ℓ_1 and ℓ_2 Regularization

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Tikhonov and Ivanov Regularization

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

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

Complexity Measures for Decision Functions

- Number of variables / features
- Depth of a decision tree
- Degree of polynomial
- How about for **linear** models?
  - ℓ_0 complexity: number of non-zero coefficients
  - 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:

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

  - If Ω is a norm on $\mathcal{F}$, this is a **ball of radius** r in $\mathcal{F}$.
- Increasing complexities: $r = 0, 1.2, 2.6, 5.4, \ldots$ gives nested spaces:

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

Constrained Empirical Risk Minimization

Constrained ERM (Ivanov regularization)

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

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

$$\text{s.t. } \Omega(f) \leqslant r$$

- 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 $\Omega : \mathcal{F} \to \mathbf{R}^{\geqslant 0}$ 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 #1 is of this form.)

Ivanov vs Tikhonov Regularization

- Let $L : \mathcal{F} \to \mathbf{R}$ be any performance measure of f
  - 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.

Proof of equivalence based on Lagrangian duality – a topic of Lecture 3.

Ivanov vs Tikhonov Regularization (Details)

Ivanov and Tikhonov regularization are equivalent if:

1. For any choice of $r>0$, the Ivanov solution

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

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

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

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

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

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

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

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 $\mathcal{D}_n = ((x_1, y_1), \ldots, (x_n, y_n))$
- Linear least squares regression is ERM for ℓ over $\mathcal{F}$:

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

- 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

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

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 $r \geqslant 0$ is

$$\hat{w} = \operatorname*{arg\,min}_{\|w\|_2^2 \leqslant r^2} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2.$$

How does ℓ_2 penalty induce "regularity"?

- Let $\hat{f}(x) = \hat{w}^T x$ be a solution to the Ivanov form of ridge regression:

$$\hat{w} = \operatorname*{arg\,min}_{\|w\|_2^2 \leqslant r^2} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 .$$

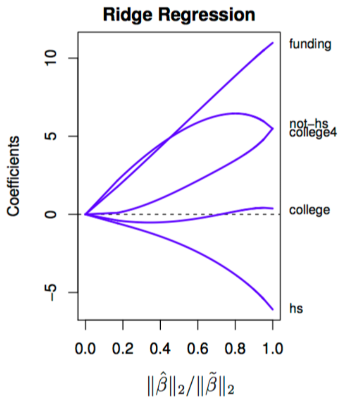
- Suppose x and x' are "close" — that is, $\|x - x'\|_2 < \varepsilon$.

- Then $f(x)$ and $f(x')$ are also "close" if $\|\hat{w}\|_2 \leqslant r$ is small:

$$\begin{aligned} \left| f(x) - f(x') \right| &= \left| \hat{w}^T x - \hat{w}^T x' \right| = \left| \hat{w}^T (x - x') \right| \\ &\leqslant \|\hat{w}\|_2 \|x - x'\|_2 (\text{Cauchy-Schwarz inequality}) \end{aligned}$$

f is **Lipschitz continuous** with Lipschitz constant $r \geqslant \|\hat{w}\|_2$.

Ridge Regression: Regularization Path



$\tilde{\beta}$ is unregularized solution; $\hat{\beta}$ is the ridge solution. (Which side has more regularization?)

Plot from Hastie, Tibshirani, and Wainwright's Statistical Learning with Sparsity, Figure 2.1. Data about predicting crime rate in 50 US cities.

Lasso Regression: Workhorse (2) of Modern Data Science

Lasso Regression (Tikhonov Form)

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

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

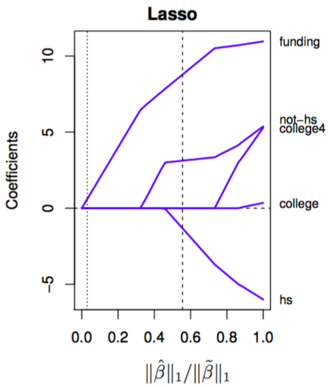
where $\|w\|_1 = |w_1| + \cdots + |w_d|$ is the ℓ_1-norm.

