Complexity Analysis of the Lasso Regularization Path

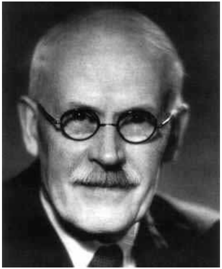
Julien Mairal, Inria, Grenoble

joint work with Bin Yu (UC Berkeley)

Journées MAS, Grenoble, 2016

Early thoughts about parsimony

(a) Dorothy Wrinch
1894–1980



(b) Harold Jeffreys
1891–1989

> *The existence of simple laws is, then, apparently, to be regarded as a quality of nature; and accordingly we may infer that it is justifiable to prefer a simple law to a more complex one that fits our observations slightly better.*

[Wrinch and Jeffreys, 1921]. Philosophical Magazine Series.

Historical overview of parsimony

- 14th century: Ockham's razor;
- 1921: Wrinch and Jeffreys' simplicity principle;
- 1952: Markowitz's portfolio selection;
- 60 and 70's: best subset selection in statistics;
- 70's: use of the ℓ_1-norm for signal recovery in geophysics;
- 90's: wavelet thresholding in signal processing;
- 1996: Olshausen and Field's dictionary learning;
- 1996–1999: Lasso (statistics) and basis pursuit (signal processing);
- 2006: compressed sensing (signal processing) and Lasso consistency (statistics);

What this work is about

- another paper about the Lasso/Basis Pursuit [Tibshirani, 1996, Chen et al., 1999]:

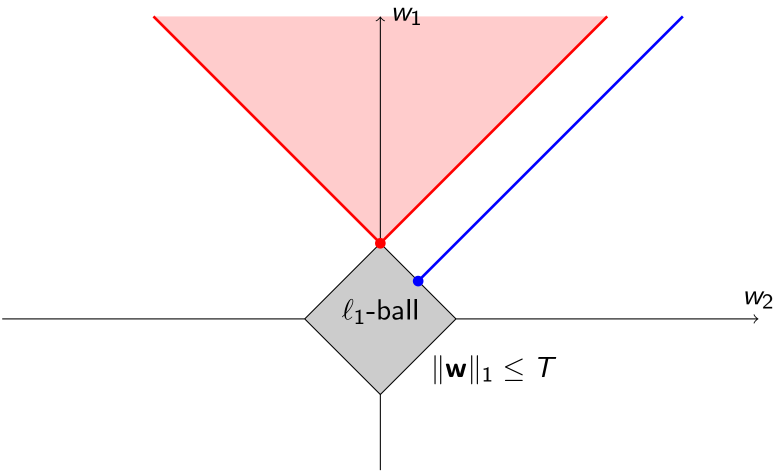
$$\min_{\mathbf{w}\in\mathbb{R}^p} \frac{1}{2}\|\mathbf{y}-\mathbf{X}\mathbf{w}\|_2^2 + \lambda\|\mathbf{w}\|_1; \tag{1}$$

- the first complexity analysis of the homotopy method [Ritter, 1962, Osborne et al., 2000, Efron et al., 2004] for solving (1);

A story similar to

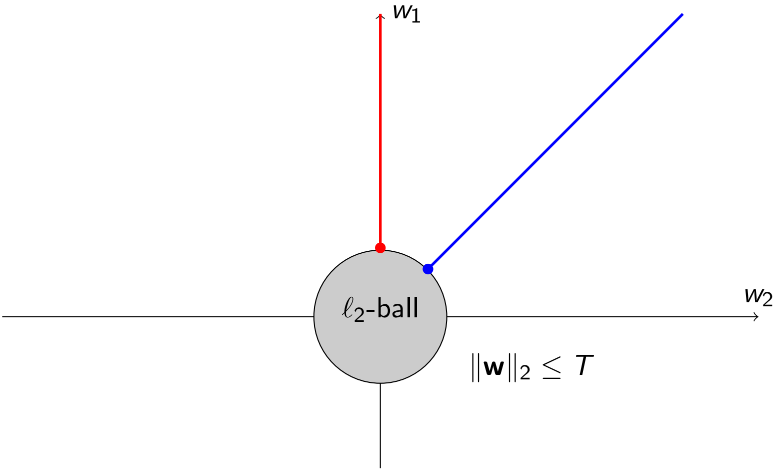
- the simplex algorithm for linear programs [Klee and Minty, 1972];
- the SVM regularization path [Gärtner, Jaggi, and Maria, 2010].

