)$$

where $\frac{1}{n} X_S^T X_S \geq \gamma I_s$.

- a generalized Grönwall-Bellman-Bihari (differential) inequality:

$$\frac{d}{dt}(D(\tilde{\beta}^*_S, \beta'_S)) \leq -\gamma F^{-1}(D(\tilde{\beta}^*_S, \beta'_S))$$

where F is a piecewise polynomial and D is the Bregman distance associated to $\| \cdot \|_1$.

Idea of Proof: II

3 Sign-consistency and l_2-consistency are reached by setting these stopping time $\tilde{\tau}_i \leq \bar{\tau}$ where oracle dynamics meets Bregman ISS

$$\tilde{\tau}_1 := \inf\{t > 0 : \mathrm{sign}(\beta'_S(t)) = \mathrm{sign}(\tilde{\beta}^*_S)\} \leq O(\log s / \beta^*_{\min})$$

$$\tilde{\tau}_2(C) := \inf\left\{ t > 0 : ||\beta'_S(t) - \tilde{\beta}^*_S||_2 \leq C\sqrt{\frac{s \log p}{n}} \right\} \leq O\left(\frac{1}{C}\sqrt{\frac{n}{p}}\right)$$

Discussion

These results can be extended to discrete algorithm, the simple 1-line Linearized Bregman iteration:

- achieve mean path sign-consistency, **statistically equivalent to LASSO**
- and path sign-consistency with less bias, **better than LASSO**
- LB iteration is as simple as ISTA, but more powerful
  - cost: two free-parameters, κ and step-size α_k
  - tips: $\alpha_k \kappa \|\Sigma_n\| < 2$, large κ to remove Elastic-net effect
- Early stopping regularization maybe better than penalization (e.g. Engl-Hanke-Neubauer'00, Y.-Rosasco-Caponnetto'07)
- A simple dynamics acts as if nonconvex optimization...

Reference

- Osher, Ruan, Xiong, Yao, and Yin, *Sparse Recovery via Differential Equations*, arXiv:1406.7728
- Xu, Xiong, Huang, and Yao, *Robust Statistical Ranking: Theory and Algorithms*, arXiv:1408.3467

- Matlab and R packages are available

Acknowledgement

- Theory
  - *Stanley Osher*, *Wotao Yin* (UCLA)
  - *Feng Ruan*, *Jiechao Xiong* (PKU)
- Applications: *Ming Yan* (UCLA); *Qianqian Xu*, *Chendi Huang* (PKU)
- Discussions: *Ming Yuan* (U Wisconsin), *Lie Wang* (MIT), *Peter Bickel* and *Bin Yu* (UCB)
- Grants:
  - IPAM, National Basic Research Program of China (973 Program), NSFC