Condition Number Analysis of Logistic Regression, and its Implications for First-Order Solution Methods

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How can optimization inform statistics (and machine learning)?

Paper in preparation (this talk):

Condition Number Analysis of Logistic Regression, and its Implications for First-Order Solution Methods

A "cousin" paper of ours:

A New Perspective on Boosting in Linear Regression via Subgradient Optimization and Relatives

Outline

- Optimization review: Greedy Coordinate Descent (GCD) and Stochastic Gradient Descent (SGD)

- A pair of condition numbers for the logistic regression problem:
  - when the sample data is non-separable:
    - a condition number for the degree of non-separability of the dataset
    - informing the convergence guarantees of GCD and SGD
    - guarantees on reaching linear convergence (thanks to Bach)

  - when the sample data is separable:
    - a condition number for the degree of separability of the dataset
    - informing convergence guarantees of GCD and SGD to deliver an approximate maximum margin classifier

Review of Greedy Coordinate Descent (GCD) and Stochastic Gradient Descent (SGD)

Two Basic First-Order Methods for Convex Optimization:

- Greedy Coordinate Descent method: "go in the best coordinate direction"
- Stochastic Gradient Descent (SGD) method: "go in the direction of the negative of the stochastic estimate of the gradient"

Convex Optimization

The problem of interest is:

$$F^* \quad := \quad \min_x \quad F(x) \qquad \text{s.t.} \quad x \in \mathbb{R}^p$$

where $F(\cdot)$ is differentiable and convex:

$$F(\lambda x + (1-\lambda)y) \leq \lambda F(x) + (1-\lambda)F(y) \quad \text{for all } x,\ y, \text{ and all } \lambda \in [0,1]$$

Let $\|x\|$ denote the given norm on the variables $x \in \mathbb{R}^p$

Norms and Dual Norms

Let $\|x\|$ be the given norm on the variables $x \in \mathbb{R}^p$

The dual norm is $\|s\|_* := \max_x \{s^T x : \|x\| \le 1\}$

Some common norms and their dual norms:

Name	Norm	Definition	Dual Norm
ℓ_2-norm	$\|x\|_2$	$\|x\|_2 = \sqrt{\sum_{j=1}^p \|x_j\|^2}$	$\|s\|_* = \|s\|_2$
ℓ_1-norm	$\|x\|_1$	$\|x\|_1 = \sum_{j=1}^p \|x_j\|$	$\|s\|_* = \|s\|_\infty$
ℓ_∞-norm	$\|x\|_\infty$	$\|x\|_\infty = \max\{\|x_1\|, \ldots, \|x_p\|\}$	$\|s\|_* = \|s\|_1$

Lipschitz constant for the Gradient

$$F^* \; := \; \min_x \; F(x) \quad \text{s.t.} \quad x \in \mathbb{R}^p$$

We say that $\nabla F(\cdot)$ is Lipschitz with parameter L_F if:

$$\|\nabla F(x) - \nabla F(y)\|_* \; \leq \; L_F \|x - y\| \quad \text{for all } x, y \in \mathbb{R}^p$$

$\| \cdot \|_*$ is the dual norm

Matrix Operator Norm

Let M be a linear operator (matrix) $M : \mathbb{R}^p \to \mathbb{R}^n$ with norm $\|x\|_a$ on $\mathbb{R}^p$ and norm $\|v\|_b$ on $\mathbb{R}^n$

The operator norm of M is given by:

$$\|M\|_{a,b} := \max_{x \neq 0} \frac{\|Mx\|_b}{\|x\|_a}$$

Greedy Coordinate Descent Method: "go in the best coordinate direction"

$$F^* := \min_x \; F(x) \quad \text{s.t.} \; x \in \mathbb{R}^p$$

Greedy Coordinate Descent

Initialize at $x^0 \in \mathbb{R}^p$, $k \leftarrow 0$

At iteration k :

1. Compute gradient $\nabla F(x^k)$
2. Compute
   - $j_k \in \arg \max_{j \in \{1,\ldots,p\}} \{|\nabla F(x^k)_j|\}$ and
   - $d^k \leftarrow \text{sgn}(\nabla F(x^k)_{j_k}) e_{j_k}$
3. Choose step-size α_k
4. Set $x^{k+1} \leftarrow x^k - \alpha_k d^k$

Metrics for Evaluating Greedy Coordinate Descent

$$F^* := \min_x \; F(x) \quad \text{s.t.} \quad x \in \mathbb{R}^p$$

Assume $F(\cdot)$ is convex and $\nabla F(\cdot)$ is Lipschitz with parameter L_F:

$$\|\nabla F(x) - \nabla F(y)\|_\infty \le L_F\|x - y\|_1 \quad \text{for all } x, y \in \mathbb{R}^p$$

Two sets of interest:

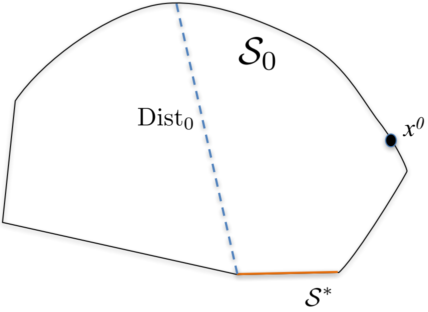
$\mathcal{S}_0 := \{x \in \mathbb{R}^p : F(x) \le F(x^0)\}$ is the level set of the initial point x^0

$\mathcal{S}^* := \{x \in \mathbb{R}^p : F(x) = F^*\}$ is the set of optimal solutions

Metrics for Evaluating Greedy Coordinate Descent, cont.