Regularizing with the ℓ_1-norm



The projection onto a convex set is “biased” towards singularities.

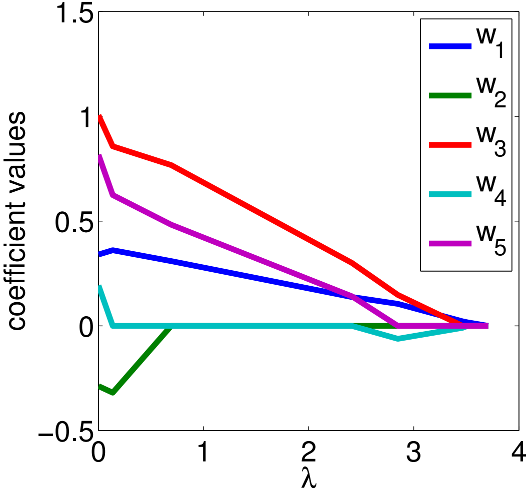
Regularizing with the ℓ_2-norm



The ℓ_2-norm is isotropic.

The Lasso Regularization Path and the Homotopy

Under uniqueness assumption of the Lasso solution, the regularization path is piecewise linear:



Our Main Results

Theorem - worst case analysis

In the worst-case, the regularization path of the Lasso has exactly $(3^p + 1)/2$ *linear segments.*

Proposition - approximate analysis

There exists an ε*-approximate path with* $O(1/\sqrt{\varepsilon})$ *linear segments.*

Brief Introduction to the Homotopy Algorithm

Optimality conditions of the Lasso

$\mathbf{w}^\star$ in $\mathbb{R}^p$ is a solution of Eq. (1) if and only if for all j in $\{1, \ldots, p\}$,

$$\begin{aligned} \mathbf{x}^{j\top}(\mathbf{y} - \mathbf{X}\mathbf{w}^\star) &= \lambda \operatorname{sign}(\mathbf{w}_j^\star) \quad \text{if} \quad \mathbf{w}_j^\star \neq 0, \\ |\mathbf{x}^{j\top} \underbrace{(\mathbf{y} - \mathbf{X}\mathbf{w}^\star)}_{\text{residual}}| &\leq \lambda \quad \text{otherwise.} \end{aligned}$$

Brief Introduction to the Homotopy Algorithm

Optimality conditions of the Lasso

$\mathbf{w}^\star$ in $\mathbb{R}^p$ is a solution of Eq. (1) if and only if for all j in $\{1, \ldots, p\}$,

$$\mathbf{x}^{j\top}(\mathbf{y} - \mathbf{X}\mathbf{w}^\star) = \lambda \operatorname{sign}(\mathbf{w}_j^\star) \;\text{ if }\; \mathbf{w}_j^\star \neq 0,$$
$$|\mathbf{x}^{j\top} \underbrace{(\mathbf{y} - \mathbf{X}\mathbf{w}^\star)}_{\text{residual}}| \leq \lambda \;\text{ otherwise.}$$

Uniqueness of the solution

Define $J \triangleq \{j \in \{1, \ldots, p\} : |\mathbf{x}^{j\top}(\mathbf{y} - \mathbf{X}\mathbf{w}^\star)| = \lambda\}$.
If the matrix $\mathbf{X}_J^\top \mathbf{X}_J$ is invertible, the solution is unique and

$$\mathbf{w}_J^\star = (\mathbf{X}_J^\top \mathbf{X}_J)^{-1}(\mathbf{X}_J^\top \mathbf{y} - \lambda \boldsymbol{\eta}_J) = \mathbf{a} + \lambda \mathbf{b},$$

where $\boldsymbol{\eta} \triangleq \operatorname{sign}(\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}^\star))$.

