Sparse Learning via Inverse Scale Space Method: from Linear Models to Neural Networks

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Sparsity lies in everywhere ...

In "compressive sensing",

- signals are sparse w.r.t. certain basis (e.g. Fourier, Wavelet)
- signals are piecewise constant or smooth
- signals might be of low rank matrix or tensor
- sparse graphical models, e.g. Ising, Potts

In "deep learning",

- sparse (local) inputs in convolutional networks (Minsky et al.)
- symmetry: translation invariance, weight sharing (Fukushima, LeCun)
- Compositional Sparsity (Poggio)
- pruning: Lottery Ticket Hypothesis (Frankle & Carbin)

1 DessiLBI (Python)
- The Lottery Ticket Hypothesis

2 From LASSO to Inverse Scale Space
- The LASSO
- LASSO and Bias
- Differential Inclusion of Inverse Scale Space
- Statistical Path Consistency with Early Stopping
- Large Scale Algorithm: Linearized Bregman Iteration (LBI)

3 Variable Splitting: Split LBI
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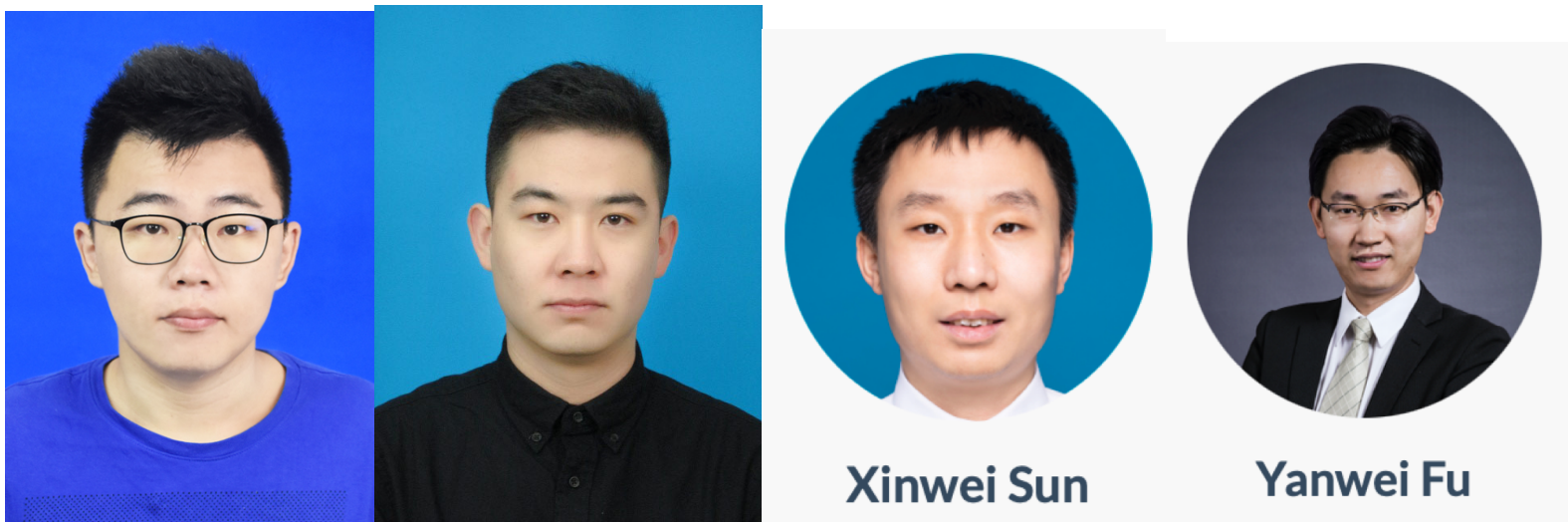
- Application: Finding Sparse Subnets in Deep Learning

4 Summary

5 *Appendix: Libra (R)

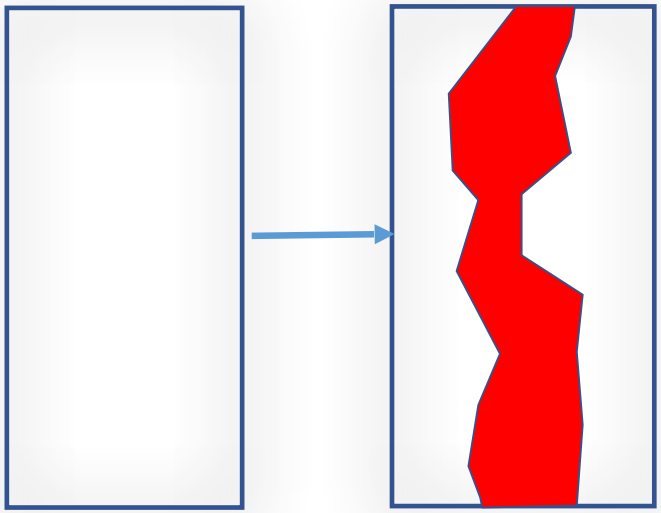
DessiLBI: Deep structurally splitting Linearized Bregman Iteration

https://github.com/DessiLBI2020/DessiLBI



Courtesy of Chen Liu/Donghao Li (HKUST-Fudan), Xinwei Sun/Yanwei Fu (Fudan)

Lottery Ticket Hypothesis: Sparse Subnetworks



Over-parameterized Networks W

Compressive Networks W_s

Lottery Ticket Hypothesis

- *Dense, randomly-initialized, feed-forward networks contain subnetworks (winning tickets) that – when trained in isolation – reach test accuracy comparable to the original network in a similar number of iterations.* (Frankle & Carbin, 2019)

Rewinding the network from the initialization, and find "winning ticket" subnet

Finding the "winning tickets"

- Existing approaches typically adopt the following 2-stage algorithms:
  - [(i)] Train dense overparameterized networks (overparameterization helps optimization landscape without hurting the generalization, yet expensive)
  - [(ii)] Prune+retrain to produce sparse subnets
- **DessiLBI** gives us 1-stage procedure (end-to-end) to render sparse subnet structures with *Early Stopping*
  - [Reference] Yanwei Fu, et al. ICML 2020 and TPAMI 2022, with a CVPR 2022 tutorial at `https://sparse-learning.github.io/`

DessiLBI: Sparse Filters Learned on MNIST

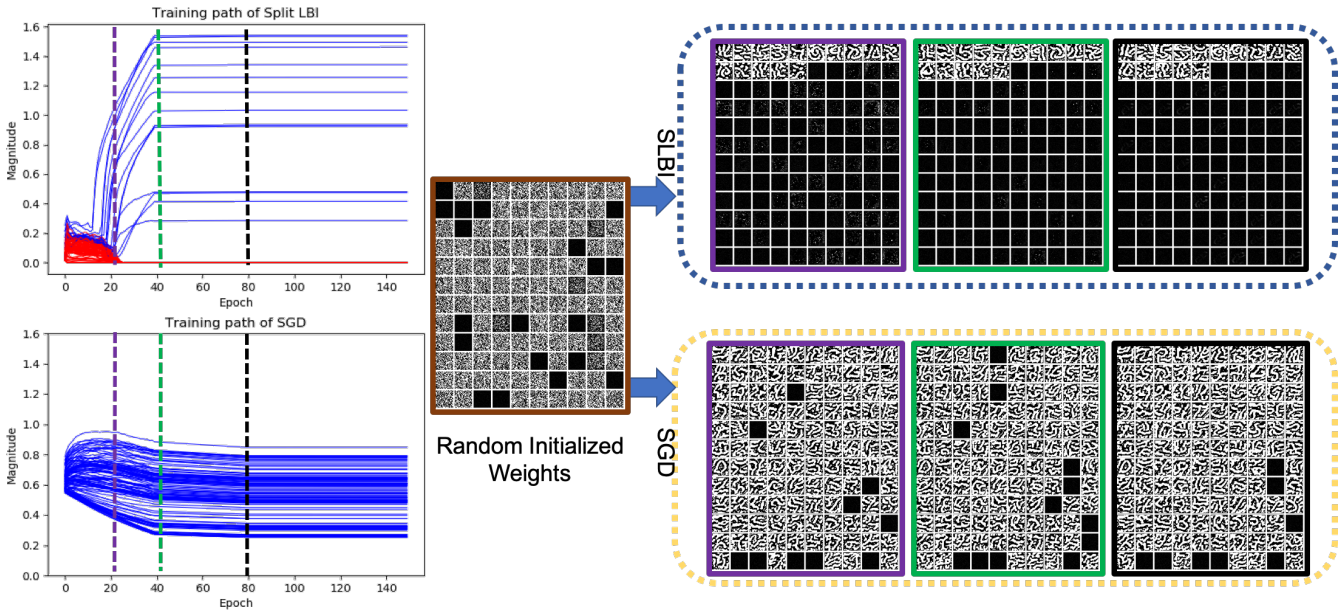


Figure: [Fu et al. ICML 2020/TPAMI 2022]Visualization of solution path and filter patterns in the third convolutional layer (i.e., conv.c5) of LetNet-5, trained on MNIST, showing a sparse selection of filters without sacrificing accuracy.

Sparse Neural Nets in Early Stopping (Lottery Tickets)

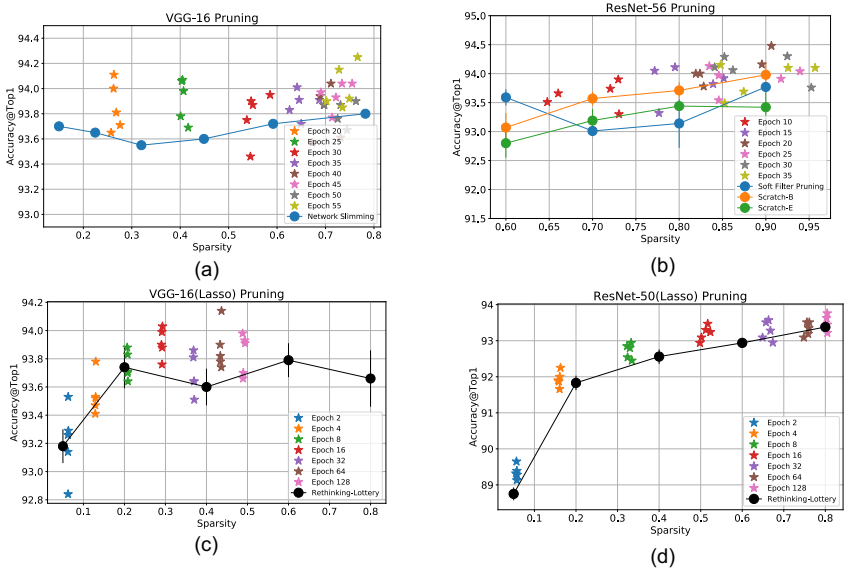


Figure: SplitLBI with early stopping finds sparse subnets whose test accuracies (stars) after retrain are comparable or even better than the baselines (Network Slimming, Soft-Filter Pruning, Scratch-B, Scratch-E, and "Rethinking-Lottery" as reported in Rethink the Value of Pruning. Sparse filters of VGG-16 and ResNet-56 are show in (a) and (b), while sparse weights of VGG-16 and ResNet-50 are shown in (c) and (d).

