COMS 4721: Machine Learning for Data Science
Lecture 6, 2/2/2017

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UNDERDETERMINED LINEAR EQUATIONS

We now consider the regression problem $y = Xw$ where $X \in \mathbb{R}^{n\times d}$ is "fat" (i.e., $d \gg n$). This is called an "underdetermined" problem.

- There are more dimensions than observations.
- w now has an infinite number of solutions satisfying $y = Xw$.

$$\begin{bmatrix} \; y \; \end{bmatrix} = \begin{bmatrix} \qquad\qquad & X & \qquad\qquad \end{bmatrix} \begin{bmatrix} \\ w \\ \\ \end{bmatrix}$$

These sorts of high-dimensional problems often come up:

- In gene analysis there are 1000's of genes but only 100's of subjects.
- Images can have millions of pixels.
- Even polynomial regression can quickly lead to this scenario.

Minimum ℓ_2 regression

One solution (least norm)

One possible solution to the underdetermined problem is

$$w_{\text{ln}} = X^T(XX^T)^{-1}y \quad \Rightarrow \quad Xw_{\text{ln}} = XX^T(XX^T)^{-1}y = y.$$

We can construct another solution by adding to w_{ln} a vector $\delta \in \mathbb{R}^d$ that is in the *null space* $\mathcal{N}$ of X:

$$\delta \in \mathcal{N}(X) \quad \Rightarrow \quad X\delta = 0 \ \text{ and } \ \delta \neq 0$$

and so $X(w_{\text{ln}} + \delta) = Xw_{\text{ln}} + X\delta = y + 0$.

In fact, there are an infinite number of possible δ, because $d > n$.

We can show that w_{ln} is the solution with smallest ℓ_2 norm. We will use the proof of this fact as an excuse to introduce two general concepts.

TOOLS: ANALYSIS

We can use *analysis* to prove that w_{ln} satisfies the optimization problem

$$w_{\text{ln}} = \arg\min_w \ \|w\|^2 \quad \text{subject to} \quad Xw = y.$$

(Think of mathematical analysis as the use of inequalities to prove things.)

Proof: Let w be another solution to $Xw = y$, and so $X(w - w_{\text{ln}}) = 0$. Also,

$$\begin{aligned}(w - w_{\text{ln}})^T w_{\text{ln}} &= (w - w_{\text{ln}})^T X^T (XX^T)^{-1} y \\ &= (\underbrace{X(w - w_{\text{ln}})}_{=0})^T (XX^T)^{-1} y \ = \ 0\end{aligned}$$

As a result, $w - w_{\text{ln}}$ is *orthogonal* to w_{ln}. It follows that

$$\|w\|^2 = \|w - w_{\text{ln}} + w_{\text{ln}}\|^2 = \|w - w_{\text{ln}}\|^2 + \|w_{\text{ln}}\|^2 + 2\,\underbrace{(w - w_{\text{ln}})^T w_{\text{ln}}}_{=0} > \|w_{\text{ln}}\|^2$$

TOOLS: LAGRANGE MULTIPLIERS

Instead of starting from the solution, start from the problem,

$$w_{\text{ln}} = \arg\min_{w}\; w^T w \quad \text{subject to} \quad Xw = y.$$

- Introduce Lagrange multipliers: $\mathcal{L}(w, \eta) = w^T w + \eta^T(Xw - y)$.
- Minimize $\mathcal{L}$ over w maximize over η. If $Xw \neq y$, we can get $\mathcal{L} = +\infty$.
- The optimal conditions are

$$\nabla_w \mathcal{L} = 2w + X^T \eta = 0, \qquad \nabla_\eta \mathcal{L} = Xw - y = 0.$$

We have everything necessary to find the solution:

1. From first condition: $w = -X^T \eta / 2$
2. Plug into second condition: $\eta = -2(XX^T)^{-1} y$
3. Plug this back into #1: $w_{\text{ln}} = X^T(XX^T)^{-1} y$

SPARSE ℓ_1 REGRESSION

LS and RR in high dimensions

Usually not suited for high-dimensional data

- Modern problems: Many dimensions/features/predictors
- Only a few of these may be important or relevant for predicting y
- Therefore, we need some form of "feature selection"

- Least squares and ridge regression:
  - Treat all dimensions equally without favoring subsets of dimensions
  - The relevant dimensions are averaged with irrelevant ones
  - Problems: Poor generalization to new data, interpretability of results

Regression with Penalties

Penalty terms

Recall: General ridge regression is of the form

$$\mathcal{L} = \sum_{i=1}^{n} (y_i - f(x_i; w))^2 + \lambda \|w\|^2$$

We've referred to the term $\|w\|^2$ as a *penalty term* and used $f(x_i; w) = x_i^T w$.

