ℓ_1 and ℓ_2 Regularization

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Hypothesis Spaces

- We've spoken vaguely about "bigger" and "smaller" hypothesis spaces
- In practice, convenient to work with a **nested sequence** of spaces:

$$\mathcal{F}_1 \subset \mathcal{F}_2 \subset \mathcal{F}_n \cdots \subset \mathcal{F}$$

Polynomial Functions

- $\mathcal{F} = \{\text{all polynomial functions}\}\$
- $\mathcal{F}_d = \{\text{all polynomials of degree } \leq d\}$

Complexity Measures for Decision Functions

- Number of variables / features
- Depth of a decision tree
- Degree of polynomial
- How about for linear decision functions, i.e. $x \mapsto w^T x = w_1 x_1 + \dots + w_d x_d$?
 - ℓ_0 complexity: number of non-zero coefficients $\sum_{i=1}^d \mathbb{1}(w_i \neq 0)$.
 - ℓ_1 "lasso" complexity: $\sum_{i=1}^{d} |w_i|$, for coefficients w_1, \ldots, w_d
 - ℓ_2 "ridge" complexity: $\sum_{i=1}^{d} w_i^2$ for coefficients w_1, \ldots, w_d

Nested Hypothesis Spaces from Complexity Measure

- Hypothesis space: \mathcal{F}
- Complexity measure $\Omega: \mathcal{F} \to [0, \infty)$
- Consider all functions in \mathcal{F} with complexity at most r:

$$\mathcal{F}_r = \{ f \in \mathcal{F} \mid \Omega(f) \leqslant r \}$$

• Increasing complexities: $r = 0, 1.2, 2.6, 5.4, \dots$ gives nested spaces:

$$\mathfrak{F}_0\subset \mathfrak{F}_{1.2}\subset \mathfrak{F}_{2.6}\subset \mathfrak{F}_{5.4}\subset \cdots \subset \mathfrak{F}$$

Constrained Empirical Risk Minimization

Constrained ERM (Ivanov regularization)

For complexity measure $\Omega: \mathcal{F} \to [0, \infty)$ and fixed $r \geqslant 0$,

$$\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i)$$
s.t. $\Omega(f) \leqslant r$

- Choose r using validation data or cross-validation.
- Each r corresponds to a different hypothesis spaces. Could also write:

$$\min_{f \in \mathcal{F}_r} \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i)$$

Penalized Empirical Risk Minimization

Penalized ERM (Tikhonov regularization)

For complexity measure $\Omega: \mathfrak{F} \to [0,\infty)$ and fixed $\lambda \geqslant 0$,

$$\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) + \lambda \Omega(f)$$

- Choose λ using validation data or cross-validation.
- (Ridge regression in homework is of this form.)

Ivanov vs Tikhonov Regularization

- Let $L: \mathcal{F} \to \mathbf{R}$ be any performance measure of f
 - \bullet e.g. L(f) could be the empirical risk of f
- For many L and Ω , Ivanov and Tikhonov are "equivalent".
- What does this mean?
 - Any solution f^* you could get from Ivanov, can also get from Tikhonov.
 - Any solution f^* you could get from Tikhonov, can also get from Ivanov.
- In practice, both approaches are effective.
- Tikhonov convenient because it's unconstrained minimization.

Can get conditions for equivalence from Lagrangian duality theory – details in homework.

Ivanov vs Tikhonov Regularization (Details)

Ivanov and Tikhonov regularization are equivalent if:

• For any choice of r > 0, any Ivanov solution

$$f_r^* \in \operatorname*{arg\,min} L(f) \text{ s.t. } \Omega(f) \leqslant r$$

is also a Tikhonov solution for some $\lambda > 0$. That is, $\exists \lambda > 0$ such that

$$f_r^* \in \underset{f \in \mathcal{F}}{\arg\min} L(f) + \lambda \Omega(f).$$

② Conversely, for any choice of $\lambda > 0$, any Tikhonov solution:

$$f_{\lambda}^* \in \operatorname*{arg\,min}_{f \in \mathcal{F}} L(f) + \lambda \Omega(f)$$

is also an Ivanov solution for some r > 0. That is, $\exists r > 0$ such that

$$f_{\lambda}^* \in \operatorname*{arg\,min}_{f \in \mathcal{F}} \mathit{L}(f) \text{ s.t. } \Omega(f) \leqslant r$$