DessiLBI: Non-semantic Features Learned on ImageNet

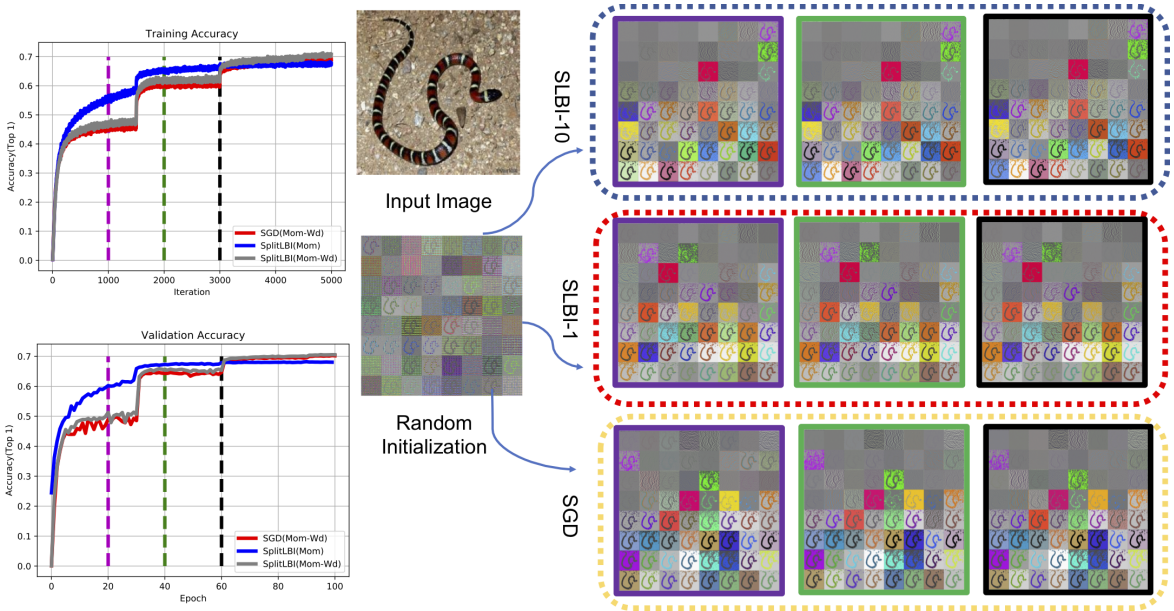


Figure: Visualization of the first convolutional layer filters of ResNet-18 trained on ImageNet-2012, where texture features are more important than colour/shapes. Given the input image and initial weights visualized in the middle, filter response gradients at 20 (purple), 40 (green), and 60 (black) epochs are visualized. SGD with Momentum (Mom) and Weight Decay (WD), is compared with SLBI.

How does it work?

In the sequel, we shall see a story on statistical model selection consistency with early stopping:

- A simple iterative algorithm shadows a particular kind of dynamics: differential inclusions of inverse scale spaces, as special cases of Mirror Descent, where important features are learned fast
- Simple discretized algorithm, amenable for parallel implementation
- Under nearly the same condition as LASSO, it reaches model selection consistency via early stopping
- but may incur less bias than LASSO
- Equipped with variable splitting, it weakens the conditions of generalized LASSO in feature selection

Sparse Linear Regression

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

$$y = X\beta^* + \epsilon, \qquad y \in \mathbb{R}^n$$

where $\epsilon \sim \mathcal{N}(0, \sigma^2)$ is **noise**.

- Basic Sparsity: $S := \mathrm{supp}(\beta^*)$ ($s = |S|$) and T be its complement.
  - X_S (X_T) be the columns of X with indices restricted on S (T)
  - X is n-by-p, with $p \gg n \geq s$.
- Generalized Structural/Transformational Sparsity: $\gamma^* = D\beta^*$ is sparse, where D is a linear transform (wavelet, gradient, etc.), $S = \mathrm{supp}(\gamma^*)$
- *How to recover β^* (or γ^*) sparsity pattern (sparsistency) and estimate values with variations (consistency)?*

Best Possible in Basic Setting: The Oracle Estimator

Had God revealed S to us, the *oracle estimator* was the subset least square solution (MLE) with $\tilde{\beta}^*_T = 0$ and

$$\tilde{\beta}^*_S = \beta^*_S + \frac{1}{n}\Sigma_n^{-1} X_S^T \epsilon, \quad \text{where } \Sigma_n = \tfrac{1}{n} X_S^T X_S \tag{1}$$

"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. $\mathbb{E}[\tilde{\beta}^*] = \beta^*$.

The Lasso

- Lasso stands for **Least Absolute Shrinkage and Selection Operator**.
  - Chen-Donoho-Saunders'1996 (BPDN)
  - Tibshirani'1996 (LASSO)
- The Lasso estimator $\hat{\beta}^L_\lambda$ is the minimizer of

$$\sum_{i=1}^{n}(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij})^2 + \lambda \sum_{j=1}^{p}|\beta_j|$$

- We may use $\|\beta\|_1 = \sum_{j=1}^{p}|\beta_j|$, which is the l_1 norm.
- LASSO often shrinks coefficients to be identically 0. (This is not the case for ridge)
- Hence it performs variable selection, and yields sparse models.

Example: Lasso Regularization Path in Credit data.

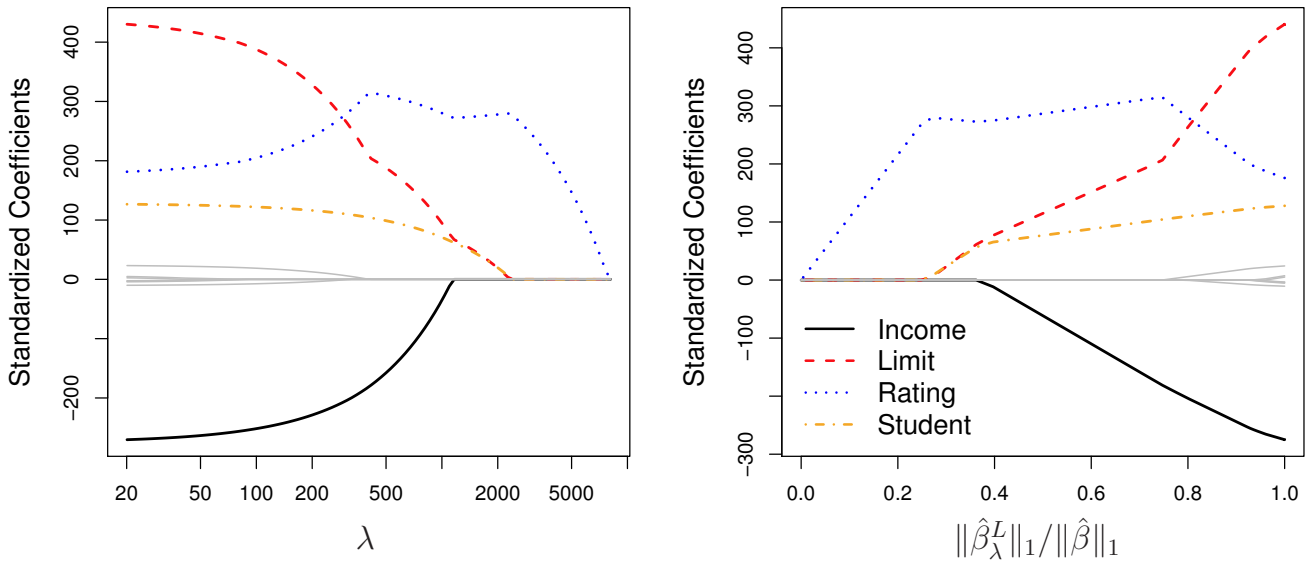


Figure: The standardized lasso coefficients on the Credit data (ISLR Chapter 6)set are shown as a function of λ and $\|\hat{\beta}^L_\lambda\|_1/\|\hat{\beta}\|_1$.

Another formulation

- For Lasso: Minimize

$$\sum_{i=1}^{n}(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij})^2 \text{ subject to } \sum_{j=1}^{p}|\beta_j| \leq s$$

- For Ridge: Minimize

$$\sum_{i=1}^{n}(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij})^2 \text{ subject to } \sum_{j=1}^{p}\beta_j^2 \leq s$$

- For l_0: Minimize

$$\sum_{i=1}^{n}(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij})^2 \text{ subject to } \sum_{j=1}^{p} I(\beta \neq 0) \leq s$$

l_0 method penalizes number of non-zero coefficients. A difficult (NP-hard) problem for optimization.

Variable selection property for Lasso

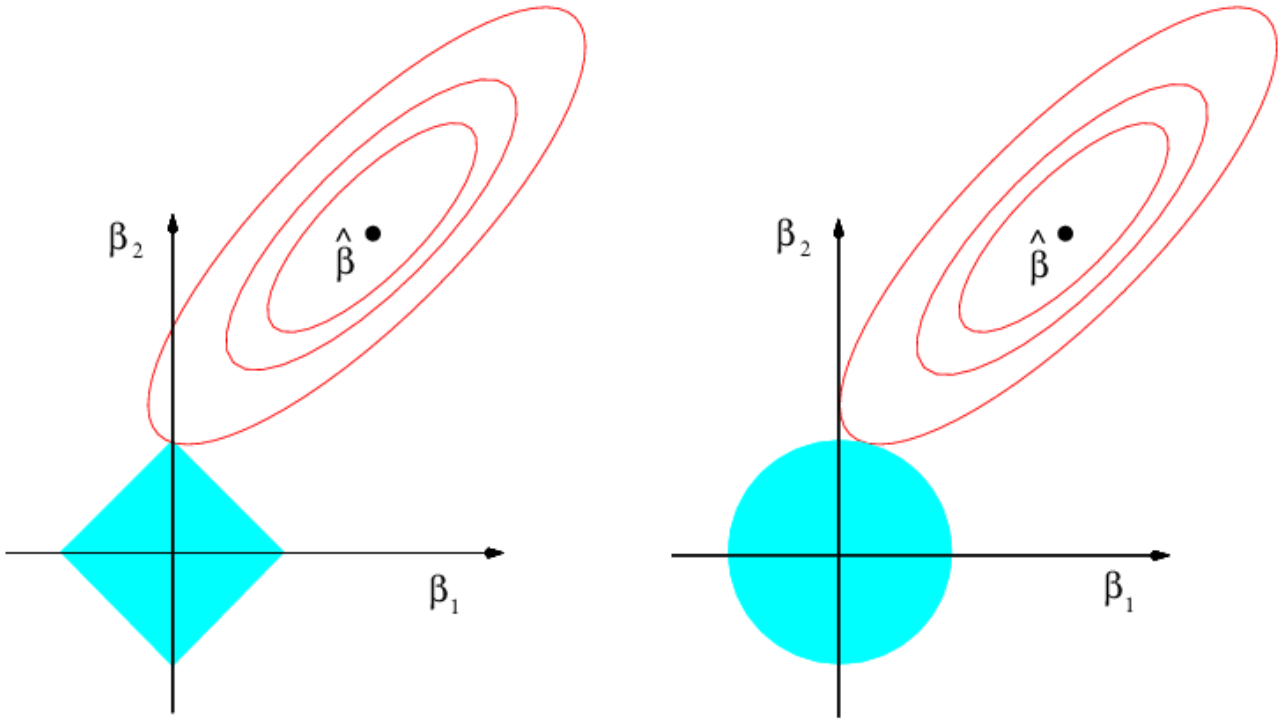


Figure: Contours of the error and constraint functions for the lasso (left) and ridge regression (right). The solid blue areas are the constraint regions, $|\beta_1| + |\beta_2| \leq s$ and $\beta_1^2 + \beta_2^2 \leq s$, while the red ellipses are the contours of the RSS.