$\mathcal{S}_0 := \{x \in \mathbb{R}^p : F(x) \leq F(x^0)\}$ is the level set of the initial point x^0
$\mathcal{S}^* := \{x \in \mathbb{R}^p : F(x) = F^*\}$ is the set of optimal solutions

$$\mathrm{Dist}_0 := \max_{x \in \mathcal{S}_0} \min_{x^* \in \mathcal{S}^*} \|x - x^*\|_1$$



(In high-dimensional machine learning problems, $\mathcal{S}^*$ can be very big)

Computational Guarantees for Greedy Coordinate Descent

$$\mathrm{Dist}_0 := \max_{x \in \mathcal{S}_0} \min_{x^* \in \mathcal{S}^*} \|x - x^*\|_1$$

Theorem: Objective Function Value Convergence (essentially [Beck and Tetruashvil 2014], [Nesterov 2003])

If the step-sizes are chosen using the rule:

$$\alpha_k = \frac{\|\nabla F(x^k)\|_\infty}{L_F} \quad \text{for all } k \geq 0 \ ,$$

then for each $k \geq 0$ the following inequality holds:

$$F(x^k) - F^* \ \leq \ \frac{2L_F(\mathrm{Dist}_0)^2}{\hat{K}^0 + k} \ < \ \frac{2L_F(\mathrm{Dist}_0)^2}{k}$$

where $\hat{K}^0 := \dfrac{2L_F(\mathrm{Dist}_0)^2}{F(x^0) - F^*}$.

Computational Guarantees for GCD, cont.

Theorem: Gradient Norm Convergence and Iterate Bounds ("Shrinkage")

If the step-sizes are chosen using the rule:

$$\alpha_k = \frac{\|\nabla F(x^k)\|_\infty}{L_F} \quad \text{for all } k \geq 0 \ ,$$

then for each $k \geq 0$ the following inequality holds:

$$\min_{i \in \{0,\ldots,k\}} \|\nabla F(x^i)\|_\infty \ \leq \ \sqrt{\frac{2L_F(F(x^0) - F^*)}{k+1}} \quad ,$$

and also

$$\|x^k - x^0\|_1 \ \leq \ \sqrt{k}\sqrt{\frac{2(F(x^0) - F^*)}{L_F}} \ .$$

Stochastic Gradient Descent (SGD) Method

The problem of interest is:

$$F^* := \min_x \; F(x) \quad \text{s.t.} \; x \in \mathbb{R}^p$$

Let $\tilde{\nabla} f(x)$ be a stochastic estimate of the gradient $\nabla F(x)$ at each x

Stochastic Gradient Descent method for minimizing $F(x)$

Initialize at $x^0 \in \mathbb{R}^p$, $k \leftarrow 0$

At iteration k :

1. Compute stochastic gradient $\tilde{\nabla} F(x^k)$
2. Choose step-size α_k
3. Set $x^{k+1} \leftarrow x^k - \alpha_k \tilde{\nabla} F(x^k)$

Stochastic Gradient Descent (SGD) Method, cont.

The canonical setting for SGD is minimizing a large sum (or average) of losses:

$$
\begin{array}{rrl}
F^* \quad := & \displaystyle\min_{x} & F(x) := \frac{1}{n}\sum_{j=1}^{n} F_j(x) \\
& \text{s.t.} & x \in \mathbb{R}^p
\end{array}
$$

where $n \gg 0$ and $\tilde{\nabla} F(x)$ is computed as follows:

1. Choose $j \sim \{1, \ldots, n\}$ uniformly and independently
2. $\tilde{\nabla} F(x) \leftarrow \nabla F_j(x)$

Then the stochastic gradient is unbiased: $\mathbb{E}[\tilde{\nabla} F(x) | x] = \nabla F(x)$

Computational Guarantees for Stochastic Gradient Descent [Bertsekas, others]

Assume that
(i) the stochastic gradient is unbiased, namely

$$\mathbb{E}[\tilde{\nabla} F(x)|x] = \nabla F(x) \text{ for any } x \text{ , and}$$

(ii) $F(\cdot)$ is G-stochastically smooth: there exists G such that:

$$\mathbb{E}[\|\tilde{\nabla} F(x)\|_2^2 \mid x] \le G^2 \text{ for any } x$$

Theorem: Expected Convergence of Stochastic Gradient Descent

If the step-sizes are constant:

$$\alpha_k = \bar{\alpha} \quad \text{for all } k \ge 0 \text{ ,}$$

then for each $k \ge 0$ the following inequality holds:

$$\mathbb{E}[F(\bar{x}^k)] - F^* \le \frac{\bar{\alpha} G^2}{2} + \frac{\|x^0 - x^*\|_2^2}{2\bar{\alpha}(k+1)} \text{ ,}$$

where $\bar{x}^k := \frac{1}{k+1} \sum_{i=0}^k x^i$.