Brief Introduction to the Homotopy Algorithm

Piecewise linearity

Under uniqueness assumptions of the Lasso solution, the regularization path $\lambda \mapsto \mathbf{w}^\star(\lambda)$ is continuous and piecewise linear.

Brief Introduction to the Homotopy Algorithm

Piecewise linearity

Under uniqueness assumptions of the Lasso solution, the regularization path $\lambda \mapsto \mathbf{w}^\star(\lambda)$ is continuous and piecewise linear.

Recipe of the homotopy method - main ideas

1. finds a trivial solution $\mathbf{w}^\star(\lambda_\infty) = 0$ with $\lambda_\infty = \|\mathbf{X}^\top \mathbf{y}\|_\infty$;
2. compute the direction of the current linear segment of the path;
3. follow the direction of the path by decreasing λ;
4. stop at the next "kink" and go back to 2.

Brief Introduction to the Homotopy Algorithm

Piecewise linearity

Under uniqueness assumptions of the Lasso solution, the regularization path $\lambda \mapsto \mathbf{w}^\star(\lambda)$ is continuous and piecewise linear.

Recipe of the homotopy method - main ideas

1. finds a trivial solution $\mathbf{w}^\star(\lambda_\infty) = 0$ with $\lambda_\infty = \|\mathbf{X}^\top \mathbf{y}\|_\infty$;
2. compute the direction of the current linear segment of the path;
3. follow the direction of the path by decreasing λ;
4. stop at the next "kink" and go back to 2.

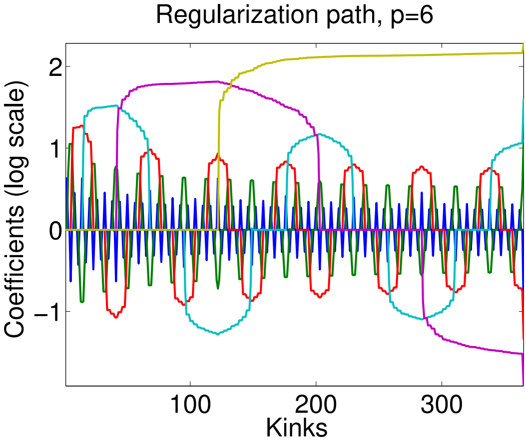
Caveats

- kinks can be very close to each other;
- the direction of the path can involve ill-conditioned matrices;
- worst-case exponential complexity (main result of this work).

Worst case analysis

Theorem - worst case analysis

In the worst-case, the regularization path of the Lasso has exactly $(3^p + 1)/2$ *linear segments.*



Worst case analysis

Consider a Lasso problem ($\mathbf{y} \in \mathbb{R}^n$, $\mathbf{X} \in \mathbb{R}^{n \times p}$).
Define the vector $\tilde{\mathbf{y}}$ in $\mathbb{R}^{n+1}$ and the matrix $\tilde{\mathbf{X}}$ in $\mathbb{R}^{(n+1)\times(p+1)}$ as follows:

$$\tilde{\mathbf{y}} \triangleq \begin{bmatrix} \mathbf{y} \\ y_{n+1} \end{bmatrix}, \quad \tilde{\mathbf{X}} \triangleq \begin{bmatrix} \mathbf{X} & 2\alpha\mathbf{y} \\ 0 & \alpha y_{n+1} \end{bmatrix},$$

where $y_{n+1} \neq 0$ and $0 < \alpha < \lambda_1/(2\mathbf{y}^\top\mathbf{y} + y_{n+1}^2)$.

Adverserial strategy

If the regularization path of the Lasso ($\mathbf{y}$,$\mathbf{X}$) has k linear segments, the path of $(\tilde{\mathbf{y}}, \tilde{\mathbf{X}})$ has $3k - 1$ linear segments.