Simple cases

- Consider the simple model $y_i = \beta_i + \epsilon_i$, $i = 1, ..., n$ and $n = p$. Then,
  - The least squares: $\hat{\beta}_j^{\mathrm{LSE}} = y_j$;
  - The ridge: $\hat{\beta}_j^R = y_j/(1+\lambda)$;
  - The Lasso: $\hat{\beta}_j^L = \mathrm{sign}(y_j)(|y_j| - \lambda/2)_+$.
- Slightly more generally, suppose input columns of the X are standardized to be mean 0 and variance 1 and are orthogonal.

$$\hat{\beta}_j^R = \hat{\beta}_j^{\mathrm{LSE}}/(1+\lambda)$$

$$\hat{\beta}_j^L = \mathrm{sign}(\hat{\beta}_j^{\mathrm{LSE}})(|\hat{\beta}_j^{\mathrm{LSE}}| - \lambda/2)_+$$

for $j = 1, ..., p$.

Example

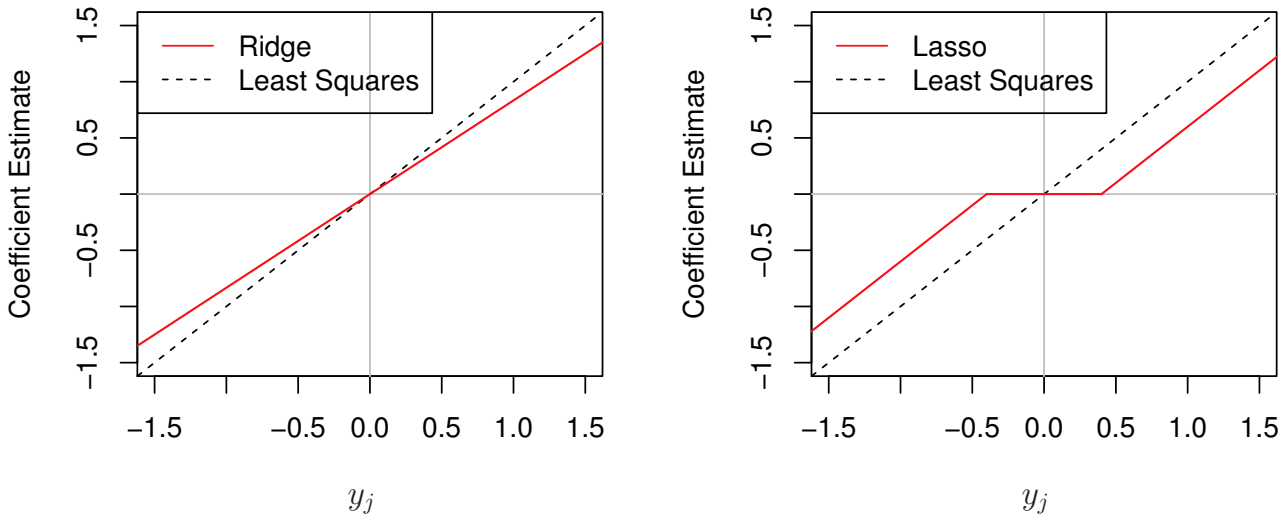


Figure: The ridge regression and lasso coefficient estimates for a simple setting with $n = p$ and X a diagonal matrix with 1 on the diagonal. Left: The ridge regression coefficient estimates are shrunken proportionally towards zero, relative to the least squares estimates. Right: The lasso coefficient estimates are soft-thresholded towards zero.

The First Order KKT Condition of LASSO

Rewrite **LASSO** as:

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

1^{st} order 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 we set $t = 2n/\lambda$ for the later convenience.

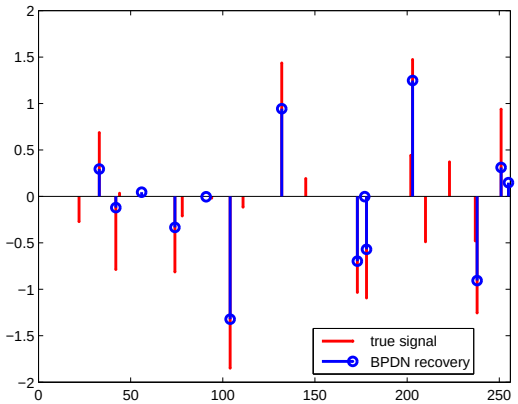
The Bias of LASSO

LASSO is biased, i.e. $\mathbb{E}(\hat{\beta}) \neq \beta^*$

- e.g. $X = Id$, $n = p = 1$, LASSO is soft-thresholding

$$\hat{\beta}_\tau = \begin{cases} 0, & \text{if } \tau < 1/\tilde{\beta}^*; \\ \tilde{\beta}^* - \frac{1}{\tau}, & \text{otherwise,} \end{cases}$$

- e.g. $n = 100$, $p = 256$, $X_{ij} \sim \mathcal{N}(0, 1)$, $\epsilon_i \sim \mathcal{N}(0, 0.1)$



True vs LASSO (t hand-tuned, courtesy of Wotao Yin)

LASSO Estimator is Biased at Path Consistency

Even when the following **path consistency** (conditions given by Zhao-Yu'06, Zou'06, Yuan-Lin'07, Wainwright'09, etc.) is reached at τ_n:

$$\exists \tau_n \in (0, \infty) \text{ s.t. } \mathrm{supp}(\hat{\beta}_{\tau_n}) = S,$$

LASSO estimate is biased away from the oracle estimator

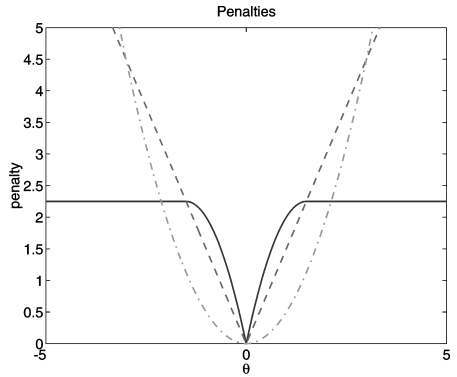
$$(\hat{\beta}_{\tau_n})_S = \tilde{\beta}^*_S - \frac{1}{\tau_n} \Sigma^{-1}_{n,S} \mathrm{sign}(\beta^*_S), \quad \tau_n > 0.$$

How to remove the bias and return the Oracle Estimator?

Nonconvex Regularization?

- To reduce bias, **non-convex** regularization was proposed (Fan-Li's SCAD, Zhang's MPLUS, Zou's Adaptive LASSO, l_q $(q < 1)$, etc.)

$$\min_{\beta} \sum_i p(|\beta_i|) + \frac{t}{2n}\|y - X\beta\|_2^2.$$



- Yet it is generally hard to locate the global optimizer
- *Any other simple scheme?*

New Idea

- LASSO:

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

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

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

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- Assuming sign-consistency in a neighborhood of τ_n,

$$\text{for } i \in S,\ \rho_{\tau_n}(i) = \text{sign}(\beta^*(i)) \in \pm 1 \Rightarrow \dot{\rho}_{\tau_n}(i) = 0,$$

$$\Rightarrow \dot{\beta}_{\tau_n}\tau_n + \beta_{\tau_n} = \tilde{\beta}^*$$

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- LASSO:

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$$\Rightarrow \dot{\beta}_{\tau_n}\tau_n + \beta_{\tau_n} = \tilde{\beta}^*$$

- Equivalently, the blue part removes bias of LASSO automatically

$$\beta^{lasso}_{\tau_n} = \tilde{\beta}^* - \frac{1}{\tau_n}\Sigma_n^{-1}\text{sign}(\beta^*) \Rightarrow \dot{\beta}^{lasso}_{\tau_n}\tau_n + \beta^{lasso}_{\tau_n} = \tilde{\beta}^*(oracle)!$$

Differential Inclusion: Inverse Scaled Spaces (ISS)

Differential inclusion replacing $\dot{\beta}^{lasso}_{\tau_n}\tau_n + \beta^{lasso}_{\tau_n}$ by β_t

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

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

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

- Replace ρ/t in LASSO KKT by $\mathrm{d}\rho/\mathrm{d}t$

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

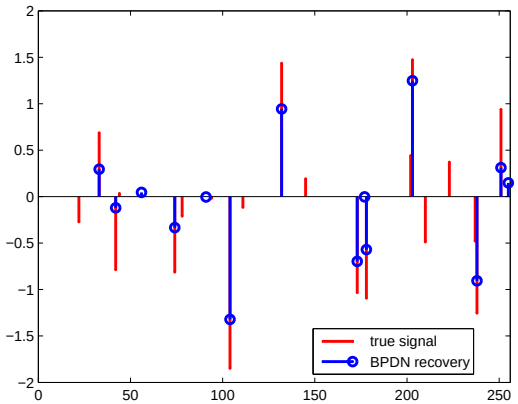
- Burger-Gilboa-Osher-Xu'06 (in image recovery it recovers the objects in an inverse-scale order as t increases (larger objects appear in β_t first))

Examples

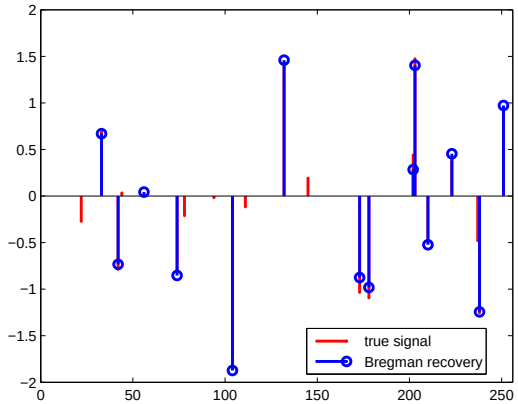
- e.g. $X = Id$, $n = p = 1$, hard-thresholding

$$\beta_\tau = \begin{cases} 0, & \text{if } \tau < 1/(\tilde{\beta}^*); \\ \tilde{\beta}^*, & \text{otherwise,} \end{cases}$$

- the same example shown before (figures by courtesy of Wotao Yin)



True vs LASSO



True vs ISS

Solution Path: Sequential Restricted Maximum Likelihood Estimate

- ρ_t is piece-wise linear in t,

$$\rho_t = \rho_{t_k} + \frac{t - t_k}{n} X^T (y - X\beta_{t_k}), \quad t \in [t_k, t_{k+1})$$

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

- β_t is piece-wise constant in t: $\beta_t = \beta_{t_k}$ for $t \in [t_k, t_{k+1})$ and $\beta_{t_{k+1}}$ is the **sequential restricted Maximum Likelihood Estimate** by solving nonnegative least square (Burger et al.'13; Osher et al.'16)

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

- Note: Sign consistency $\rho_t = \mathrm{sign}(\beta^*) \Rightarrow \beta_t = \tilde{\beta}^*$ the oracle estimator

