$\ell_1$ and $\ell_2$ 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

- \( \mathcal{F} = \{ \text{all polynomial functions} \} \)
- \( \mathcal{F}_d = \{ \text{all polynomials of degree } \leq d \} \)
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. $x \mapsto w_1 x_1 + \cdots + w_d x_d$?
  - $\ell_0$ complexity: number of non-zero coefficients
  - $\ell_1$ “lasso” complexity: $\sum_{i=1}^{d} |w_i|$, for coefficients $w_1, \ldots, w_d$
  - $\ell_2$ “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 $r$:
  \[ \mathcal{F}_r = \{ f \in \mathcal{F} \mid \Omega(f) \leq r \} \]
- 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 $r \geq 0$,

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

s.t. $\Omega(f) \leq r$

- 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 $\Omega : \mathcal{F} \rightarrow [0, \infty)$ and fixed $\lambda \geq 0$,

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

- Choose $\lambda$ using validation data or cross-validation.
- (Ridge regression in homework is of this form.)
Let $L : \mathcal{F} \to \mathbb{R}$ be any performance measure of $f$
- e.g. $L(f)$ could be the empirical risk of $f$

For many $L$ and $\Omega$, Ivanov and Tikhonov are “equivalent”.

What does this mean?
- Any solution $f^\ast$ you could get from Ivanov, can also get from Tikhonov.
- Any solution $f^\ast$ 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:

1. For any choice of \( r > 0 \), any Ivanov solution

\[
 f_r^* \in \arg \min_{f \in \mathcal{F}} L(f) \text{ s.t. } \Omega(f) \leq r
\]

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

\[
 f_r^* \in \arg \min_{f \in \mathcal{F}} L(f) + \lambda \Omega(f).
\]

2. Conversely, for any choice of \( \lambda > 0 \), any Tikhonov solution:

\[
 f_\lambda^* \in \arg \min_{f \in \mathcal{F}} L(f) + \lambda \Omega(f)
\]

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

\[
 f_\lambda^* \in \arg \min_{f \in \mathcal{F}} L(f) \text{ s.t. } \Omega(f) \leq r
\]
\( l_1 \) and \( l_2 \) Regularization
Linear Least Squares Regression

- Consider linear models
  \[ \mathcal{F} = \{ f : \mathbb{R}^d \to \mathbb{R} \mid f(x) = w^T x \text{ for } w \in \mathbb{R}^d \} \]

- 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 \( \ell \) over \( \mathcal{F} \):
  \[
  \hat{w} = \arg \min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left( w^T x_i - y_i \right)^2
  \]

- 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 (Tikhonov Form)

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

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

where $\| w \|^2_2 = w_1^2 + \cdots + w_d^2$ is the square of the $\ell_2$-norm.

Ridge Regression (Ivanov Form)

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

$$
\hat{w} = \arg\min_{\| w \|^2_2 \leq r^2} \frac{1}{n} \sum_{i=1}^{n} \left( w^T x_i - y_i \right)^2.
$$
How does $\ell_2$ regularization induce “regularity”? 

- For $\hat{f}(x) = \hat{w}^T x$,
  - $\hat{f}$ is **Lipschitz continuous** with Lipschitz constant $\|\hat{w}\|_2$.
  - That is, when moving from $x$ to $x + h$, $\hat{f}$ changes no more than $\|\hat{w}\|_2\|h\|$.
- So $\ell_2$ regularization controls the maximum rate of change of $\hat{f}$.

**Proof:**

$$\left| \hat{f}(x + h) - \hat{f}(x) \right| = |\hat{w}^T (x + h) - \hat{w}^T x| = |\hat{w}^T h| \leq \|\hat{w}\|_2\|h\|_2 \text{(Cauchy-Schwarz inequality)}$$
Ridge Regression: Regularization Path

\[ \hat{w}_r = \arg \min_{\|w\|_2^2 \leq r^2} \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2 \]

\[ \hat{w} = \hat{w}_\infty = \text{Unconstrained ERM} \]

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

Modified from Hastie, Tibshirani, and Wainwright's *Statistical Learning with Sparsity*, Fig 2.1. About predicting crime in 50 US cities.
Lasso Regression: Workhorse (2) of Modern Data Science

Lasso Regression (Tikhonov Form)

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

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

where $\| w \|_1 = |w_1| + \cdots + |w_d|$ is the $\ell_1$-norm.

Lasso Regression (Ivanov Form)

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

$$\hat{w} = \arg\min_{\| w \|_1 \leq r} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2.$$
Lasso Regression: Regularization Path

\[ \hat{w}_r = \arg \min_{\|w\|_1 \leq r} \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2 \]

\[ \hat{w} = \hat{w}_\infty = \text{Unconstrained ERM} \]

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

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Modified from Hastie, Tibshirani, and Wainwright’s *Statistical Learning with Sparsity*, Fig 2.1. About predicting crime in 50 US cities.
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.

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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
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.
Why does Lasso regression give sparse solutions?
Illustrate affine prediction functions in parameter space.
The $\ell_1$ and $\ell_2$ Norm Constraints

- For visualization, restrict to 2-dimensional input space
- $\mathcal{F} = \{ f(x) = w_1 x_1 + w_2 x_2 \}$ (linear hypothesis space)
- Represent $\mathcal{F}$ by $\{(w_1, w_2) \in \mathbb{R}^2 \}$.

- $\ell_2$ contour: $w_1^2 + w_2^2 = r$
- $\ell_1$ contour: $|w_1| + |w_2| = r$

Where are the “sparse” solutions?
The Famous Picture for $\ell_1$ Regularization

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

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

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 $\hat{w} = (X^T X)^{-1} X^T y$, the OLS solution.