Worst case analysis

$$\tilde{\mathbf{y}} \triangleq \begin{bmatrix} \mathbf{y} \\ y_{n+1} \end{bmatrix}, \quad \tilde{\mathbf{X}} \triangleq \begin{bmatrix} \mathbf{X} & 2\alpha\mathbf{y} \\ 0 & \alpha y_{n+1} \end{bmatrix},$$

Let us denote by $\{\boldsymbol{\eta}^1, \ldots, \boldsymbol{\eta}^k\}$ the sequence of k sparsity patterns in $\{-1, 0, 1\}^p$ encountered along the path of the Lasso $(\mathbf{y}, \mathbf{X})$.

The new sequence of sparsity patterns for $(\tilde{\mathbf{y}}, \tilde{\mathbf{X}})$ is

$$\Bigg\{ \overbrace{\begin{bmatrix} \boldsymbol{\eta}^1 = 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \boldsymbol{\eta}^2 \\ 0 \end{bmatrix}, \ldots, \begin{bmatrix} \boldsymbol{\eta}^k \\ 0 \end{bmatrix}}^{\text{first } k \text{ patterns}}, \overbrace{\begin{bmatrix} \boldsymbol{\eta}^k \\ 1 \end{bmatrix}, \begin{bmatrix} \boldsymbol{\eta}^{k-1} \\ 1 \end{bmatrix}, \ldots, \begin{bmatrix} \boldsymbol{\eta}^1 = 0 \\ 1 \end{bmatrix}}^{\text{middle } k \text{ patterns}},$$
$$\underbrace{\begin{bmatrix} -\boldsymbol{\eta}^2 \\ 1 \end{bmatrix}, \begin{bmatrix} -\boldsymbol{\eta}^3 \\ 1 \end{bmatrix}, \ldots, \begin{bmatrix} -\boldsymbol{\eta}^k \\ 1 \end{bmatrix}}_{\text{last } k-1 \text{ patterns}} \Bigg\}.$$

Worst case analysis

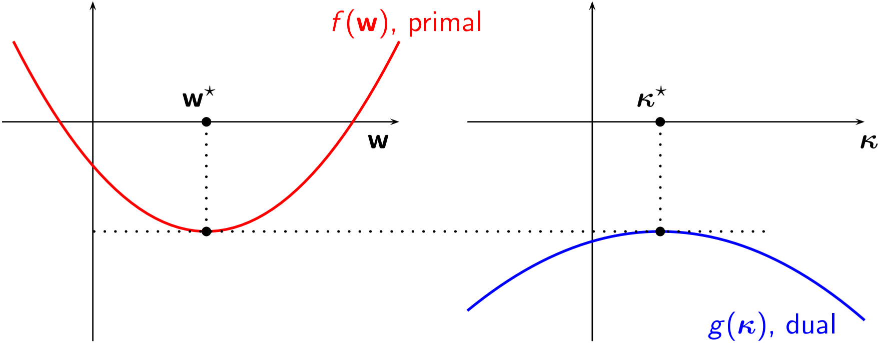
We are now in shape to build a pathological path with $(3^p+1)/2$ linear segments. Note that this lower-bound complexity is tight.

$$\mathbf{y} \triangleq \begin{bmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}, \quad \mathbf{X} \triangleq \begin{bmatrix} \alpha_1 & 2\alpha_2 & 2\alpha_3 & \dots & 2\alpha_p \\ 0 & \alpha_2 & 2\alpha_3 & \dots & 2\alpha_p \\ 0 & 0 & \alpha_3 & \dots & 2\alpha_p \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \alpha_p \end{bmatrix},$$