 ℓ_1 and ℓ_2 Regularization

Linear Least Squares Regression

Consider linear models

$$\mathcal{F} = \left\{ f : \mathbf{R}^d \to \mathbf{R} \mid f(x) = w^T x \text{ for } w \in \mathbf{R}^d \right\}$$

- Loss: $\ell(\hat{y}, y) = (y \hat{y})^2$
- Training data $\mathfrak{D}_n = ((x_1, y_1), \dots, (x_n, y_n))$
- Linear least squares regression is ERM for ℓ over \mathcal{F} :

$$\hat{w} = \operatorname*{arg\,min}_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n \left\{ w^T x_i - y_i \right\}^2$$

- Can **overfit** when *d* is large compared to *n*.
- e.g.: $d \gg n$ very common in Natural Language Processing problems (e.g. a 1M features for 10K documents).

Ridge Regression: Workhorse of Modern Data Science

Ridge Regression (Tikhonov Form)

The ridge regression solution for regularization parameter $\lambda \geqslant 0$ is

$$\hat{w} = \arg\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n \left\{ w^T x_i - y_i \right\}^2 + \lambda ||w||_2^2,$$

where $||w||_2^2 = w_1^2 + \cdots + w_d^2$ is the square of the ℓ_2 -norm.

Ridge Regression (Ivanov Form)

The ridge regression solution for complexity parameter $r \ge 0$ is

$$\hat{w} = \arg\min_{\|w\|_2^2 \le r^2} \frac{1}{n} \sum_{i=1}^n \left\{ w^T x_i - y_i \right\}^2.$$

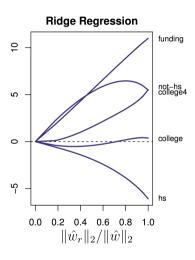
How does ℓ_2 regularization induce "regularity"?

- For $\hat{f}(x) = \hat{w}^T x$, \hat{f} is **Lipschitz continuous** with Lipschitz constant $L = \|\hat{w}\|_2$.
- That is, when moving from x to x+h, \hat{f} changes no more than L||h||.
- So ℓ_2 regularization controls the maximum rate of change of \hat{f} .
- Proof:

$$\begin{aligned} \left| \hat{f}(x+h) - \hat{f}(x) \right| &= \left| \hat{w}^T(x+h) - \hat{w}^T x \right| = \left| \hat{w}^T h \right| \\ &\leqslant \|\hat{w}\|_2 \|h\|_2 \text{(Cauchy-Schwarz inequality)} \end{aligned}$$

• Since $\|\hat{w}\|_1 \ge \|\hat{w}\|_2$, an ℓ_1 constraint will also give a Lipschitz bound.

Ridge Regression: Regularization Path



$$\begin{array}{rcl} \hat{w}_r & = & \displaystyle \arg\min_{\|w\|_2^2 \le r^2} \frac{1}{n} \sum_{i=1}^n \left(w^T x_i - y_i \right)^2 \\ \hat{w} & = & \hat{w}_\infty = \text{Unconstrained ERM} \end{array}$$

- For r = 0, $||\hat{w}_r||_2 / ||\hat{w}||_2 = 0$.
- For $r = \infty$, $||\hat{w}_r||_2 / ||\hat{w}||_2 = 1$

Lasso Regression: Workhorse (2) of Modern Data Science

Lasso Regression (Tikhonov Form)

The lasso regression solution for regularization parameter $\lambda \geqslant 0$ is

$$\hat{w} = \arg\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n \left\{ w^T x_i - y_i \right\}^2 + \lambda ||w||_1,$$

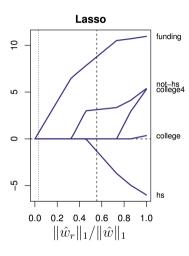
where $||w||_1 = |w_1| + \cdots + |w_d|$ is the ℓ_1 -norm.