Penalized fitting

The general structure of the optimization problem is

$$\text{total cost} \;=\; \text{goodness-of-fit term} \;+\; \text{penalty term}$$

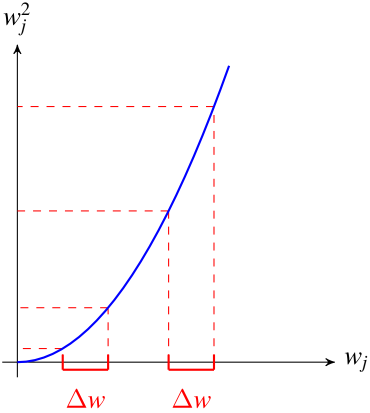
- Goodness-of-fit measures how well our model f approximates the data.
- Penalty term makes the solutions we don't want more "expensive".

What kind of solutions does the choice $\|w\|^2$ favor or discourage?

Quadratic Penalties

Intuitions

- Quadratic penalty: Reduction in cost depends on $|w_j|$.
- Suppose we reduce w_j by Δw. The effect on $\mathcal{L}$ depends on the starting point of w_j.
- Consequence: We should favor vectors w whose entries are of similar size, preferably small.



Sparsity

Setting

- Regression problem with n data points $x \in \mathbb{R}^d$, $d \gg n$.
- Goal: Select a small subset of the d dimensions and switch off the rest.
- This is sometimes referred to as "feature selection".

What does it mean to "switch off" a dimension?

- Each entry of w corresponds to a dimension of the data x.
- If $w_k = 0$, the prediction is

$$f(x, w) = x^T w = w_1 x_1 + \cdots + 0 \cdot x_k + \cdots + w_d x_d,$$

  so the prediction does not depend on the kth dimension.
- Feature selection: Find a w that (1) predicts well, and (2) has only a small number of non-zero entries.
- A w for which most dimensions $= 0$ is called a *sparse* solution.

Penalty goal

Find a penalty term which encourages sparse solutions.

Quadratic penalty vs sparsity

- Suppose w_k is large, all other w_j are very small but non-zero
- Sparsity: Penalty should keep w_k, and push other w_j to zero
- Quadratic penalty: Will favor entries w_j which all have similar size, and so it will push w_k towards small value.

Overall, a quadratic penalty favors many small, but non-zero values.

Solution

Sparsity can be achieved using *linear* penalty terms.

Sparse regression

LASSO: Least Absolute Shrinkage and Selection Operator

With the LASSO, we replace the ℓ_2 penalty with an ℓ_1 penalty:

$$w_{\text{lasso}} = \arg\min_{w} \|y - Xw\|_2^2 + \lambda \|w\|_1$$

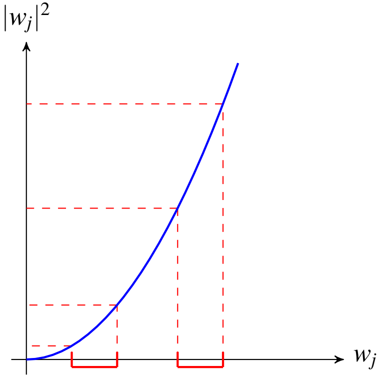
where

$$\|w\|_1 = \sum_{j=1}^{d} |w_j|.$$

This is also called ℓ_1-regularized regression.

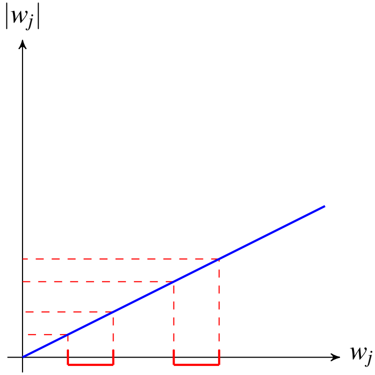
QUADRATIC PENALTIES

Quadratic penalty



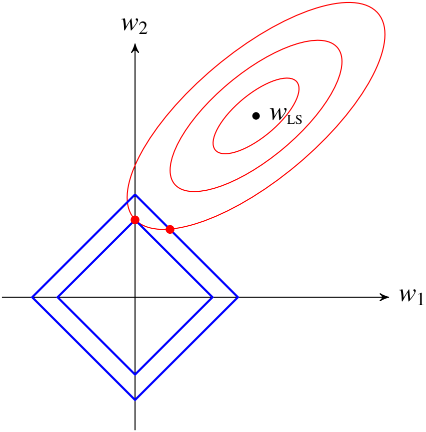
Reducing a large value w_j achieves a larger cost reduction.