Logistic Regression

Logistic Regression

Logistic Regression Example: Predicting Parole Violation

Predict P(violate parole) based on age, gender, time served, offense class, multiple convictions, NYC, etc.

	Violator	Male	Age	TimeServed	Class	Multiple	InCity
1	0	1	49.4	3.15	D	0	1
2	1	1	26.0	5.95	D	1	0
3	0	1	24.9	2.25	D	1	0
4	0	1	52.1	29.22	A	0	0
5	0	1	35.9	12.78	A	1	1
6	0	1	25.9	1.18	C	1	1
7	0	1	19.0	0.54	D	0	0
8	0	1	43.2	1.07	C	0	1
9	0	1	31.6	1.17	E	0	0
10	0	1	40.7	4.64	B	1	1
11	0	1	53.9	21.61	A	0	1
12	0	1	28.5	3.23	D	1	0
13	0	1	36.1	3.71	D	0	1
14	0	1	48.8	1.17	D	0	0
15	0	1	37.6	4.62	C	0	0
16	0	1	42.5	1.75	D	0	1
...	...	...	...	...	...	...	...
6098	0	1	55.0	0.72	E	0	0
6099	0	1	49.6	29.88	A	0	1
6100	0	1	22.4	2.85	D	0	1
6101	0	1	44.8	1.76	D	1	0
6102	0	0	45.3	1.03	E	0	0

Logistic Regression for Prediction

$Y \in \{-1, 1\}$ is a Bernoulli random variable:

$$P(Y = 1) = p$$

$$P(Y = -1) = 1 - p$$

$x = (x_1, \ldots, x_p) \in \mathbb{R}^p$ is the vector of independent variables

$P(Y = 1)$ depends on the values of the independent variables $x_1, \ldots, x_p$

Logistic regression model is:

$$P(Y = 1 \mid x) \;=\; \frac{1}{1 + e^{-\beta^T x}}$$

Logistic Regression for Prediction, continued

Logistic regression model is:

$$P(Y = 1 \mid x) = \frac{1}{1 + e^{-\beta^T x}}$$

Data records are (x_i, y_i), $i = 1, \ldots, n$

	Violator	Male	Age	TimeServed	Class	Multiple	InCity
1	0	1	49.4	3.15	D	0	1
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6101	0	1	44.8	1.76	D	1	0
6102	0	0	45.3	1.03	E	0	0

Let us construct an estimate of β based on the data (x_i, y_i), $i = 1, \ldots, n$

Logistic Regression: Maximum Likelihood Estimation

$$\max_{\beta} \left(\prod_{y_i=1} \frac{1}{1+e^{-\beta^T x_i}} \right) \left(\prod_{y_i=-1} \left(1 - \frac{1}{1+e^{-\beta^T x_i}} \right) \right)$$

$$= \max_{\beta} \left(\prod_{i=1}^{n} \frac{1}{1+e^{-y_i \beta^T x_i}} \right)$$

$$\equiv \min_{\beta} \frac{1}{n} \sum_{i=1}^{n} \ln \left(1 + e^{-y_i \beta^T x_i} \right) \quad =: \quad L_n(\beta)$$

Logistic Regression Optimization Problem

Logistic regression optimization problem is:

$$\begin{array}{rlll} L_n^* & := & \min\limits_{\beta} & L_n(\beta) := \frac{1}{n}\sum_{i=1}^{n} \ln(1+\exp(-y_i\beta^T x_i)) \\ & & \text{s.t.} & \beta \in \mathbb{R}^p \end{array}$$

If $y_i = +1$, we ideally want $\beta^T x_i \gg 0$

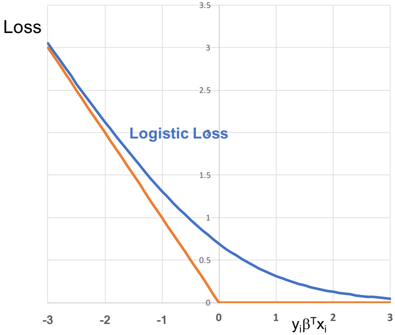
If $y_i = -1$, we ideally want $\beta^T x_i \ll 0$

Therefore we ideally want β for which $y_i\beta^T x_i \gg 0$ for very many i

Logistic Regression Optimization Problem, continued

Logistic regression optimization problem is:

$$
\begin{array}{rll}
L_n^* \;:= & \min\limits_{\beta} & L_n(\beta) := \frac{1}{n}\sum_{i=1}^{n} \ln(1+\exp(-y_i\beta^T x_i)) \\
 & \text{s.t.} & \beta \in \mathbb{R}^p
\end{array}
$$