Approximate Complexity

Refinement of Giesen, Jaggi, and Laue [2010] for the Lasso

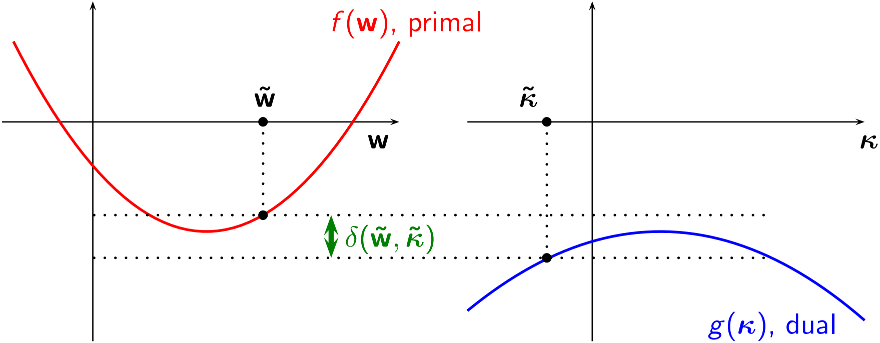
Strong Duality



Strong duality means that $\max_{\boldsymbol{\kappa}} g(\boldsymbol{\kappa}) = \min_{\mathbf{w}} f(\mathbf{w})$

Approximate Complexity

Duality Gaps



Strong duality means that $\max_{\boldsymbol{\kappa}} g(\boldsymbol{\kappa}) = \min_{\mathbf{w}} f(\mathbf{w})$

The duality gap guarantees us that $0 \leq f(\tilde{\mathbf{w}}) - f(\mathbf{w}^\star) \leq \delta(\tilde{\mathbf{w}}, \tilde{\boldsymbol{\kappa}})$.

Approximate Complexity

$$\min_{\mathbf{w}} \left\{ f_\lambda(\mathbf{w}) \triangleq \frac{1}{2}\|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 + \lambda\|\mathbf{w}\|_1 \right\}, \qquad \text{(primal)}$$

$$\max_{\boldsymbol{\kappa}} \left\{ g_\lambda(\boldsymbol{\kappa}) \triangleq -\frac{1}{2}\boldsymbol{\kappa}^\top\boldsymbol{\kappa} - \boldsymbol{\kappa}^\top\mathbf{y} \;\text{ s.t. }\; \|\mathbf{X}^\top\boldsymbol{\kappa}\|_\infty \leq \lambda \right\}. \qquad \text{(dual)}$$

ε-approximate solution

$\mathbf{w}$ satisfies $APPROX_\lambda(\varepsilon)$ when there exists a dual variable $\boldsymbol{\kappa}$ s.t.

$$\delta_\lambda(\mathbf{w}, \boldsymbol{\kappa}) = f_\lambda(\mathbf{w}) - g_\lambda(\boldsymbol{\kappa}) \leq \varepsilon f_\lambda(\mathbf{w}).$$

ε-approximate path

A path $\mathcal{P} : \lambda \mapsto \mathbf{w}(\lambda)$ is an approximate path if it always contains ε-approximate solutions.

(see Giesen et al. [2010] for generic results on approximate paths)

Approximate Complexity

Main relation

$$APPROX_\lambda(0) \Longrightarrow APPROX_{\lambda(1-\sqrt{\varepsilon})}(\varepsilon)$$

Key: find an appropriate dual variable $\boldsymbol{\kappa}(\mathbf{w})$ + simple calculation;

Proposition - approximate analysis

there exists an ε-approximate path with at most $\left\lceil \frac{\log(\lambda_\infty/\lambda_1)}{\sqrt{\varepsilon}} \right\rceil$ *segments.*

Approximate homotopy - main ideas

- Maintain approximate optimality conditions along the path;
- Make steps in λ greater than or equal to $\lambda(1-\theta\sqrt{\varepsilon})$;
- When the kinks are too close to each other, make a large step and switch to first-order method;

A Few Messages to Conclude

- **Despite its exponential complexity, the homotopy algorithm remains extremely powerful in practice**;
- numerical stability is still an issue of the homotopy algorithm;
- when one does not care about precision, the worst-case complexity of the path can be significantly reduced.

References I

S. S. Chen, D. L. Donoho, and M. A. Saunders. Atomic decomposition by basis pursuit. *SIAM Journal on Scientific Computing*, 20:33–61, 1999.

B. Efron, T. Hastie, I. Johnstone, and R. Tibshirani. Least angle regression. *Annals of statistics*, 32(2):407–499, 2004.

B. Gärtner, M. Jaggi, and C. Maria. An exponential lower bound on the complexity of regularization paths. *preprint arXiv:0903.4817v2*, 2010.