Lasso Regression (Ivanov Form)

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

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

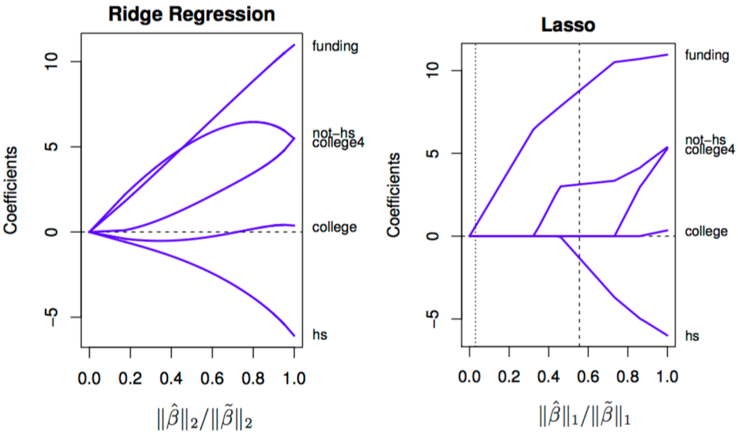
Lasso Regression: Regularization Path



$\tilde{\beta}$ is unregularized solution; $\hat{\beta}$ is the lasso solution.

Plot from Hastie, Tibshirani, and Wainwright's Statistical Learning with Sparsity, Figure 2.1

Ridge vs. Lasso: Regularization Paths



Plot from Hastie, Tibshirani, and Wainwright's Statistical Learning with Sparsity, Figure 2.1

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

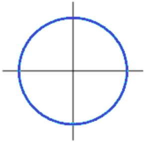
Ivanov and Tikhonov Equivalent?

- For ridge regression and lasso regression (and much more)
  - the Ivanov and Tikhonov formulations are equivalent
  - [Homework assignment 3 or 4.]
- We will use whichever form is most convenient.

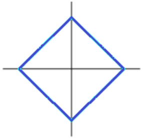
The ℓ_1 and ℓ_2 Norm Constraints

- 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 $\left\{(w_1, w_2) \in \mathbf{R}^2\right\}$.

- ℓ_2 contour: $w_1^2 + w_2^2 = r$



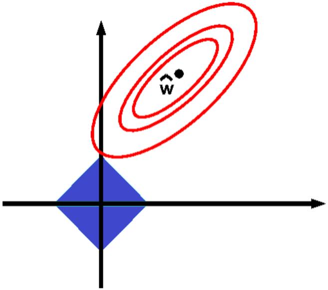
- ℓ_1 contour: $|w_1| + |w_2| = r$



Where are the "sparse" solutions?

The Famous Picture for ℓ_1 Regularization

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



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

KPM Fig. 13.3

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 $\hat{w} = \left(X^T X\right)^{-1} X^T y$, 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 $w \in \mathbf{R}^d$:

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

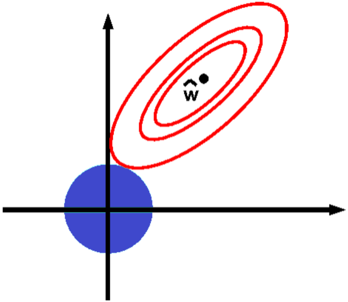
- Set of w with $\hat{R}_n(w)$ exceeding $\hat{R}_n(\hat{w})$ by $c > 0$ is

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

  which is an **ellipsoid centered at $\hat{w}$.**
- We'll derive this in homework #2.

The Famous Picture for ℓ_2 Regularization

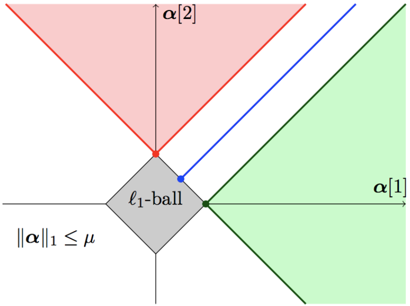
- $f_r^* = \arg\min_{w \in \mathbf{R}^2} \sum_{i=1}^n \left(w^T x_i - y_i\right)^2$ subject to $w_1^2 + w_2^2 \leqslant r$



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

KPM Fig. 13.3

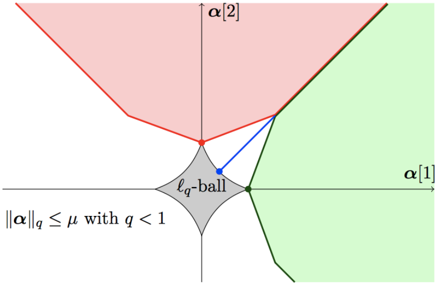
Why are Lasso Solutions Often Sparse?