Lasso Regression (Ivanov Form)

The lasso regression solution for complexity parameter $r \ge 0$ is

$$\hat{w} = \underset{\|w\|_1 \leq r}{\arg \min} \frac{1}{n} \sum_{i=1}^{n} \{w^T x_i - y_i\}^2.$$

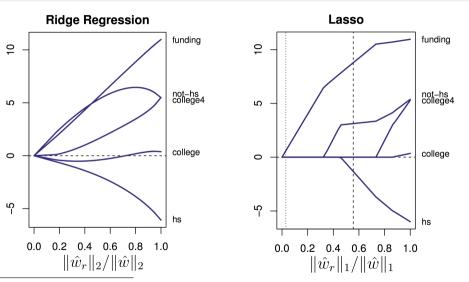
Lasso Regression: Regularization Path



$$\begin{array}{rcl} \hat{w}_r & = & \displaystyle \mathop{\arg\min}_{\|w\|_1 \le r} \frac{1}{n} \sum_{i=1}^n \left(w^T x_i - y_i \right)^2 \\ \hat{w} & = & \hat{w}_\infty = \text{Unconstrained ERM} \end{array}$$

- For r = 0, $||\hat{w}_r||_1/||\hat{w}||_1 = 0$.
- For $r = \infty$, $\|\hat{w}_r\|_1 / \|\hat{w}\|_1 = 1$

Ridge vs. Lasso: Regularization Paths



Modified from Hastie. Tibshirani. and Wainwright's Statistical Learning with Sparsity, Fig 2.1. About predicting crime in 50 US cities. Julia Kempe & David S. Rosenberg (CDS, NYU)

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Lasso Gives Feature Sparsity: So What?

Coefficient are $0 \implies$ don't need those features. What's the gain?

- Time/expense to compute/buy features
- Memory to store features (e.g. real-time deployment)
- Identifies the important features
- Better prediction? sometimes
- As a feature-selection step for training a slower non-linear model

Ivanov and Tikhonov Equivalent?

- For ridge regression and lasso regression (and much more)
 - the Ivanov and Tikhonov formulations are equivalent
 - [Optional homework problem, upcoming.]
- We will use whichever form is most convenient.



Parameter Space

• Illustrate affine prediction functions in parameter space.

The ℓ_1 and ℓ_2 Norm Constraints

- For visualization, restrict to 2-dimensional input space
- $\mathcal{F} = \{f(x) = w_1x_1 + w_2x_2\}$ (linear hypothesis space)
- Represent \mathcal{F} by $\{(w_1, w_2) \in \mathbb{R}^2\}$.
 - ℓ_2 contour: $w_1^2 + w_2^2 = r$



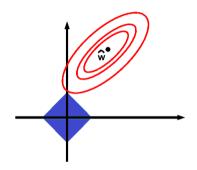
Where are the "sparse" solutions?

•
$$\ell_1$$
 contour: $|w_1| + |w_2| = r$



The Famous Picture for ℓ_1 Regularization

• $f_r^* = \arg\min_{w \in \mathbb{R}^2} \frac{1}{n} \sum_{i=1}^n (w^T x_i - y_i)^2$ subject to $|w_1| + |w_2| \le r$



- Blue region: Area satisfying complexity constraint: $|w_1| + |w_2| \le r$
- Red lines: contours of $\hat{R}_n(w) = \sum_{i=1}^n (w^T x_i y_i)^2$.

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The Empirical Risk for Square Loss

• Denote the empirical risk of $f(x) = w^T x$ by

$$\hat{R}_n(w) = \frac{1}{n} ||Xw - y||^2,$$

where X is the **design matrix**.

- \hat{R}_n is minimized by $\hat{w} = (X^T X)^{-1} X^T y$, the OLS solution.
- What does \hat{R}_n look like around \hat{w} ?

The Empirical Risk for Square Loss

• By "completing the square", we can show for any $w \in \mathbb{R}^d$:

$$\hat{R}_{n}(w) = \frac{1}{n}(w - \hat{w})^{T}X^{T}X(w - \hat{w}) + \hat{R}_{n}(\hat{w})$$

• Set of w with $\hat{R}_n(w)$ exceeding $\hat{R}_n(\hat{w})$ by c>0 is

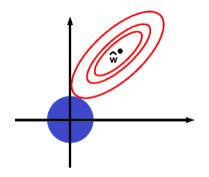
$$\{w \mid \hat{R}_n(w) = c + \hat{R}_n(\hat{w})\} = \{w \mid (w - \hat{w})^T X^T X (w - \hat{w}) = nc\},$$

which is an ellipsoid centered at \hat{w} .