Example: Regularization Paths of LASSO vs. ISS

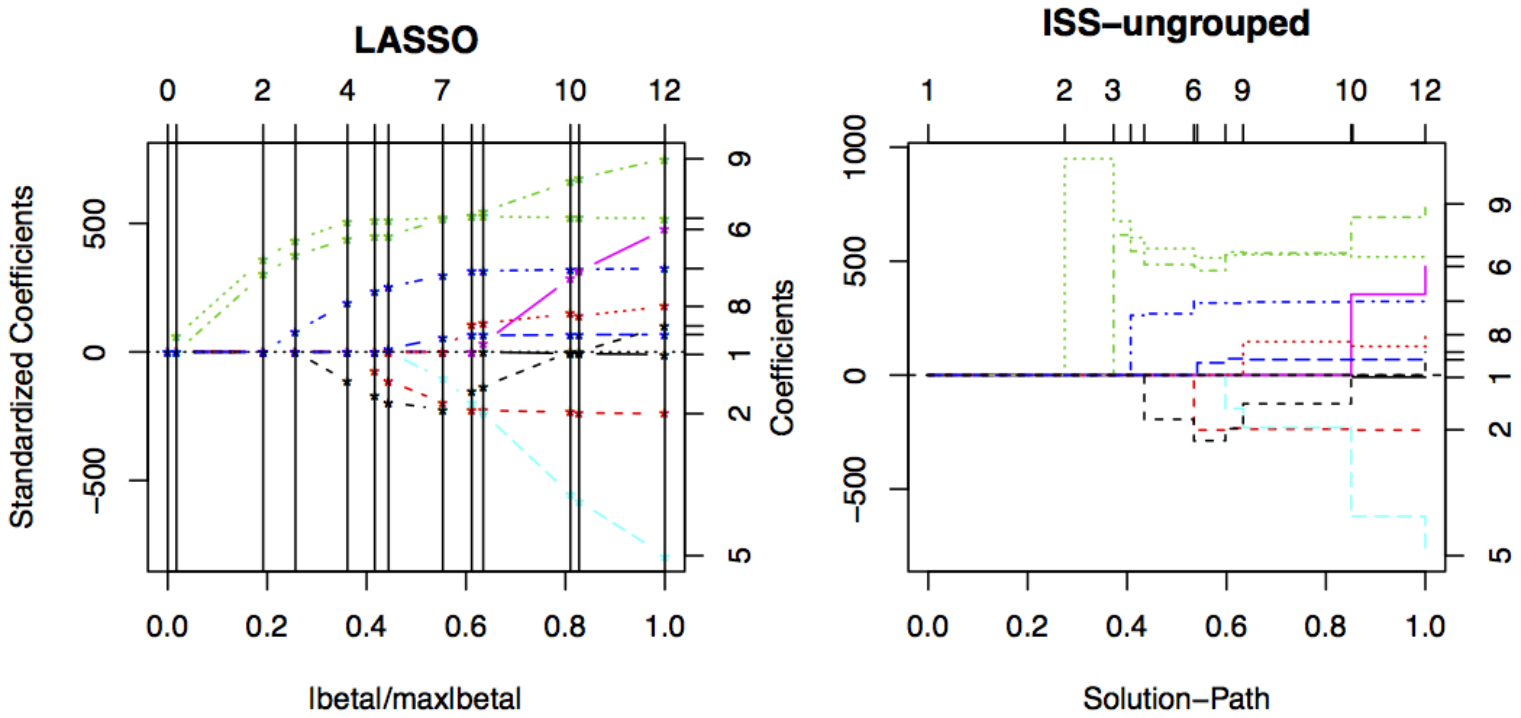


Figure: Diabetes data (Efron et al.'04) and regularization paths are different, yet bearing similarities on the order of parameters being nonzero

Why? A Path Consistency Theory

Our aim is to show that under nearly the same conditions for sign-consistency of LASSO, 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)
- the oracle estimator which is unbiased, better than the LASSO estimate.
- Early stopping regularization is necessary to prevent overfitting noise!

Assumptions

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

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

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

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

- "Irrepresentable" means that one can not represent (regress) column vectors in X_T by covariates in X_S.
- The incoherence/irrepresentable condition is used independently in Tropp'04, Yuan-Lin'05, Zhao-Yu'06, Zou'06, Wainwright'09, etc.

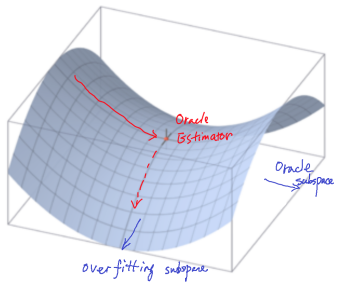
Understanding the Dynamics

ISS as restricted gradient descent:

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

such that

- incoherence condition and strong signals ensure it firstly evolves on index set S (Oracle Subspace) 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 overfitting noise



Path Consistency

Theorem (Osher-Ruan-Xiong-Y.-Yin'2016)

Assume (A1) and (A2). Define an early stopping time

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

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

- *No-false-positive: for all* $t \le \bar{\tau}$, *the path has no-false-positive with high probability,* $\mathrm{supp}(\beta(t)) \subseteq S$;
- *Consistency: moreover if the signal is strong enough such that*

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

there is $\tau \le \bar{\tau}$ *such that solution path* $\beta(t)) = \tilde{\beta}^*$ *for every* $t \in [\tau, \bar{\tau}]$.

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

Large scale algorithm: Linearized Bregman Iteration

Damped Dynamics: continuous solution path

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

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

$$\rho_{k+1} + \frac{1}{\kappa}\beta_{k+1} = \rho_k + \frac{1}{\kappa}\beta_k + \frac{\alpha_k}{n}X^T(y - X\beta_k), \tag{6}$$

where

- Damping factor: $\kappa > 0$
- Step size: $\alpha_k > 0$ s.t. $\alpha_k\kappa\|\Sigma_n\| \leq 2$
- Moreau Decomposition: $z_k := \rho_k + \frac{1}{\kappa}\beta_k \Leftrightarrow \beta_k = \kappa \cdot \mathit{Shrink}(z_k, 1)$

Comparison with ISTA

Linearized Bregman (LB) iteration:

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

which is not **ISTA**:

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

Comparison:

- **ISTA**:
  - as $t \to \infty$ solves **LASSO**: $\frac{1}{n}\|y - X\beta\|_2^2 + \lambda\|\beta\|_1$
  - parallel run ISTA with $\{\lambda_k\}$ for LASSO regularization paths
- **LB**: a single run generates the whole regularization path at same cost of ISTA-LASSO estimator for a fixed regularization

LBI generates regularization paths

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

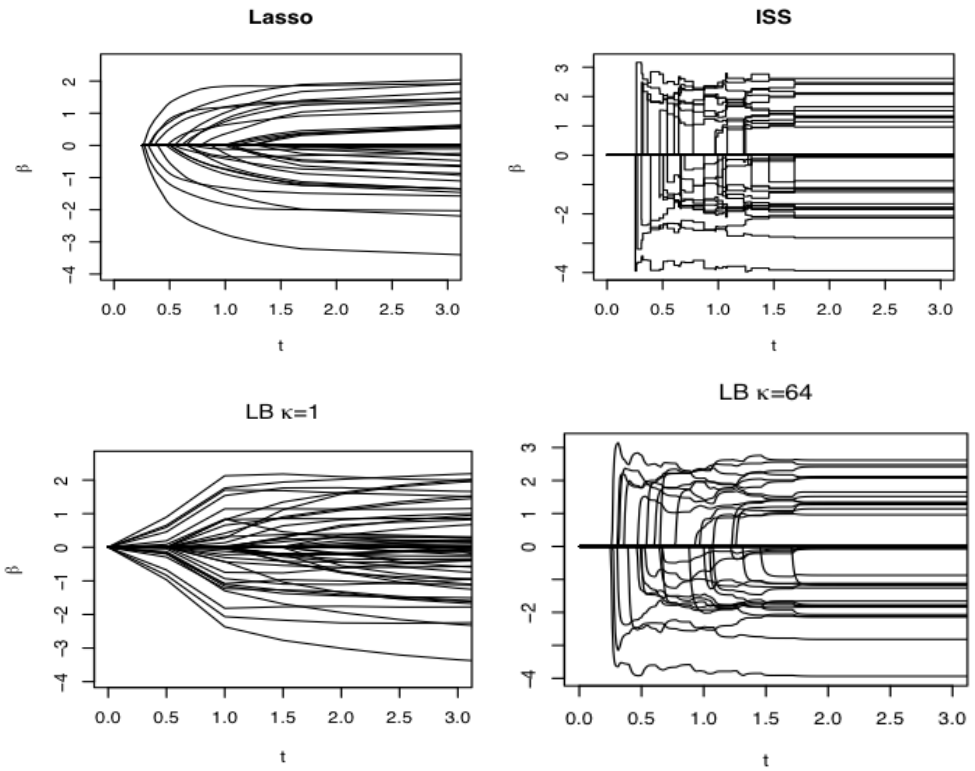


Figure: As $\kappa \to \infty$, LB paths have a limit as piecewise-constant ISS path

General Loss and Regularizer

$$\dot{\eta}_t = -\frac{\kappa_0}{n}\sum_{i=1}^{n}\nabla_\eta \ell(x_i, \theta_t, \eta_t) \tag{7a}$$

$$\dot{\rho}_t + \frac{\dot{\theta}_t}{\kappa_1} = -\frac{1}{n}\sum_{i=1}^{n}\nabla_\theta \ell(x_i, \theta_t, \eta_t) \tag{7b}$$

$$\rho_t \in \partial\|\theta_t\|_* \tag{7c}$$

- $\ell(x_i, \theta)$ is a loss function: negative logarithmic likelihood, non-convex loss (neural networks), etc.
- $\|\theta_t\|_*$ is the Minkowski-functional (gauge) of dictionary convex hulls:

$$\|\theta\|_* := \inf\{\lambda \geq 0 : \theta \in \lambda K\}, \quad K \text{ is a symmetric convex hull of } \{a_i\}$$

  - it can be generalized to non-convex regularizers

More reference on generalizations

- **Logistic Regression**: loss – conditional likelihood, regularizer – l_1 (Shi-Yin-Osher-Saijda'10,Huang-Yao'18)
- **Graphical Models** (Gaussian/Ising/Potts Model): loss – likelihood, composite conditional likelihood, regularizer – l_1 and group l_1 (Huang-Yao'18)
- **Fused LASSO/TV**: split Bregman with composite l_2 loss and l_1 gauge (Osher-Burger-Goldfarb-Xu-Yin'06, Burger-Gilboa-Osher-Xu'06, Yin-Osher-Goldfarb-Darbon'08, Huang-Sun-Xiong-Yao'16)
- **Matrix Completion/Regression**: gauge – the matrix nuclear norm (Cai-Candès-Shen'10)
- for more examples, see Appendix: Libra (R) (by Ruan-Xiong-Y. downloadable at `https://cran.r-project.org/web/packages/Libra/`)

Structural or Transformational Sparsity

Structural/Transformational Sparse Regression:

$$y = X\beta^\star + \epsilon, \tag{8a}$$

$$\gamma^\star = D\beta^\star, \tag{8b}$$

where

$$S = \mathrm{supp}\left(\gamma^\star\right), \quad s := |S| \ll p.$$

Split LBI vs. Generalized LASSO

- Generalized LASSO (`genlasso`):

$$\arg\min_{\beta} \left(\frac{1}{2n} \|y - X\beta\|_2^2 + \lambda \|D\beta\|_1 \right). \tag{9}$$

- Split LBI: Loss that splits prediction vs. sparsity control

$$\ell(\beta, \gamma) := \frac{1}{2n} \|y - X\beta\|_2^2 + \frac{1}{2\nu} \|\gamma - D\beta\|_2^2 \quad (\nu > 0). \tag{10}$$