- What does $\hat{R}_n$ look like around $\hat{w}$?
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

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

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

We'll derive this in homework.
The Famous Picture for $\ell_2$ Regularization

- $f^*_r = \arg \min_{w \in \mathbb{R}^2} \sum_{i=1}^{n} (w^T x_i - y_i)^2$ subject to $w_1^2 + w_2^2 \leq r$

Blue region: Area satisfying complexity constraint: $w_1^2 + w_2^2 \leq r$

Red lines: contours of $\hat{R}_n(w) = \sum_{i=1}^{n} (w^T x_i - y_i)^2$.

KPM Fig. 13.3

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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 $\ell_1$ constrained solution will be at corner

Fig from Mairal et al.’s Sparse Modeling for Image and Vision Processing Fig 1.6
The \((\ell_q)^q\) Constraint

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

- Suppose design matrix \( X \) is orthogonal, so \( X^T X = I \), and contours are circles.
- Then OLS solution in green or red regions implies \( \ell_q \) constrained solution will be at corner \( \ell_q \)-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]” (google it)

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

Figure from https://www.quora.com/Why-is-L1-regularization-supposed-to-lead-to-sparsity-than-L2.
Finding the Lasso Solution
How to find the Lasso solution?

- How to solve the Lasso?

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

- $\|w\|_1 = |w_1| + |w_2|$ is not differentiable!
Consider any number $a \in \mathbb{R}$.

Let the **positive part** of $a$ be

$$a^+ = a 1(a \geq 0).$$

Let the **negative part** of $a$ be

$$a^- = -a 1(a \leq 0).$$

Do you see why $a^+ \geq 0$ and $a^- \geq 0$?

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

\[ \min_{\mathbf{w} \in \mathbb{R}^d} \sum_{i=1}^{n} \left( \mathbf{w}^T \mathbf{x}_i - y_i \right)^2 + \lambda \| \mathbf{w} \|_1 \]

- Replace each \( w_i \) by \( w_i^+ - w_i^- \).
- Write \( w^+ = (w_1^+, \ldots, w_d^+) \) and \( w^- = (w_1^-, \ldots, w_d^-) \).
The Lasso as a Quadratic Program

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

\[
\min_{w^+, w^-} \sum_{i=1}^{n} \left( (w^+ - w^-)^T x_i - y_i \right)^2 + \lambda 1^T (w^+ + w^-)
\]

subject to \( w_i^+ \geq 0 \) for all \( i \), \( w_i^- \geq 0 \) 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:

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

subject to \( w_i^+ \geq 0 \) for all \( i \) \( w_i^- \geq 0 \) for all \( i \),

- When we plug this optimization problem into a QP solver,
  - it just sees \( 2d \) variables and \( 2d \) constraints.
  - Doesn’t see that 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 be eliminate confusion, let’s start by calling them \( a_i \) and \( b_i \) and prove our claim...
The Lasso as a Quadratic Program

Lasso problem is trivially equivalent to the following:

$$\min_w \min_{a,b} \sum_{i=1}^n \left( (a-b)^T x_i - y_i \right)^2 + \lambda 1^T (a+b)$$

subject to

- $a_i \geq 0$ for all $i$
- $b_i \geq 0$ 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 $a + b = |w|$.
The Lasso as a Quadratic Program

\[
\begin{align*}
\min_w \min_{a,b} & \sum_{i=1}^n \left( (a-b)^T x_i - y_i \right)^2 + \lambda 1^T (a+b) \\
\text{subject to} & \quad a_i \geq 0 \text{ for all } i, \quad b_i \geq 0 \text{ for all } i, \\
& \quad a - b = w
\end{align*}
\]

- Claim: Don’t need constraint \( a - b = w \).
- For any \( a, b \geq 0 \), there’s some \( w = a - b \).
- So our constraint set has all \( a, b \geq 0 \).
So lasso optimization problem is equivalent to

$$
\min_{a,b} \sum_{i=1}^{n} \left( (a - b)^T x_i - y_i \right)^2 + \lambda 1^T (a + b)
$$

subject to $a_i \geq 0$ for all $i$, $b_i \geq 0$ 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.)
Projected SGD

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

subject to \( w_i^+ \geq 0 \) for all \( i \)
\( w_i^- \geq 0 \) for all \( i \)

- 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.
Coordinate Descent Method

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

  $$w_i^{\text{new}} = \arg \min_{w_i} L(w_1, \ldots, w_i-1, w_i, w_i+1, \ldots, w_d)$$

  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

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

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

\[ \hat{w}_j = \arg \min_{w_j \in \mathbb{R}} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda |w|_1 \]

Then

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

\[ a_j = 2 \sum_{i=1}^{n} x_{i,j}^2 \]

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

where \( w_{-j} \) is \( w \) without component \( j \) and similarly for \( x_{i,-j} \).
Coordinate Descent: When does it work?

- Suppose we’re minimizing $f : \mathbb{R}^d \to \mathbb{R}$.
- Sufficient conditions:
  1. $f$ 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...
Theorem

If the objective $f$ has the following structure

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

where

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

then the coordinate descent algorithm converges to the global minimum.

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 $\ell_1$ regularization!
  - Shalev-Shwartz & Tewari’s “Stochastic Methods...” (2011)
Stochastic Coordinate Descent for Lasso – Variation

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

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

Stochastic Coordinate Descent for Lasso - Variation

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

- Initialize \( \tilde{w}^{(0)} = 0 \)

- while not converged:
  - Randomly choose a coordinate \( j \in \{1, \ldots, 2d\} \)
  - \( \tilde{w}_j \leftarrow \tilde{w}_j + \max \{ -\tilde{w}_j, -\nabla_j L(\tilde{w}) \} \)