Linear penalty



Cost reduction does not depend on the magnitude of w_j.

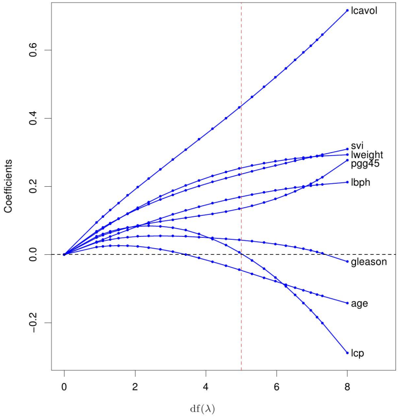
Ridge Regression vs LASSO



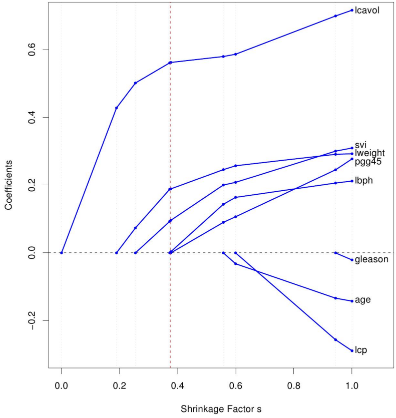
This figure applies to $d < n$, but gives intuition for $d \gg n$.

- Red: Contours of $(w - w_{\text{LS}})^T (X^T X)(w - w_{\text{LS}})$ (see Lecture 3)
- Blue: (left) Contours of $\|w\|_1$, and (right) contours of $\|w\|_2^2$

COEFFICIENT PROFILES: RR VS LASSO



(a) $||w||_2$ penalty



(b) $||w||_1$ penalty

ℓ_p Regression

ℓ_p-norms

These norm-penalties can be extended to all norms:

$$\|w\|_p = \Big(\sum_{j=1}^{d} |w_j|^p\Big)^{\frac{1}{p}} \qquad \text{for } 0 < p \leq \infty$$

ℓ_p-regression

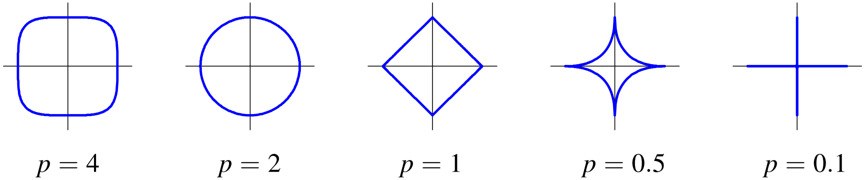
The ℓ_p-regularized linear regression problem is

$$w_{\ell_p} := \arg\min_{w} \|y - Xw\|_2^2 + \lambda \|w\|_p^p$$

We have seen:

- ℓ_1-regression = LASSO
- ℓ_2-regression = ridge regression

ℓ_p Penalization Terms



p	Behavior of $\| . \|_p$
$p = \infty$	Norm measures largest absolute entry, $\|w\|_\infty = \max_j |w_j|$
$p > 2$	Norm focuses on large entries
$p = 2$	Large entries are expensive; encourages similar-size entries
$p = 1$	Encourages sparsity
$p < 1$	Encourages sparsity as for $p = 1$, but contour set is not convex (i.e., no “line of sight” between every two points inside the shape)
$p \to 0$	Simply records whether an entry is non-zero, i.e. $\|w\|_0 = \sum_j \mathbb{I}\{w_j \neq 0\}$

COMPUTING THE SOLUTION FOR ℓ_p

Solution of ℓ_p problem

ℓ_2 aka ridge regression. Has a closed form solution

ℓ_p **($p \geq 1, p \neq 2$)** — By "convex optimization". We won't discuss convex analysis in detail in this class, but two facts are important

- There are no "local optimal solutions" (i.e., local minimum of $\mathcal{L}$)
- The true solution can be found *exactly* using iterative algorithms

($p < 1$) — We can only find an approximate solution (i.e., the best in its "neighborhood") using iterative algorithms.

Three techniques formulated as optimization problems

Method	Good-o-fit	penalty	Solution method
Least squares	$\|\|y - Xw\|\|_2^2$	none	Analytic solution exists if $X^T X$ invertible
Ridge regression	$\|\|y - Xw\|\|_2^2$	$\|\|w\|\|_2^2$	Analytic solution exists always
LASSO	$\|\|y - Xw\|\|_2^2$	$\|\|w\|\|_1$	Numerical optimization to find solution