Each logistic loss term is a 1-smoothing of $\max\{0, -y_i\beta^T x_i\}$

Basic Properties of the Logistic Loss Function

$$\begin{array}{rcll} L_n^* & := & \min\limits_{\beta} & L_n(\beta) := \frac{1}{n}\sum_{i=1}^n \ln(1+\exp(-y_i\beta^T x_i)) \\ & & \text{s.t.} & \beta \in \mathbb{R}^p \end{array}$$

- $L_n(\cdot)$ is convex
- $\nabla L_n(\cdot)$ is $L = \frac{1}{4n}\|\mathbf{X}\|_{1,2}^2$-Lipschitz:

$$\|\nabla L_n(\beta) - \nabla L_n(\beta')\|_\infty \le \frac{1}{4n}\|\mathbf{X}\|_{1,2}^2 \|\beta - \beta'\|_1$$

  where $\mathbf{X} := \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$

- For $\beta^0 := 0$ it holds that $L_n(\beta^0) = \ln(2)$
- $L_n^* \ge 0$
- If $L_n^* = 0$, then the optimum is not attained (something is "wrong" or "very wrong")
- We will see later that "very wrong" might actually be very good....

Logistic Regression Problem of Interest, continued

Alternate versions of optimization problem add regularization and/or sparsification:

$$
\begin{array}{lll}
L_n^* \;:=\; & \min\limits_{\beta} & L_n(\beta) := \frac{1}{n}\sum_{i=1}^n \ln(1+\exp(-y_i\beta^T x_i)) + \lambda\|\beta\|_p \\
& \text{s.t.} & \beta \in \mathbb{R}^p \\
& & \|\beta\|_0 \le k
\end{array}
$$

Overall aspirations:

- Good predictive performance on new (out of sample) observations
- Models that are more interpretable (e.g., sparse)

How do GCD and SGD Inform Logistic Regression?

Some questions:

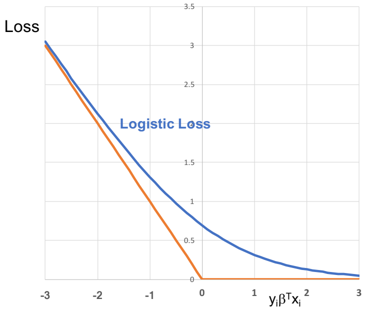
- How do the computational guarantees for Greedy Coordinate Descent and Stochastic Gradient Descent specialize to the case of Logistic Regression?
- Can we say anything further about the convergence properties of these methods in the special case of Logistic Regression?
- What role does problem structure/conditioning play in these guarantees?

Elementary Properties of the Logistic Loss Function

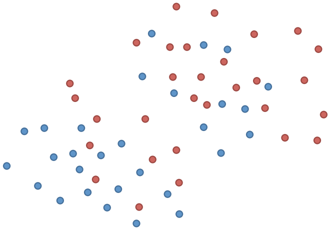
$$L_n^* \quad := \quad \min_{\beta} \quad L_n(\beta) := \tfrac{1}{n}\sum_{i=1}^{n} \ln(1+\exp(-y_i\beta^T x_i))$$

Recall that logistic regression "ideally" seeks β for which $y_i x_i^T \beta \gg 0$ for all i :

- $y_i = +1 \Rightarrow x_i^T\beta \gg 0$
- $y_i = -1 \Rightarrow x_i^T\beta \gg 0$

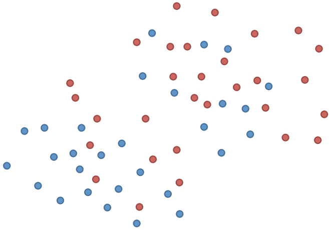


Geometry of the Data: Separable and Non-Separable Data

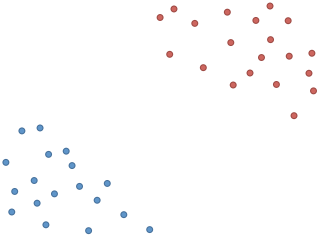


(a) Data is Non-Separable (b) Data is Separable

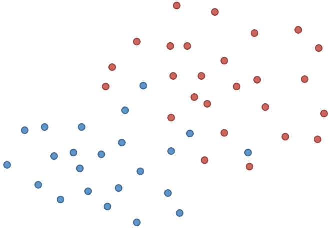
Very/Mild Separable/Non-Separable Data



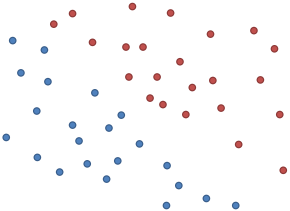
(a) Data is Very Non-Separable



(b) Data is Very Separable



(c) Data is Mildly Non-Separable



(d) Data is Mildly Separable

Separable and Non-Separable Data

Separable Data

The data is separable if there exists $\bar{\beta}$ for which

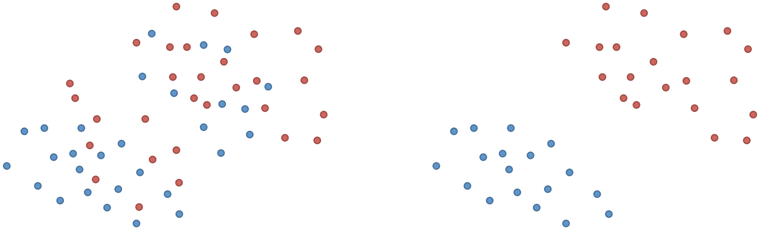
$$y_i \cdot (\bar{\beta})^T x_i > 0 \quad \text{for all } i = 1, \ldots, n$$