• We'll derive this in homework.

The Famous Picture for ℓ_2 Regularization

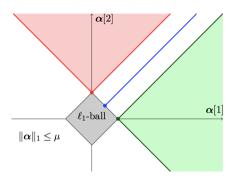
• $f_r^* = \operatorname{arg\,min}_{w \in \mathbb{R}^2} \sum_{i=1}^n (w^T x_i - y_i)^2$ subject to $w_1^2 + w_2^2 \leqslant r$



- Blue region: Area satisfying complexity constraint: $w_1^2 + w_2^2 \leqslant r$
- Red lines: contours of $\hat{R}_n(w) = \sum_{i=1}^n (w^T x_i y_i)^2$.

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Why are Lasso Solutions Often Sparse?



- Suppose design matrix X is orthogonal, so $X^TX = I$, and contours are circles.
- ullet Then OLS solution in green or red regions implies ℓ_1 constrained solution will be at corner

The $(\ell_q)^q$ Constraint

- Generalize to ℓ_a : $(\|w\|_a)^q = |w_1|^q + |w_2|^q$.
- Note: $||w||_q$ is a norm if $q \ge 1$, but not for $q \in (0,1)$
- $\mathcal{F} = \{f(x) = w_1x_1 + w_2x_2\}.$
- Contours of $||w||_q^q = |w_1|^q + |w_2|^q$:



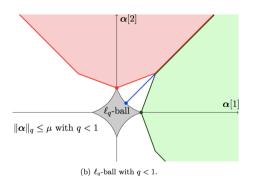








ℓ_q Even Sparser

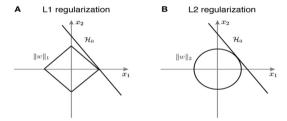


- Suppose design matrix X is orthogonal, so $X^TX = I$, and contours are circles.
- ullet Then OLS solution in green or red regions implies ℓ_q constrained solution will be at corner

 ℓ_q -ball constraint is not convex, so more difficult to optimize.

The Quora Picture

From Quora: "Why is L1 regularization supposed to lead to sparsity than L2? [sic]" (google it)



- Does this picture have any interpretation that makes sense? (Aren't those lines supposed to be ellipses?)
- Yes... we can revisit.



How to find the Lasso solution?

• How to solve the Lasso?

$$\min_{w \in \mathbf{R}^d} \sum_{i=1}^n \left(w^T x_i - y_i \right)^2 + \lambda \|w\|_1$$

• $||w||_1 = |w_1| + |w_2|$ is not differentiable!

Splitting a Number into Positive and Negative Parts

- Consider any number $a \in \mathbb{R}$.
- Let the **positive part** of a be

$$a^+ = a1(a \geqslant 0).$$

• Let the **negative part** of a be

$$a^{-} = -a1(a \leq 0).$$

- Do you see why $a^+ \ge 0$ and $a^- \ge 0$?
- How do you write a in terms of a^+ and a^- ?
- How do you write |a| in terms of a^+ and a^- ?

How to find the Lasso solution?

The Lasso problem

$$\min_{w \in \mathbf{R}^d} \sum_{i=1}^n (w^T x_i - y_i)^2 + \lambda ||w||_1$$

- Replace each w_i by $w_i^+ w_i^-$.
- Write $w^+ = (w_1^+, \dots, w_d^+)$ and $w^- = (w_1^-, \dots, w_d^-)$.

The Lasso as a Quadratic Program

We will show: substituting $w = w^+ - w^-$ and $|w| = w^+ + w^-$ gives an equivalent problem:

$$\min_{w^+,w^-} \quad \sum_{i=1}^n \left(\left(w^+ - w^- \right)^T x_i - y_i \right)^2 + \lambda 1^T \left(w^+ + w^- \right)$$
subject to $w_i^+ \geqslant 0$ for all i , $w_i^- \geqslant 0$ for all i ,

- Objective is differentiable (in fact, convex and quadratic)
- 2d variables vs d variables and 2d constraints vs no constraints
- A "quadratic program": a convex quadratic objective with linear constraints.
 - Could plug this into a generic QP solver.