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

Fig from Mairal et al.'s Sparse Modeling for Image and Vision Processing Fig 1.6

ℓ_q Even Sparser



(b) ℓ_q-ball with $q < 1$.

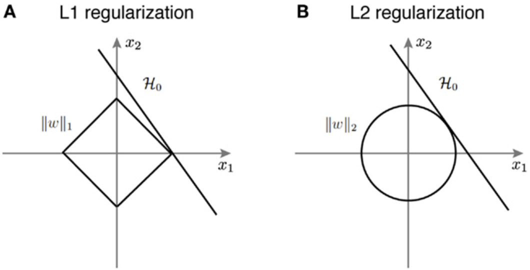
- Suppose design matrix X is orthogonal, so $X^T X = I$, and contours are circles.
- Then OLS solution in green or red regions implies ℓ_q constrained solution will be at corner

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

Fig from Mairal et al.'s Sparse Modeling for Image and Vision Processing Fig 1.9

The Quora Picture

- From Quora: "Why is L1 regularization supposed to lead to sparsity than L2? [sic]"



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

Finding the Lasso Solution

How to find the Lasso solution?

- How to solve the Lasso?

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

- $\|w\|_1$ is not differentiable!

Splitting a Number into Positive and Negative Parts

- Consider any number $a \in \mathbf{R}$.
- Let the **positive part** of a be
$$a^{+} = a1(a \geqslant 0).$$
- Let the **negative part** of a be
$$a^{-} = -a1(a \leqslant 0).$$
- Do you see why $a^{+} \geqslant 0$ and $a^{-} \geqslant 0$?
- 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
$$\min_{w \in \mathbf{R}^d} \sum_{i=1}^{n} \left(w^T x_i - y_i\right)^2 + \lambda \|w\|_1$$
- Replace each w_i by $w_i^+ - w_i^-$.
- Write $w^+ = \left(w_1^+, \ldots, w_d^+\right)$ and $w^- = \left(w_1^-, \ldots, w_d^-\right)$.

The Lasso as a Quadratic Program

- Substituting $w = w^+ - w^-$ and $|w| = w^+ + w^-$, Lasso problem is:

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

$$\text{subject to } w_i^+ \geqslant 0 \text{ for all } i$$

$$w_i^- \geqslant 0 \text{ for all } i,$$

  where 1 represents a column vector of 1's in $\mathbf{R}^d$.

- 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.

Projected SGD

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

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

Coordinate Descent Method

- **Goal:** Minimize $L(w) = L(w_1, \ldots, w_d)$ over $w = (w_1, \ldots, w_d) \in \mathbf{R}^d$.
- 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

$$w_i^{\text{new}} = \operatorname*{arg\,min}_{w_i} L(w_1, \ldots, w_{i-1}, \mathbf{w_i}, w_{i+1}, \ldots, w_d)$$

- 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 $w = (w_1, \dots, w_d) \in \mathbf{R}^d$.

- **Initialize** $w^{(0)} = 0$
- **while** not converged:
  - Choose a coordinate $j \in \{1, \dots, d\}$
  - $w_j^{\text{new}} \leftarrow \arg\min_{w_j} L(w_1^{(t)}, \dots, w_{j-1}^{(t)}, \mathbf{w_j}, w_{j+1}^{(t)}, \dots, w_d^{(t)})$
  - $w_j^{(t+1)} \leftarrow w_j^{\text{new}}$ and $w^{(t+1)} \leftarrow w^{(t)}$
  - $t \leftarrow t + 1$

- 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

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

Then

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

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

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

Coordinate Descent: When does it work?

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

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

  is not differentiable...
- Luckily there are weaker conditions...

Coordinate Descent: The Separability Condition

Theorem

[a] *If the objective f has the following structure*

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

where

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

then the coordinate descent algorithm converges to the global minimum.

[a] Tseng 1988: "Coordinate ascent for maximizing nondifferentiable concave functions", Technical Report LIDS-P

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

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

Stochastic Coordinate Descent for Lasso - Variation

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

- **Initialize** $\tilde{w}^{(0)} = 0$
  - **while** not converged:
    - Randomly choose a coordinate $j \in \{1, \ldots, 2d\}$
    - $\tilde{w}_j \leftarrow \tilde{w}_j + \max\left\{-\tilde{w}_j, -\nabla_j L(\tilde{w})\right\}$