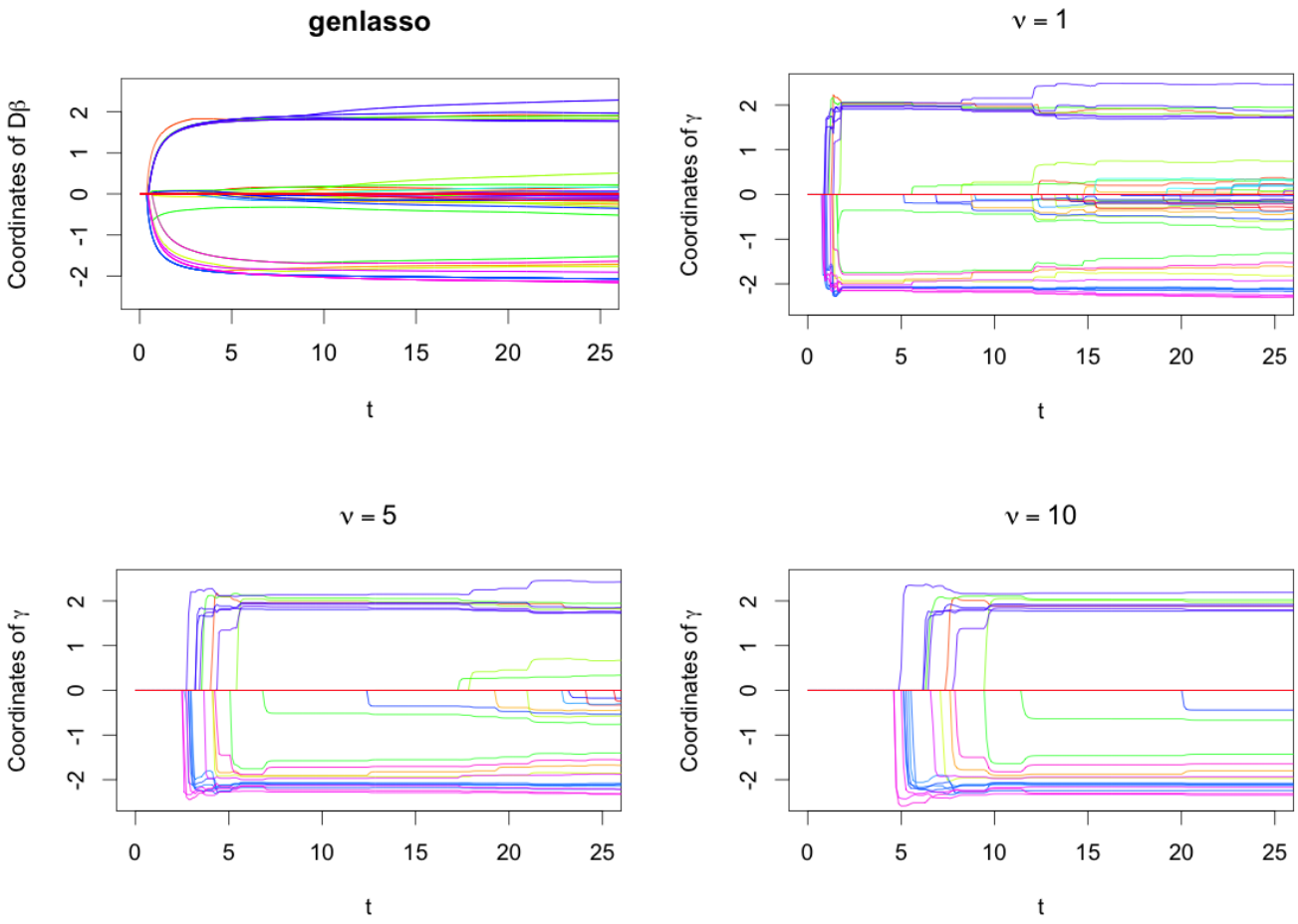
Algorithm [Huang-Sun-Xiong-Y. 2016] :

$$\beta_{k+1} = \beta_k - \kappa\alpha \nabla_\beta \ell(\beta_k, \gamma_k), \tag{11a}$$

$$z_{k+1} = z_k - \alpha \nabla_\gamma \ell(\beta_k, \gamma_k), \tag{11b}$$

$$\gamma_{k+1} = \kappa \cdot \mathrm{prox}_{\|\cdot\|_1}(z_{k+1}), \tag{11c}$$

Split LBI vs. Generalized LASSO paths



Split LBI may beat Generalized LASSO in Model Selection

genlasso	Split LBI			genlasso	Split LBI		
	$\nu = 1$	$\nu = 5$	$\nu = 10$		$\nu = 1$	$\nu = 5$	$\nu = 10$
.9426	.9845	.9969	**.9982**	.9705	.9955	.9996	**.9998**
(.0390)	(.0185)	(.0065)	(**.0043**)	(.0212)	(.0056)	(.0014)	(**.0009**)

- Example: $n = p = 50$, $X \in \mathbb{R}^{n \times p}$ with $X_j \sim N(0, I_p)$, $\epsilon \sim N(0, I_n)$
- (Left) $D = I$ (LASSO vs. Split LBI)
- (Right) 1-D fused (generalized) LASSO vs. Split LBI
- In terms of Area Under the ROC Curve (AUC), Split LBI has less false discoveries than `genlasso`
- *Why*? Split LBI may need weaker irrepresentable conditions than generalized LASSO...

Structural Sparsity Assumptions

- Define $\Sigma(\nu) := (I - D(\nu X^* X + D^T D)^\dagger D^T)/\nu$.
- **Assumption 1**: Restricted Strong Convexity (RSC).

$$\Sigma_{S,S}(\nu) \succeq \lambda \cdot I. \tag{12}$$

- **Assumption 2**: Irrepresentable Condition (IRR).

$$\mathrm{IRR}(\nu) := \|\Sigma_{S^c,S}(\nu) \cdot \Sigma_{S,S}^{-1}(\nu)\|_\infty \leq 1 - \eta. \tag{13}$$

- $\nu \to 0$: RSC and IRR above reduce to the neccessary and sufficient for consistency of `genlasso` (Vaiter'13,LeeSunTay'13).
- $\nu \neq 0$: by allowing variable splitting in proximity, IRR above can be weaker than literature, bringing better variable selection consistency than `genlasso` (observed before)!

Remark: Identifiable Conditions (IC)

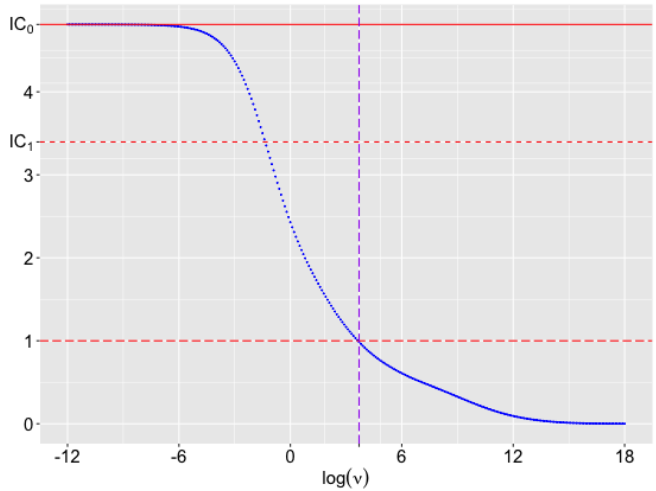
- Let the columns of W form an orthogonal basis of $\ker(D_{S^c})$.

$$\Omega^S := \left(D_{S^c}^\dagger\right)^T \left(X^*XW\left(W^TX^*XW\right)^\dagger W^T - I\right) D_S^T, \tag{14}$$

$$\mathrm{IC}_0 := \left\|\Omega^S\right\|_\infty, \ \mathrm{IC}_1 := \min_{u\in\ker(D_{S^c})} \left\|\Omega^S \mathrm{sign}\left(D_S\beta^\star\right) - u\right\|_\infty. \tag{15}$$

- The sign consistency of `genlasso` has been proved, under $\mathrm{IC}_1 < 1$ [Vaiter et al. 2013].
- The sign consistency of Split LBI is proved under $\mathrm{IRR}(\nu) < 1$ [Huang-Sun-Xiong-Y.'2016].
- As $\mathrm{IRR}(\nu) < \mathrm{IC}_1$ when ν grows, our IRR is easier to meet.

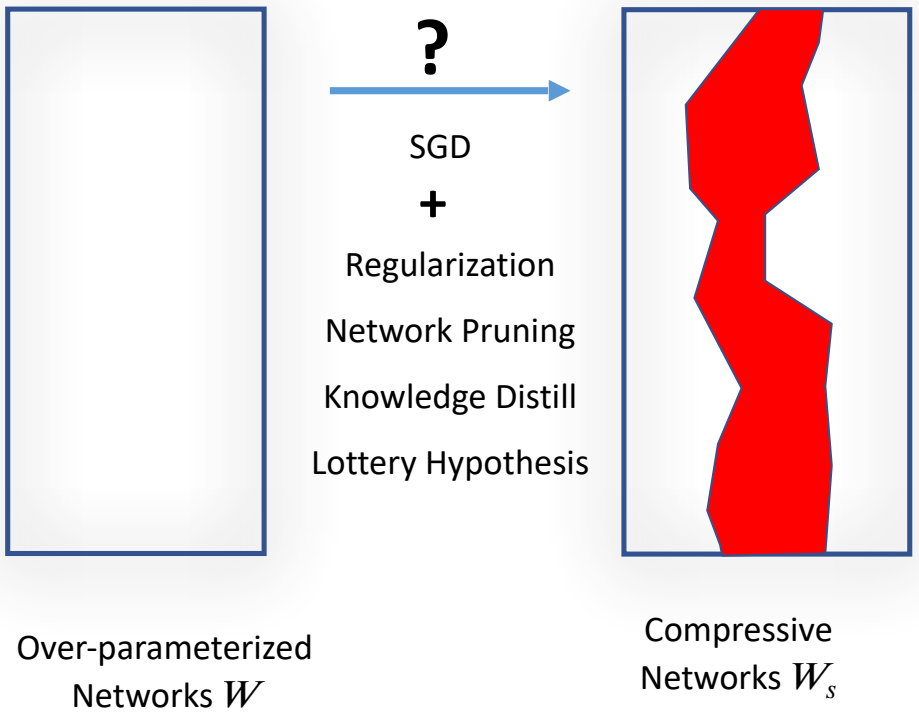
Split LBI improves Irrepresentable Condition



Theorem (Huang-Sun-Xiong-Y.'2020)

- $\mathrm{IC}_0 \geq \mathrm{IC}_1$.
- $\mathrm{IRR}(\nu) \to \mathrm{IC}_0$ $(\nu \to 0)$.
- $\mathrm{IRR}(\nu) \to C$ $(\nu \to \infty)$ *with* $C = 0 \Longleftrightarrow \ker(X) \subseteq \ker(D_S)$.