Possible point of confusion

Equivalent to lasso problem:

$$\min_{w^+,w^-} \quad \sum_{i=1}^n \left(\left(w^+ - w^- \right)^T x_i - y_i \right)^2 + \lambda 1^T \left(w^+ + w^- \right)$$
subject to $w_i^+ \geqslant 0$ for all i $w_i^- \geqslant 0$ for all i ,

- When we plug this optimization problem into a QP solver,
 - it just sees 2d variables and 2d constraints.
 - Doesn't know we want w_i^+ and w_i^- to be positive and negative parts of w_i .
- Turns out they will come out that way as a result of the optimization!
- But to eliminate confusion, let's start by calling them a_i and b_i and prove our claim...

Lasso problem is trivially equivalent to the following:

$$\min_{w} \min_{a,b} \quad \sum_{i=1}^{n} \left((a-b)^{T} x_{i} - y_{i} \right)^{2} + \lambda 1^{T} (a+b)$$
subject to $a_{i} \geqslant 0$ for all i $b_{i} \geqslant 0$ for all i ,
$$a-b = w$$

$$a+b = |w|$$

- Claim: Don't need constraint a + b = |w|.
- $a' \leftarrow a \min(a, b)$ and $b' \leftarrow b \min(a, b)$ at least as good
- So if a and b are minimizers, at least one is 0.
- Since a-b=w, we must have $a=w^+$ and $b=w^-$. So also a+b=|w|.

$$\min_{\substack{w \ a,b}} \min_{\substack{a,b}} \sum_{i=1}^{n} \left((a-b)^{T} x_{i} - y_{i} \right)^{2} + \lambda 1^{T} (a+b)$$
subject to $a_{i} \geqslant 0$ for all i $b_{i} \geqslant 0$ for all i , $a-b=w$

- Claim: Can remove min_w and the constraint a-b=w.
- One way to see this is by switching the order of minimization...

$$\min_{\substack{a,b \ w}} \min_{\substack{w}} \quad \sum_{i=1}^{n} \left((a-b)^{T} x_{i} - y_{i} \right)^{2} + \lambda 1^{T} (a+b)$$
subject to $a_{i} \geqslant 0$ for all i $b_{i} \geqslant 0$ for all i ,
$$a-b=w$$

- For any $a \ge 0$, $b \ge 0$, there's always a single w that satisfies the constraints.
- So the inner minimum is always attained at w = a b.
- Since w doesn't show up in the objective function,
 - nothing changes if we drop min_w and the constraint.

• So lasso optimization problem is equivalent to

$$\min_{a,b} \quad \sum_{i=1}^{n} \left((a-b)^{T} x_{i} - y_{i} \right)^{2} + \lambda 1^{T} (a+b)$$
subject to $a_{i} \ge 0$ for all i , $b_{i} \ge 0$ for all i ,

where at the end we take $w^* = a^* - b^*$ (and we've shown above that a^* and b^* are positive and negative parts of w^* , respectively.)

• Has constraints – how do we optimize?

Projected SGD

$$\begin{aligned} & \min_{w^+, w^- \in \mathbf{R}^d} \sum_{i=1}^n \left(\left(w^+ - w^- \right)^T x_i - y_i \right)^2 + \lambda \mathbf{1}^T \left(w^+ + w^- \right) \\ & \text{subject to } w_i^+ \geqslant 0 \text{ for all } i \\ & w_i^- \geqslant 0 \text{ for all } i \end{aligned}$$

- Just like SGD, but after each step
 - Project w^+ and w^- into the constraint set.
 - In other words, if any component of w^+ or w^- becomes negative, set it back to 0.

Finding the Lasso Solution: Coordinate Descent (Shooting Method)

Coordinate Descent Method

- Goal: Minimize $L(w) = L(w_1, ..., w_d)$ over $w = (w_1, ..., w_d) \in \mathbb{R}^d$.
- In gradient descent or SGD,
 - each step potentially changes all entries of w.
- In each step of coordinate descent,
 - we adjust only a single w_i .
- In each step, solve

$$w_i^{\text{new}} = \underset{w_i}{\text{arg min }} L(w_1, \dots, w_{i-1}, \mathbf{w_i}, w_{i+1}, \dots, w_d)$$

- Solving this argmin may itself be an iterative process.
- Coordinate descent is great when
 - it's easy or easier to minimize w.r.t. one coordinate at a time

Coordinate Descent Method

Coordinate Descent Method

Goal: Minimize $L(w) = L(w_1, \dots w_d)$ over $w = (w_1, \dots, w_d) \in \mathbb{R}^d$.