Non-Separable Data

The data is non-separable if it is not separable, namely, every β satisfies

$$y_i \cdot (\beta)^T x_i \leq 0 \quad \text{for at least one } i \in \{1, \ldots, n\}$$

Separable and Non-Separable Data



(a) Data is Non-Separable

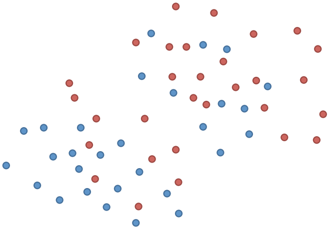
(b) Data is Separable

Results in the Non-Separable Case

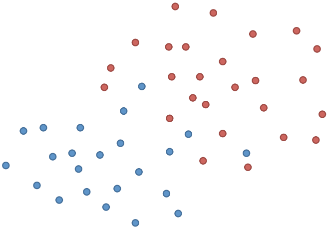
Results in the Non-Separable Case

Non-Separable Data and Problem Behavior/Conditioning

Let us quantify the degree of non-separability of the data.



(a) Very non-separable data



(b) Mildly non-separable data

We will relate this to problem behavior/conditioning....

Non-Separability Condition Number $\mathrm{DegNSEP}^*$

Definition of Non-Separability Condition Number $\mathrm{DegNSEP}^*$

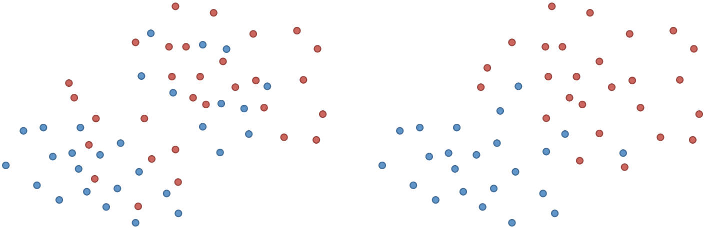
$$\begin{aligned} \mathrm{DegNSEP}^* := \quad \min_{\beta \in \mathbb{R}^p} \quad & \frac{1}{n}\sum_{i=1}^{n}[y_i\beta^T x_i]^- \\ \text{s.t.} \quad & \|\beta\|_1 = 1 \end{aligned}$$

$\mathrm{DegNSEP}^*$ is the least average misclassification error (over all normalized classifiers)

$\mathrm{DegNSEP}^* > 0$ if and only if the data is strictly non-separable

Non-Separability Measure DegNSEP*

$$\mathrm{DegNSEP}^* := \min_{\beta \in \mathbb{R}^p} \quad \frac{1}{n}\sum_{i=1}^{n}[y_i \beta^T x_i]^-$$
$$\text{s.t.} \quad \|\beta\|_1 = 1$$



(a) DegNSEP* is large (b) DegNSEP* is small

Computational Guarantees for Greedy Coordinate Descent: Non-Separable Case

Theorem: Computational Guarantees for Greedy Coordinate Descent: Non-Separable Case

Consider the GCD applied to the Logistic Regression problem with step-sizes $\alpha_k := \frac{4n\|\nabla L_n(\beta^k)\|_\infty}{\|\mathbf{X}\|_{1,2}^2}$ for all $k \geq 0$, and suppose that the data is non-separable. Then for each $k \geq 0$ it holds that:

(i) (training error): $L_n(\beta^k) - L_n^* \leq \frac{2(\ln(2))^2\|\mathbf{X}\|_{1,2}^2}{k \cdot n \cdot (\mathrm{DegNSEP}^*)^2}$

(ii) (regularization): $\|\beta^k\|_1 \leq \sqrt{k}\left(\frac{1}{\|\mathbf{X}\|_{1,2}}\right)\sqrt{8n(\ln(2) - L_n^*)}$

Computational Guarantees for Greedy Coordinate Descent: Non-Separable Case

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(ii) (regularization): $\|\beta^k\|_1 \ \leq \ \sqrt{k}\left(\frac{1}{\|\mathbf{X}\|_{1,2}}\right)\sqrt{8n(\ln(2) - L_n^*)}$

Computational Guarantees for Stochastic Gradient Descent: Non-Separable Case

Theorem: Computational Guarantees for Stochastic Gradient Descent: Non-Separable Case