Lottery Ticket Hypothesis: Learning Sparse Subnetworks

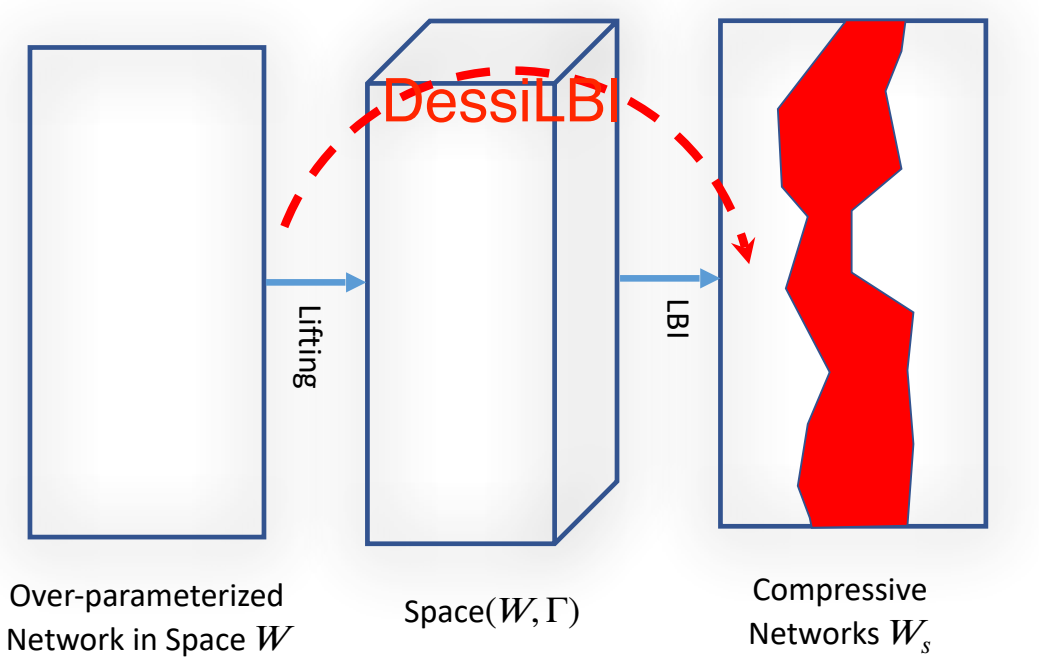


Existing 2-Stage Approaches:

- Fully training dense network,
- Finding good sparse subnets.

Our method: 1-Stage Approach (end-to-end)
Without fully training a dense model.

The key idea of DessiLBI: Lifting Parameters



1, Lifting parameter space W to (W,Γ) coupling the inverse scale space.

2, Γ learns structural sparsity in inverse scale space.

3, Network's solution path in (W,Γ) as the discretization of dynamics, and solved by LBI.

4, Our optimizer enjoys a provable global convergence guarantee.

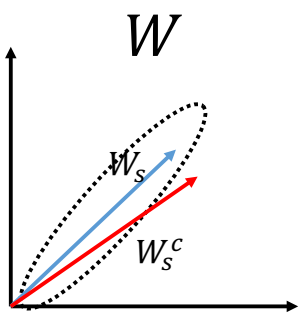
Loss

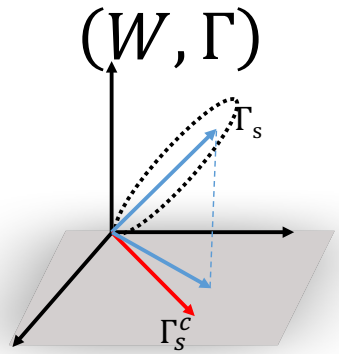
W_s: wining ticket

W: dense parameters

$W_s \cup W_{S^c} = W$

W_s and W_{S^c} correlated





$\Gamma_s \cup \Gamma_s^c = \Gamma$

Γ_s and Γ_s^c orthogonal

Differential Inclusion of Inverse Scale Space

GD of Weight Space

$$\dot{W}_t = -\nabla_W \hat{\mathcal{L}}_n(W)$$

$$\bar{\mathcal{L}}(W, \Gamma) = \hat{\mathcal{L}}_n(W) + \frac{1}{2\nu}\|W - \Gamma\|_F^2$$

DessiLBI Algorithm

$$\frac{\dot{W}_t}{\kappa} = -\nabla_W \bar{\mathcal{L}}(W_t, \Gamma_t)$$
$$\dot{V}_t = -\nabla_\Gamma \bar{\mathcal{L}}(W_t, \Gamma_t)$$
$$V_t \in \partial\left(\Omega(\Gamma) + \frac{1}{2\kappa}\|\Gamma\|^2\right)$$
$$\bar{\mathcal{L}}(W, \Gamma) = \hat{\mathcal{L}}_n(W) + \frac{1}{2\nu}\|W - \Gamma\|_F^2$$

Differential Inclusion of Inverse Scale Space

$$W_{k+1} = W_k - \kappa\alpha_k \cdot \nabla_W \bar{\mathcal{L}}(W_k, \Gamma_k)$$
$$V_{k+1} = V_k - \alpha_k \cdot \nabla_\Gamma \bar{\mathcal{L}}(W_k, \Gamma_k),$$
$$\Gamma_{k+1} = \kappa \cdot \mathrm{Prox}_{\Omega_\lambda}(V_{k+1})$$

$$W_{k+1} = W_k - \kappa\alpha_k \cdot \nabla_W \bar{\mathcal{L}}(W_k, \Gamma_k),$$
$$V_{k+1} = V_k - \alpha_k \cdot \nabla_\Gamma \bar{\mathcal{L}}(W_k, \Gamma_k)$$

Gradient Descent

$$\Gamma_{k+1} = \kappa \cdot \mathrm{Prox}_{\Omega}(V_{k+1})$$
$$\mathrm{Prox}_{\Omega}(V) = \arg\min_{\Gamma}\left\{\frac{1}{2}\|\Gamma - V\|_2^2 + \Omega(\Gamma)\right\}$$

Proximal Mapping

The Simple Discretization - DessLBI

V is the sub-gradient for some sparsity-enforced, often non-differentiable regularization $\Omega_\lambda(\Gamma) = \lambda\Omega_1(\Gamma), (\lambda \in \mathbb{R}_+)$ such as Lasso or group Lasso penalties for $\Omega_1(\Gamma)$

- W_t follows the gradient descent with ℓ_2-regularization
- Important Features of Γ_t are first selected: *Inverse Scale Space*

Proximal Map for Sparse Structure

$$\mathrm{Prox}_{\Omega}(V) = \arg\min_{\Gamma} \left\{ \frac{1}{2}\|\Gamma - V\|_2^2 + \Omega(\Gamma) \right\}$$

DessLBI enforce structural sparsity by Group lasso penalty,

$$\Omega(\Gamma) = \sum_g \|\Gamma^g\|_2 = \sum_g \sqrt{\sum_{i=1}^{|\Gamma^g|} (\Gamma_i^g)^2}$$

A close form solution:

$$\Gamma^g = \kappa \cdot \max\left(0, 1 - 1/\|V^g\|_2\right) V^g$$

Convolutional layer, $\Gamma^g = \Gamma^g(c_{in}, c_{out}, \texttt{size})$

Fully connected layer $\Gamma = \Gamma(c_{in}, c_{out})$

c_{in} :No. of input channel

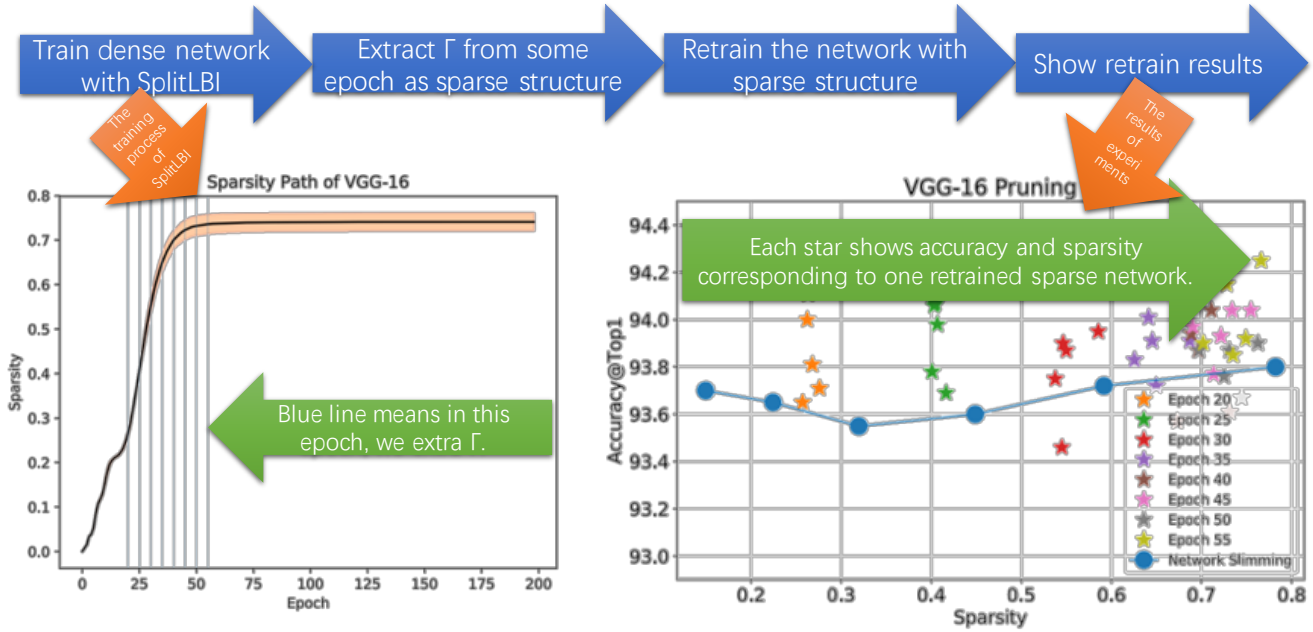
c_{out} :No. of output channel

size: kernel size

- (Batch) DessLBI w./w.o. Momentum and Weight-decay (Mom-Wd)
- We have a theorem that guarantees the global convergence of DessiLBI: from any initialization, DessiLBI sequence converges to a critical point.

A Flow Chart for Finding Sparse Structure

Experiments Design



Summary

- The limit of Linearized Bregman iteration follows differential inclusion of inverse scale space, where significant features emerge earlier on solution paths
- It renders the unbiased *Oracle Estimator* under sign-consistency
- Sign consistency under nearly the same condition as LASSO
  - Restricted Strongly Convex + Irrepresentable Condition
- Split extension: sign consistency under a weaker condition than generalized LASSO
  - under a provably weaker Irrepresentable Condition
- Early stopping regularization is exploited against overfitting noise