- Initialize $w^{(0)} = 0$
- while not converged:
 - $\begin{array}{l} \bullet \ \, \text{Choose a coordinate} \ j \in \{1,\ldots,d\} \\ \bullet \ \, w_j^{\text{new}} \leftarrow \arg\min_{w_j} L(w_1^{(t)},\ldots,w_{j-1}^{(t)},\mathbf{w_j},w_{j+1}^{(t)},\ldots,w_d^{(t)}) \\ \bullet \ \, w_j^{(t+1)} \leftarrow w_j^{\text{new}} \ \, \text{and} \ \, w^{(t+1)} \leftarrow w^{(t)} \\ \bullet \ \, t \leftarrow t+1 \end{array}$
- Random coordinate choice \implies stochastic coordinate descent
- Cyclic coordinate choice \implies cyclic coordinate descent

In general, we will adjust each coordinate several times.

Coordinate Descent Method for Lasso

- Why mention coordinate descent for Lasso?
- In Lasso, the coordinate minimization has a closed form solution!

Coordinate Descent Method for Lasso

Closed Form Coordinate Minimization for Lasso

$$\hat{w}_j = \underset{w_j \in \mathbf{R}}{\operatorname{arg\,min}} \sum_{i=1}^n \left(w^T x_i - y_i \right)^2 + \lambda |w|_1$$

Then

$$\hat{w}_j = egin{cases} (c_j + \lambda)/a_j & \text{if } c_j < -\lambda \ 0 & \text{if } c_j \in [-\lambda, \lambda] \ (c_j - \lambda)/a_j & \text{if } c_j > \lambda \end{cases}$$

$$a_j = 2\sum_{i=1}^n x_{i,j}^2$$
 $c_j = 2\sum_{i=1}^n x_{i,j}(y_i - w_{-j}^T x_{i,-j})$

where w_{-i} is w without component j and similarly for $x_{i,-i}$.

Coordinate Descent: When does it work?

- Suppose we're minimizing $f: \mathbb{R}^d \to \mathbb{R}$.
- Sufficient conditions:
 - f is continuously differentiable and
 - 2 f is strictly convex in each coordinate
- But lasso objective

$$\sum_{i=1}^{n} (w^{T} x_{i} - y_{i})^{2} + \lambda ||w||_{1}$$

is not differentiable...

• Luckily there are weaker conditions...

Coordinate Descent: The Separability Condition

Theorem

^a If the objective f has the following structure

$$f(w_1,...,w_d) = g(w_1,...,w_d) + \sum_{j=1}^d h_j(w_j),$$

where

- $g: \mathbb{R}^d \to \mathbb{R}$ is differentiable and convex, and
- each $h_j : R \to R$ is convex (but not necessarily differentiable)

then the coordinate descent algorithm converges to the global minimum.

^aTseng 2001: "Convergence of a Block Coordinate Descent Method for Nondifferentiable Minimization"

Coordinate Descent Method – Variation

- Suppose there's no closed form? (e.g. logistic regression)
- Do we really need to fully solve each inner minimization problem?
- A single projected gradient step is enough for ℓ_1 regularization!
 - Shalev-Shwartz & Tewari's "Stochastic Methods..." (2011)

Stochastic Coordinate Descent for Lasso – Variation

• Let $\tilde{w} = (w^+, w^-) \in \mathsf{R}^{2d}$ and

$$L(\tilde{w}) = \sum_{i=1}^{n} \left(\left(w^{+} - w^{-} \right)^{T} x_{i} - y_{i} \right)^{2} + \lambda \left(w^{+} + w^{-} \right)^{2}$$

Stochastic Coordinate Descent for Lasso - Variation

Goal: Minimize $L(\tilde{w})$ s.t. $w_i^+, w_i^- \ge 0$ for all i.

- Initialize $\tilde{w}^{(0)} = 0$
 - while not converged:
 - Randomly choose a coordinate $j \in \{1, \dots, 2d\}$
 - $\tilde{w}_i \leftarrow \tilde{w}_i + \max\{-\tilde{w}_i, -\nabla_i L(\tilde{w})\}$