Consider SGD applied to the Logistic Regression problem with step-sizes $\alpha_i := \frac{\sqrt{8n\ln(2)}}{\sqrt{k+1}\|\mathbf{X}\|_{2,2}\|\mathbf{X}\|_{2,\infty}}$ for $i = 0, \ldots, k$, and suppose that the data is non-separable. Then it holds that:

(i) (training error):

$$\mathbb{E}[\min_{0\leq i\leq k} L_n(\beta^i)] - L_n^* \;\leq\; \frac{1}{\sqrt{k+1}}\left(\frac{(L_n^*)^2\|\mathbf{X}\|_{2,\infty}^2}{4\sqrt{2\ln(2)}(\text{DegNSEP}^*)^2} + \frac{\sqrt{2\ln(2)n}\|\mathbf{X}\|_{2,\infty}}{\|\mathbf{X}\|_{2,2}}\right)$$

(ii) (regularization): $\|\beta^k\|_2 \;\leq\; \sqrt{k+1}\left(\frac{\sqrt{8n\ln(2)}}{\|\mathbf{X}\|_{2,2}}\right)$

Computational Guarantees for Stochastic Gradient Descent: Non-Separable Case

Theorem: Computational Guarantees for Stochastic Gradient Descent: Non-Separable Case

Consider SGD applied to the Logistic Regression problem with step-sizes $\alpha_i := \frac{\sqrt{8n\ln(2)}}{\sqrt{k+1}\|\mathbf{X}\|_{2,2}\|\mathbf{X}\|_{2,\infty}}$ for $i = 0, \ldots, k$, and suppose that the data is non-separable. Then it holds that:

(i) (training error):

$$\mathbb{E}[\min_{0\le i\le k} L_n(\beta^i)] - L_n^* \ \le \ \frac{1}{\sqrt{k+1}}\left(\frac{(L_n^*)^2\|\mathbf{X}\|_{2,\infty}^2}{4\sqrt{2\ln(2)}(\mathrm{DegNSEP}^*)^2} + \frac{\sqrt{2\ln(2)n}\|\mathbf{X}\|_{2,\infty}}{\|\mathbf{X}\|_{2,2}}\right)$$

(ii) (regularization): $\|\beta^k\|_2 \ \le \ \sqrt{k+1}\left(\frac{\sqrt{8n\ln(2)}}{\|\mathbf{X}\|_{2,2}}\right)$

Reaching Linear Convergence

Reaching Linear Convergence using Greedy Coordinate Descent for Logistic Regression

For logistic regression, does GCD exhibit linear convergence?

Some Definitions/Notation

Definitions:

- $R := \max_{i \in \{1,\ldots,n\}} \|x_i\|_2$ (maximum ℓ_2 norm of the feature vectors)
- $H(\beta^*)$ denotes the Hessian of $L_n(\cdot)$ at an optimal solution β^*
- $\lambda_{\mathrm{pmin}}(H(\beta^*))$ denotes the smallest non-zero (and hence positive) eigenvalue of $H(\beta^*)$

Reaching Linear Convergence of GCD for Logistic Regression

Theorem: Reaching Linear Convergence of GCD for Logistic Regression

Consider GCD applied to the Logistic Regression problem with step-sizes $\alpha_k := \frac{4n\|\nabla L_n(\beta^k)\|_\infty}{\|\mathbf{X}\|_{1,2}^2}$ for all $k \geq 0$, and suppose that the data is non-separable. Define:

$$\check{k} := \frac{16p\ln(2)^2\|\mathbf{X}\|_{1,2}^4 R^2}{9n^2(\mathrm{DegNSEP}^*)^2\lambda_{\mathrm{pmin}}(H(\beta^*))^2} \ .$$

Then for all $k \geq \check{k}$, it holds that:

$$L_n(\beta^k) - L_n^* \leq (L_n(\beta^{\check{k}}) - L_n^*)\left(1 - \frac{\lambda_{\mathrm{pmin}}(H(\beta^*))n}{p\cdot\|\mathbf{X}\|_{1,2}^2}\right)^{k-\check{k}} \ .$$

Reaching Linear Convergence of GCD for Logistic Regression, cont.

Some comments:

- Proof relies on (a slight generalization of) the "generalized self-concordance" property of the logistic loss function due to [Bach 2014]
- Furthermore, we can bound:

$$\lambda_{\rm pmin}(H(\beta^*)) \ \geq \ \tfrac{1}{4n}\lambda_{\rm pmin}(\mathbf{X}^T\mathbf{X}) \exp\left(-\frac{\ln(2)\|\mathbf{X}\|_{1,\infty}}{\mathrm{DegNSEP}^*}\right)$$

- As compared to results of a similar flavor for other algorithms, here we have an exact characterization of when the linear convergence "kicks in" and also what the rate of linear convergence is guaranteed to be
- Q: Can we exploit this generalized self-concordance property in other ways? (still ongoing . . .)