J. Giesen, M. Jaggi, and S. Laue. Approximating parameterized convex optimization problems. In *Algorithms - ESA*, Lectures Notes Comp. Sci. 2010.

V. Klee and G. J. Minty. How good is the simplex algorithm? In O. Shisha, editor, *Inequalities*, volume III, pages 159–175. Academic Press, New York, 1972.

References II

M. R. Osborne, B. Presnell, and B. A. Turlach. On the Lasso and its dual. *Journal of Computational and Graphical Statistics*, 9(2):319–37, 2000.

K. Ritter. Ein verfahren zur lösung parameterabhängiger, nichtlinearer maximum-probleme. *Mathematical Methods of Operations Research*, 6(4):149–166, 1962.

R. Tibshirani. Regression shrinkage and selection via the Lasso. *Journal of the Royal Statistical Society. Series B*, 58(1):267–288, 1996.

D. Wrinch and H. Jeffreys. XLII. On certain fundamental principles of scientific inquiry. *Philosophical Magazine Series 6*, 42(249):369–390, 1921.

Worst case analysis - Backup Slide

$$\tilde{\mathbf{y}} \triangleq \begin{bmatrix} \mathbf{y} \\ y_{n+1} \end{bmatrix}, \quad \tilde{\mathbf{X}} \triangleq \begin{bmatrix} \mathbf{X} & 2\alpha\mathbf{y} \\ 0 & \alpha y_{n+1} \end{bmatrix},$$

Some intuition about the adverserial strategy:

1. the patterns of the new path must be $[\boldsymbol{\eta}^{i\top}, 0]^\top$ or $[\pm\boldsymbol{\eta}^{i\top}, 1]^\top$;
2. the factor α ensures the $(p+1)$-th variable to enter late the path;
3. after the k first kinks, we have $\mathbf{y} \approx \mathbf{X}\mathbf{w}^\star(\lambda)$ and thus

$$\tilde{\mathbf{X}} \begin{bmatrix} \mathbf{w}^\star(\lambda) \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ y_{n+1} \end{bmatrix} \approx \tilde{\mathbf{y}} \approx \tilde{\mathbf{X}} \begin{bmatrix} -\mathbf{w}^\star(\lambda) \\ 1/\alpha \end{bmatrix}.$$

Worst case analysis - Backup Slide 2

$$\min_{\tilde{\mathbf{w}}\in\mathbb{R}^p, \tilde{w}\in\mathbb{R}} \frac{1}{2}\left\|\tilde{\mathbf{y}} - \tilde{\mathbf{X}}\begin{bmatrix}\tilde{\mathbf{w}}\\ \tilde{w}\end{bmatrix}\right\|_2^2 + \lambda\left\|\begin{bmatrix}\tilde{\mathbf{w}}\\ \tilde{w}\end{bmatrix}\right\|_1 =,$$

$$\min_{\tilde{\mathbf{w}}\in\mathbb{R}^p, \tilde{w}\in\mathbb{R}} \frac{1}{2}\|(1-2\alpha\tilde{w})\mathbf{y} - \mathbf{X}\tilde{\mathbf{w}}\|_2^2 + \frac{1}{2}(y_{n+1} - \alpha y_{n+1}\tilde{w})^2 + \lambda\|\tilde{\mathbf{w}}\|_1 + \lambda|\tilde{w}|.$$

is equivalent to

$$\min_{\tilde{\mathbf{w}}'\in\mathbb{R}^p} \frac{1}{2}\|\mathbf{y} - \mathbf{X}\tilde{\mathbf{w}}'\|_2^2 + \frac{\lambda}{|1-2\alpha\tilde{w}^\star|}\|\tilde{\mathbf{w}}'\|_1,$$

and then

$$\tilde{\mathbf{w}}^\star = \begin{cases} (1-2\alpha\tilde{w}^\star)\mathbf{w}^\star\left(\frac{\lambda}{|1-2\alpha\tilde{w}^\star|}\right) & \text{if } \tilde{w}^\star \neq \frac{1}{2\alpha} \\ 0 & \text{otherwise} \end{cases}.$$