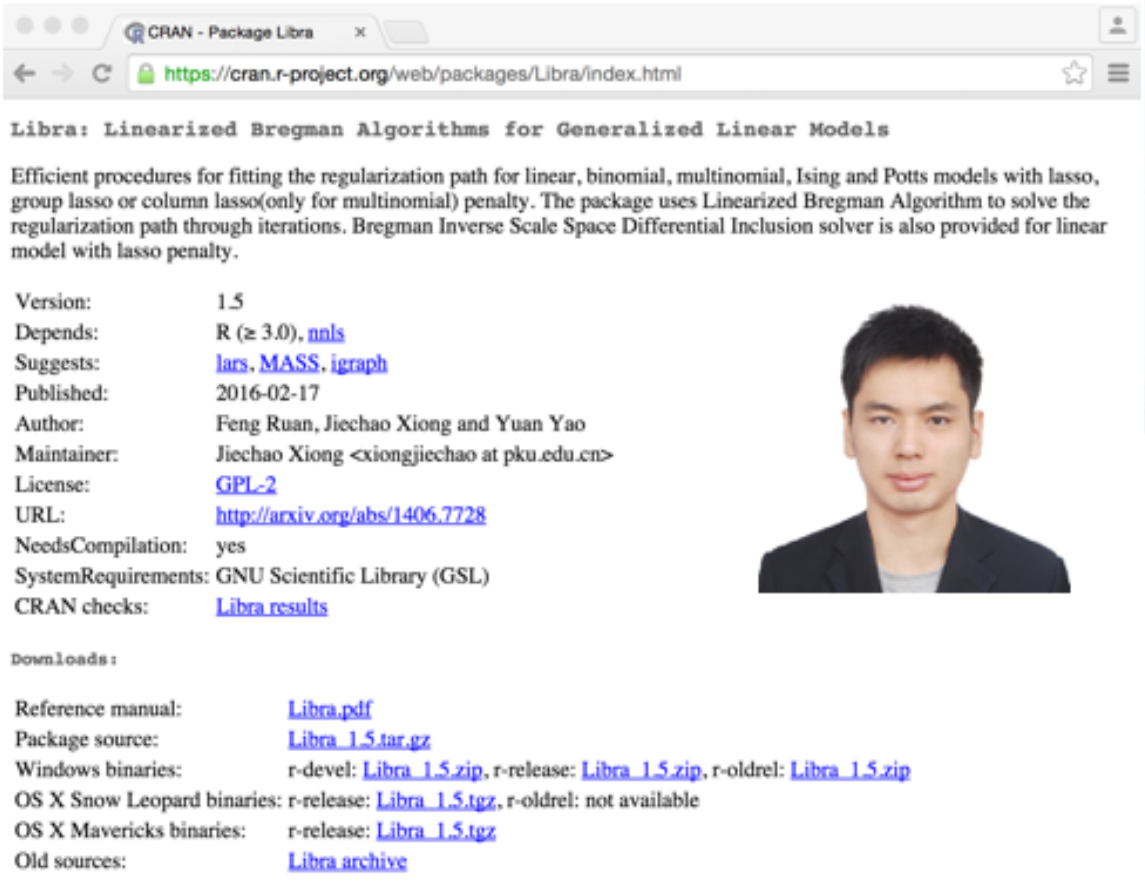
A Renaissance of Boosting as restricted gradient descent ...

Some Reference

- Osher, Ruan, Xiong, Yao, and Yin, "Sparse Recovery via Differential Equations", *Applied and Computational Harmonic Analysis*, 2016
- Xiong, Ruan, and Yao, "A Tutorial on Libra: R package for Linearized Bregman Algorithms in High Dimensional Statistics", *Handbook of Big Data Analytics*, Eds. by Wolfgang Karl Härdle, Henry Horng-Shing Lu, and Xiaotong Shen, Springer, 2017. `https://arxiv.org/abs/1604.05910`
- Xu, Xiong, Cao, and Yao, "False Discovery Rate Control and Statistical Quality Assessment of Annotators in Crowdsourced Ranking", *ICML 2016*, arXiv:1604.05910
- Huang, Sun, Xiong, and Yao, "Split LBI: an iterative regularization path with structural sparsity", *NIPS 2016*, `https://github.com/yuany-pku/split-lbi`
- Sun, Hu, Wang, and Yao, "GSplit LBI: taming the procedure bias in neuroimaging for disease prediction", *MICCAI 2017*
- Huang and Yao, "A Unified Dynamic Approach to Sparse Model Selection", *AISTATS 2018*
- Huang, Sun, Xiong, and Yao, "Boosting with Structural Sparsity: A Differential Inclusion Approach", *Applied and Computational Harmonic Analysis*, 48(1):1-45, 2020, arXiv: 1704.04833
- Qianqian Xu, Xinwei Sun, Zhiyong Yang, Qingming Huang, and Yuan Yao. "iSplit LBI: Individualized Partial Ranking with Ties via Split LBI". *NeurIPS 2019*, arXiv:1910.05905
- Yanwei Fu, Chen Liu, Donghao Li, Xinwei Sun, Jinshan Zeng, and Yuan Yao. DessiLBI: Exploring Structural Sparsity of Deep Neural Networks via Differential Inclusion Paths. *ICML 2020*, arXiv:2007.02010.
- Yanwei Fu, Chen Liu, Donghao Li, Zuyuan Zhong, Xinwei Sun, Jinshan Zeng, and Yuan Yao. Exploring Structural Sparsity of Deep Networks via Inverse Scale Spaces. IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI), 2022.
- Yang Cao, Xinwei Sun, Yuan Yao. "Controlling the False Discovery Rate in Structural Sparsity: Split Knockoffs". arXiv:2103.16159.
- Pytorch package for deep learning: `https://github.com/DessiLBI2020/DessiLBI`
- R package: `http://cran.r-project.org/web/packages/Libra/index.html`

Cran R package: Libra

http://cran.r-project.org/web/packages/Libra/



Libra (1.6) currently includes

Sparse statistical models:

- linear regression: ISS (differential inclusion), LBI
- logistic regression (binomial, multinomial): LBI
- graphical models (Gaussian, Ising, Potts): LBI

Two types of regularization:

- LASSO: l_1-norm penalty
- Group LASSO: $l_2 - l_1$ penalty

Libra computes regularization paths via Linearized Bregman Iteration (LBI)

for $\theta_0 = z_0 = \mathbf{0}$ and $k \in \mathbb{N}$,

$$z_{k+1} = z_k - \frac{\alpha_k}{n} \sum_{i=1}^{n} \nabla_\theta \ell(x_i, \theta_k) \tag{16a}$$

$$\theta_{k+1} = \kappa \cdot \mathrm{prox}_{\|\cdot\|_*}(z_{k+1}) \tag{16b}$$

where

- $\ell(x, \theta)$ is the *loss* function to minimize
- $\mathrm{prox}_{\|\cdot\|_*}(z) := \arg\min_u \left(\frac{1}{2}\|u - z\|^2 + \|u\|_* \right)$
- $\alpha_k > 0$ is step-size
- $\kappa > 0$ while $\alpha_k \kappa \|\nabla_\theta^2 \hat{\mathbb{E}} \ell(x, \theta)\| < 2$
- as simple as ISTA (easy to parallel implementation), yet different limit dynamics

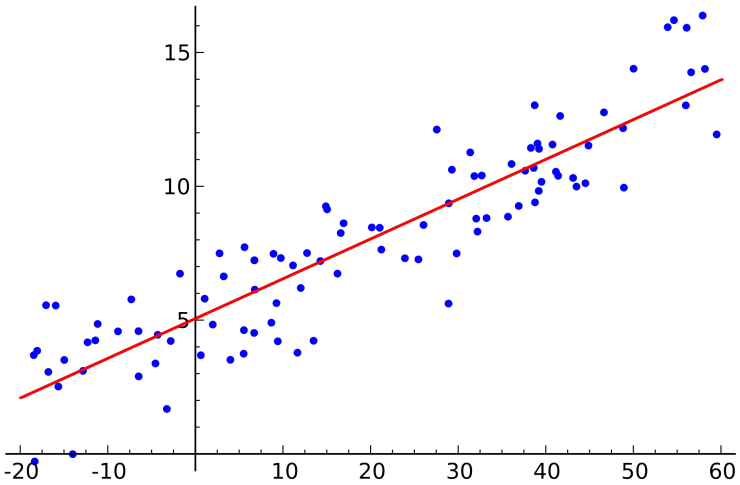
Linear Regression

Linear Regression:

$$y = X\beta + \epsilon$$

β is sparse or group sparse, with two types of penalty:

- "ungrouped": $\sum_i |\beta_i|$
- "grouped": $\sum_g \sqrt{\sum_{g_i=g} \beta_i^2}$

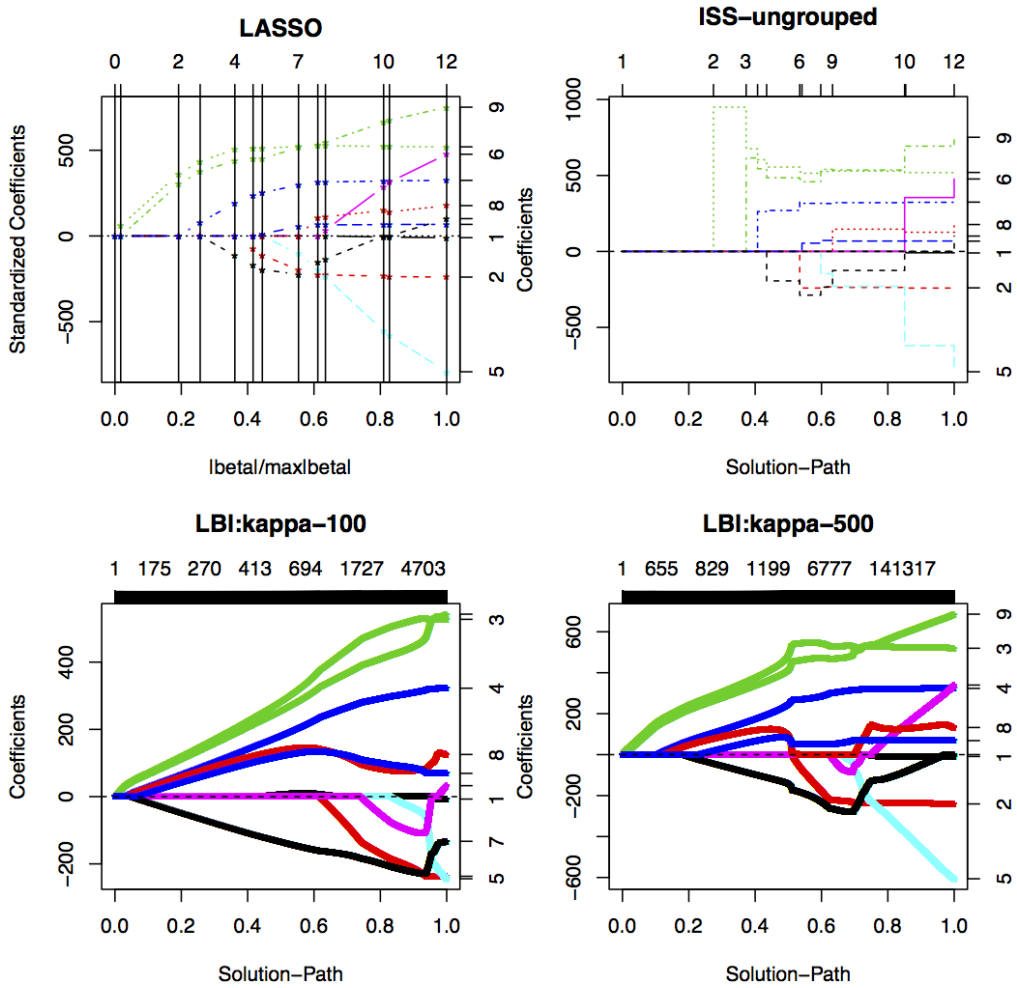


Linear Regression Example: Diabetes Data

```
data('diabetes')
attributes(x)
#$dim
# [1] 442  10
#$dimnames[[2]]
# [1] "age" "sex" "bmi" "map" "tc"  "ldl" "hdl" "tch" "ltg" "glu"

lassopath = lars(x,y)
isspath = iss(x,y)
lb(x,y,kappa=100,alpha=0.005,family="gaussian",group="ungrouped",
    intercept=FALSE,normalize=FALSE)
lb(x,y,kappa=500,alpha=0.001,family="gaussian",group="ungrouped",
    intercept=FALSE,normalize=FALSE)
```