DegNSEP* and "Perturbation to Separability"

$$\mathrm{DegNSEP}^* := \min_{\beta \in \mathbb{R}^p} \quad \frac{1}{n}\sum_{i=1}^{n}[y_i \beta^T x_i]^-$$

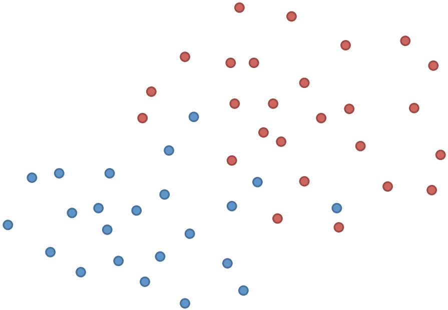
$$\text{s.t.} \quad \|\beta\|_1 = 1$$

Theorem: DegNSEP* is the "Perturbation to Separability"

$$\mathrm{DegNSEP}^* = \inf_{\Delta x_1, \ldots, \Delta x_n} \quad \frac{1}{n}\sum_{i=1}^{n} \|\Delta x_i\|_\infty$$

$$\text{s.t.} \quad (x_i + \Delta x_i, y_i), i = 1, \ldots, n \text{ are separable}$$

Illustration of Perturbation to Separability

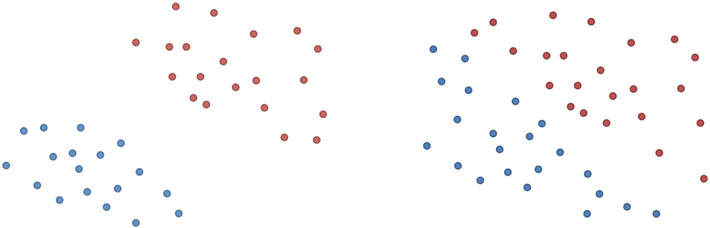


Results in the Separable Case

Results in the Separable Case

Separable Data and Problem Behavior/Conditioning

Let us quantify the degree of separability of the data.



(a) Very separable data

(b) Barely separable data

We will relate this to problem behavior/conditioning....

Separability Condition Number DegSEP^*

Definition of Separability Condition Number DegSEP^*

$$\begin{aligned} \mathrm{DegSEP}^* := \quad & \max_{\beta \in \mathbb{R}^p} \quad \min_{i \in \{1,\ldots,n\}} [y_i \beta^T x_i] \\ & \text{s.t.} \quad \|\beta\|_1 \leq 1 \end{aligned}$$

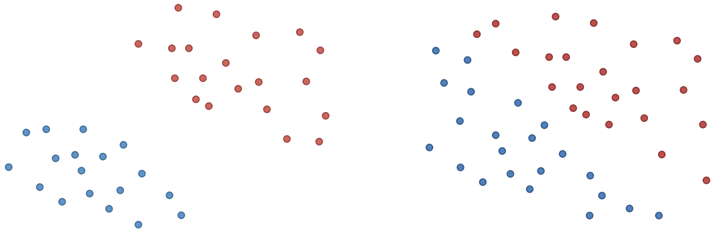
DegSEP^* maximizes the minimal classification value $[y_i \beta^T x_i]$ (over all normalized classifiers)

DegSEP^* is simply the "maximum margin" in machine learning parlance

$\mathrm{DegSEP}^* > 0$ if and only if the data is separable

Separability Measure DegSEP*

$$\mathrm{DegSEP}^* := \max_{\beta \in \mathbb{R}^p} \quad \min_{i \in \{1,\ldots,n\}} [y_i \beta^T x_i]$$
$$\text{s.t.} \quad \|\beta\|_1 \leq 1$$



(a) DegSEP* is large

(b) DegSEP* is small

DegSEP^* and Problem Behavior/Conditioning

$$L_n^* \quad := \quad \min_{\beta} \quad L_n(\beta) := \frac{1}{n}\sum_{i=1}^{n} \ln(1+\exp(-y_i\beta^T x_i))$$

$$\begin{array}{rll} \mathrm{DegSEP}^* := & \max\limits_{\beta\in\mathbb{R}^p} & \min\limits_{i\in\{1,\ldots,n\}} [y_i\beta^T x_i] \\ & \text{s.t.} & \|\beta\|_1 \le 1 \end{array}$$

Theorem: Separability and Non-Attainment

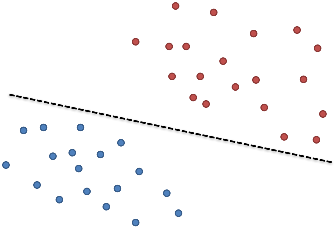
Suppose that the data is separable. Then $\mathrm{DegSEP}^* > 0$, $L_n^* = 0$, and LR does not attain its optimum.

Despite this, it turns out that Greedy Coordinate Descent and also Stochastic Gradient Descent are reasonably effective at finding an approximate margin maximizer ....

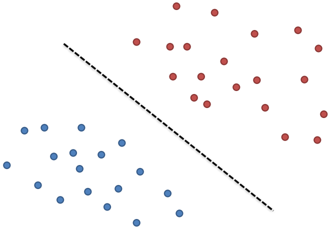
Margin function $\rho(\beta)$

Margin function $\rho(\beta)$

$$\rho(\beta) := \min_{i \in \{1,\ldots,n\}} [y_i \beta^T x_i]$$



(a) $\rho(\beta)$ is small



(b) $\rho(\beta)$ is large

Computational Guarantees for Greedy Coordinate Descent: Separable Case

Theorem: Computational Guarantees for Greedy Coordinate Descent: Separable Case

Consider GCD applied to the Logistic Regression problem with step-sizes $\alpha_k := \frac{4n\|\nabla L_n(\beta^k)\|_\infty}{\|\mathbf{X}\|_{1,2}^2}$ for all $k \geq 0$, and suppose that the data is separable.

(i) (margin bound): there exists $i \leq \left\lfloor \frac{3.7n\|\mathbf{X}\|_{1,2}^2}{(\mathrm{DegSEP}^*)^2} \right\rfloor$ for which the normalized iterate $\bar{\beta}^i := \beta^i/\|\beta^i\|_1$ satisfies

$$\rho(\bar{\beta}^i) \;\geq\; \frac{.18 \cdot \mathrm{DegSEP}^*}{n} \,.$$

(ii) (shrinkage): $\|\beta^k\|_1 \;\leq\; \sqrt{k}\left(\frac{1}{\|\mathbf{X}\|_{1,2}}\right)\sqrt{8n\ln(2)}$

Computational Guarantees for Greedy Coordinate Descent: Separable Case

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(ii) (shrinkage): $\|\beta^k\|_1 \ \leq \ \sqrt{k} \left(\frac{1}{\|\mathbf{X}\|_{1,2}} \right) \sqrt{8n\ln(2)}$

Computational Guarantees for Stochastic Gradient Descent: Separable Case

Theorem: Computational Guarantees for Stochastic Gradient Descent: Separable Case

Consider SGD applied to the Logistic Regression problem with step-sizes $\alpha_i := \frac{\sqrt{8n\ln(2)}}{\sqrt{k+1}\|\mathbf{X}\|_{2,2}\|\mathbf{X}\|_{2,\infty}}$ for $i = 0, \ldots, k$, where

$$k := \left\lfloor \frac{28.1 n^3 \|\mathbf{X}\|_{2,2}^2 \|\mathbf{X}\|_{2,\infty}^2}{\gamma^2 (\mathrm{DegSEP}^*)^4} \right\rfloor$$

and $\gamma \in (0,1]$. If the data is separable, then :

$$\mathbb{P}\left(\exists i \in \{0, \ldots, k\} \text{ s.t. } \rho(\bar{\beta}^i) \geq \frac{\gamma (\mathrm{DegSEP}^*)^2}{20 n^2 \|\mathbf{X}\|_{2,\infty}} \right) \geq 1 - \gamma \ .$$

where $\bar{\beta}^i := \beta^i / \|\beta^i\|_1$ are the normalized iterates of SGD.

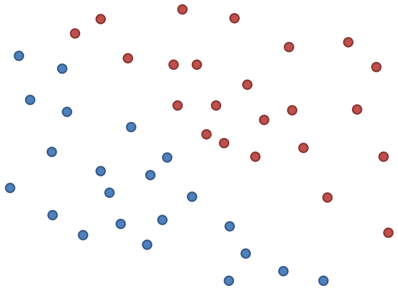
DegSEP* and "Perturbation to Non-Separability"

$$\begin{aligned} \mathrm{DegSEP}^* := \max_{\beta \in \mathbb{R}^p} \quad & \min_{i \in \{1,\ldots,n\}} [y_i \beta^T x_i] \\ \text{s.t.} \quad & \|\beta\|_1 \leq 1 \end{aligned}$$

Theorem: DegSEP* is the "Perturbation to Non-Separability"

$$\begin{aligned} \mathrm{DegSEP}^* = \inf_{\Delta x_1,\ldots,\Delta x_n} \quad & \max_{i \in \{1,\ldots,n\}} \|\Delta x_i\|_\infty \\ \text{s.t.} \quad & (x_i + \Delta x_i, y_i), i = 1, \ldots, n \text{ are non-separable} \end{aligned}$$

Illustration of Perturbation to Non-Separability



Other Issues

Some other topics not mentioned (still ongoing):

- Other first-order methods for logistic regression (gradient descent, accelerated gradient descent, other randomized methods, etc.
- High-dimensional regime $p > n$, define $\mathrm{DegNSEP}^*_k$ and DegSEP^*_k for restricting β to satisfy $\|\beta\|_0 \leq k$
- Numerical experiments comparing methods
- Other...

Summary

- Some old and new results for Greedy Coordinate Descent and Stochastic Gradient Descent
- Analyizing these methods for Logistic Regression: separable/non-separable cases
- Non-Separable case
  - condition number $\mathrm{DegNSEP}^*$
  - computational guarantees for Greedy Coordinate Descent and Stochastic Gradient Descent, including reaching linear convergence
- Separable case
  - condition number DegSEP^*
  - computational guarantees for Greedy Coordinate Descent and Stochastic Gradient Descent, including computing an approximate maximum margin classifier