LBI generates iterative regularization paths



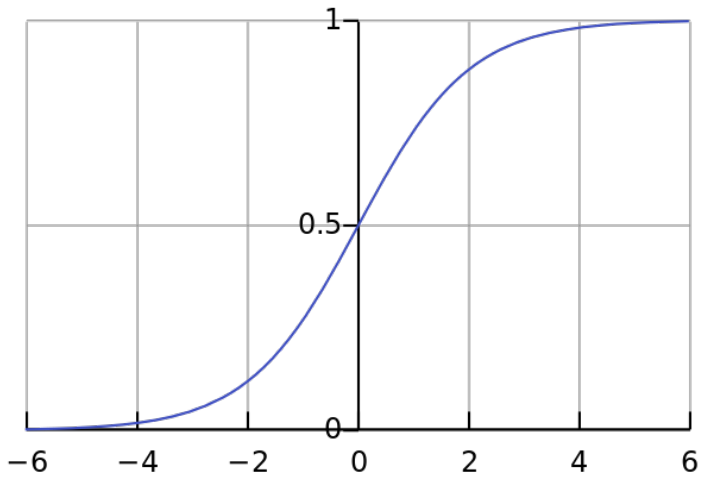
Logistic Regression

Logistic Regression:

$$\log \frac{P(y=1|X)}{P(y=-1|X)} = X\beta \Leftrightarrow P(y=1|X) = \frac{e^{X\beta}}{1+e^{X\beta}} =: \sigma(X\beta)$$

β is sparse or group sparse, with two types of penalty:

- "ungrouped": $\sum_i |\beta_i|$
- "grouped": $\sum_g \sqrt{\sum_{g_i=g} \beta_i^2}$



Example: Publications of COPSS Award Winners

- dataset is provided by Prof. Jiashun Jin @CMU
- 3248 papers by 3607 authors between 2003 and the first quarter of 2012 from:
  - the Annals of Statistics, Journal of the American Statistical Association, Biometrika and Journal of the Royal Statistical Society Series B
- a subset of 382 papers by 35 COPSS award winners
- Question: can we model the coauthorship structure to predict the out-of-sample behavior?

A logistic regression path with early stopping regularization

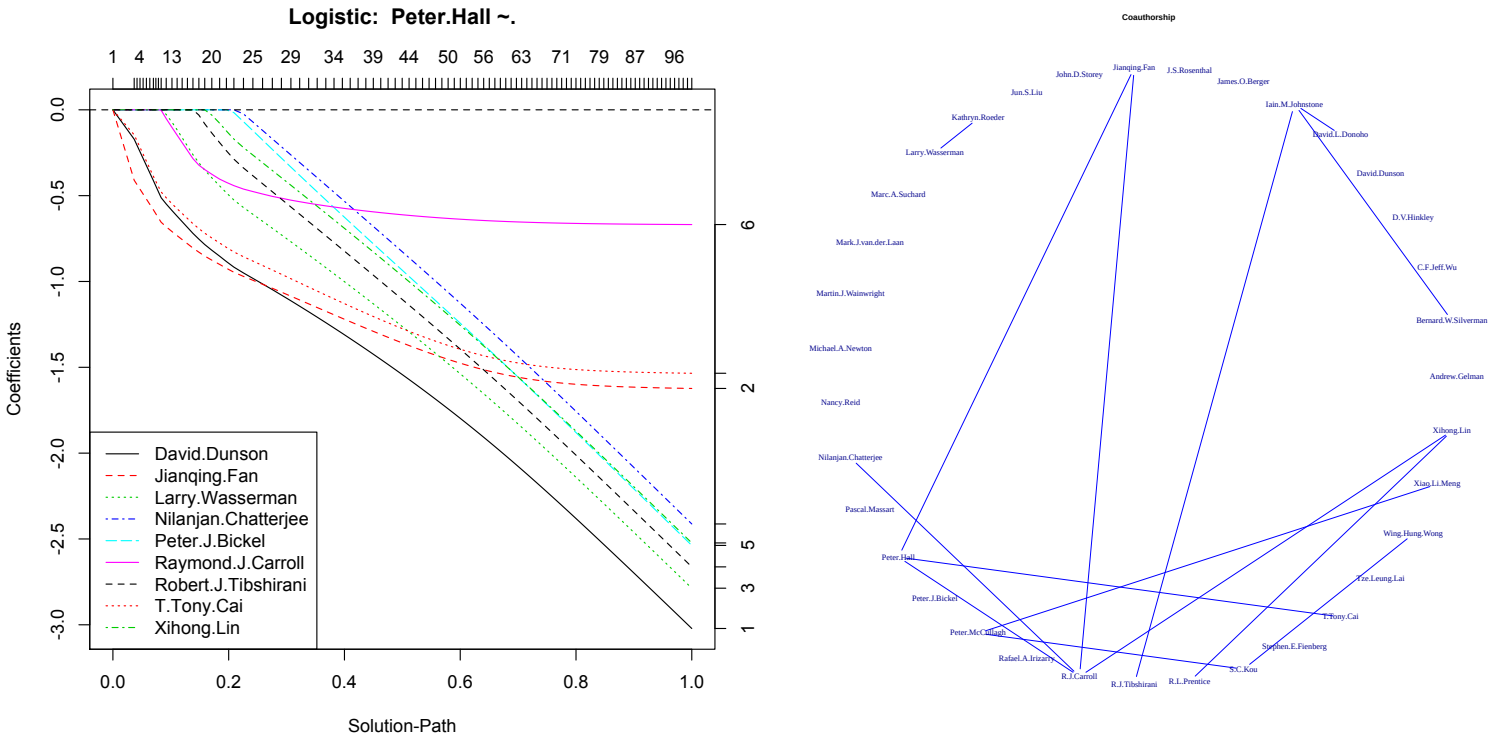


Figure: Peter Hall vs. other COPSS award winners in sparse logistic regression [papers from AoS/JASA/Biometrika/JRSSB, 2003-2012]: true coauthors are merely Tony Cai, R.J. Carroll, and J. Fan

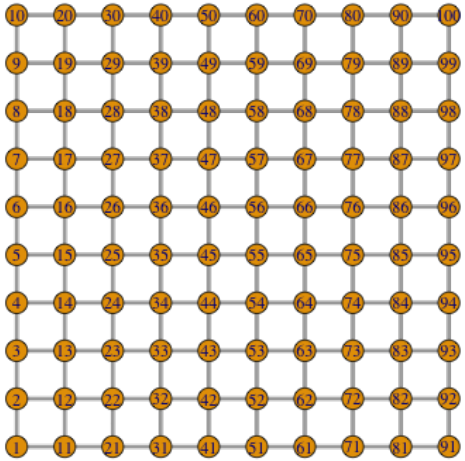
Sparse Ising Model

All models are wrong, but some are useful (George Box):

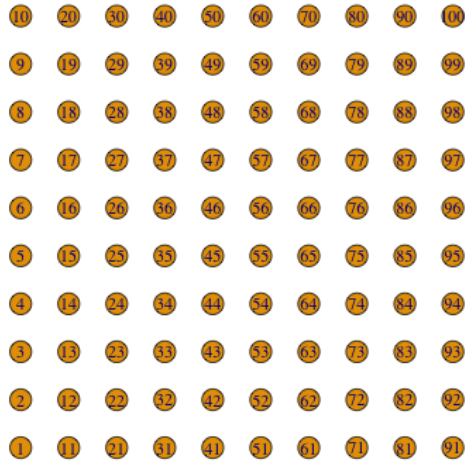
$$P(x_1, \ldots, x_p) \sim \exp\left(\sum_i H_i x_i + \sum_{i,j} J_{ij} x_i x_j\right)$$

- Ising model: $x_i = 1$ if author i appears in a paper, otherwise 0
- H_i describes the mean publication rate of author i
- J_{ij} describes the interactions between author i and j
  - $J_{ij} > 0$: author i and j collaborate more often than others
  - $J_{ij} < 0$: author i and j collaborate less frequently than others
  - sparsity: $J_{ij} = 0$ mostly, a model of collaboration network
  - learned by maximum composite conditional likelihood with LB

Early stopping against overfitting in sparse Ising model learning



a true Ising model of 2-D grid



a movie of LB path

Application: Sparse Ising Model of COPSS Award Winners

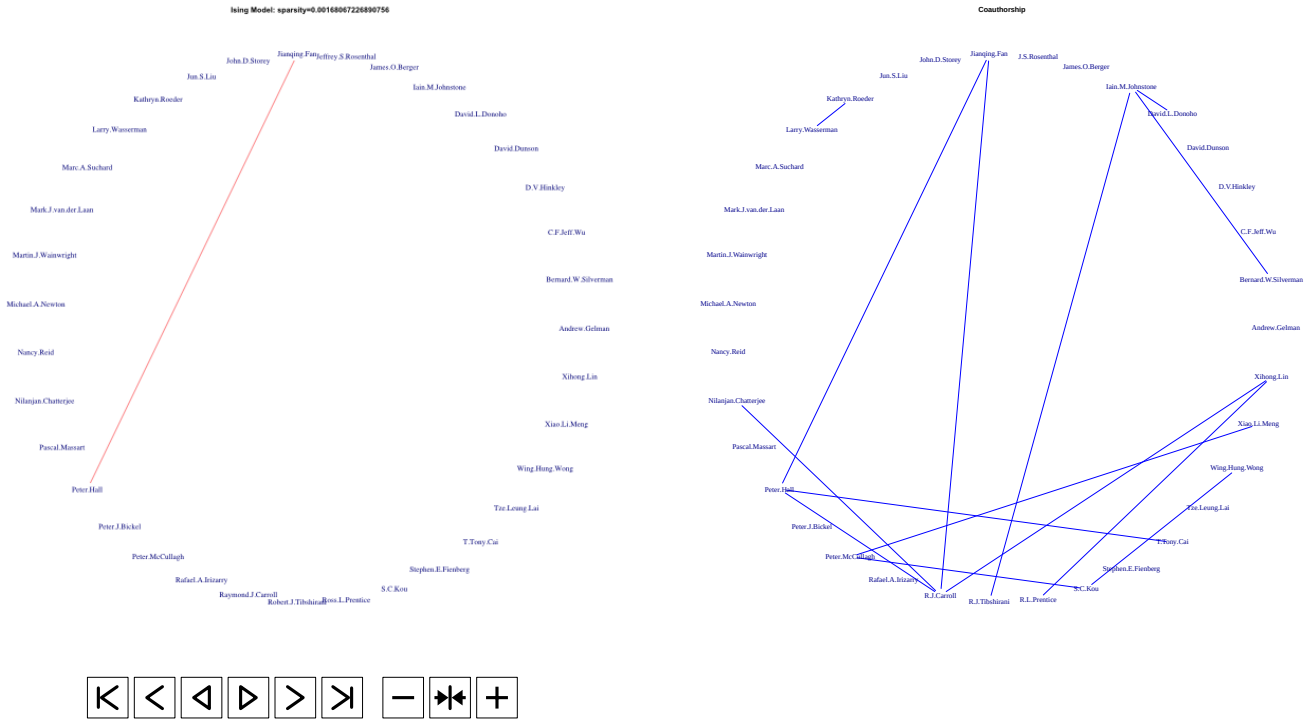


Figure: Left: LB path of Ising Model learning; Right: coauthorship network of existing data. Typically COPSS winners do not like working together; Peter Hall (1951-2016) is the hub of statisticians, like Erdös for mathematicians