Discussion on Regularization

He He

Slides based on Lecture 3a from David Rosenberg's course material.

CDS, NYU

Feb 16, 2021

Logistics

- Thanks for the course feedback!
- Piazza posting instructions
  - Search for similar questions
  - Describe your progress and clarify confusion points
- Feel free to turn on video (when talking)
- Tutorial for convex optimization (preparation for SVM) on **Thursday 9:30am–10:30am** during Marylou's OH
  - Convex functions
  - Primal/Dual problem, strong/weak duality
  - Complementary slackness, KKT conditions

Model Selection

- Goal: Select the "best" subset of features according to some **score** $\begin{cases} \text{valid loss} \\ \text{valid loss} + \lambda|S| \end{cases}$
    - Can also be formulated as ℓ_0 regularization
    - ℓ_0 "norm": number of non-zero elements
    - **Forward/Backward selection** is a greedy method often used in practice
- Pitfalls in feature selection
    - Is it possible to include irrelevant features (false positives)?
    - What happens when we have dependence among features (e.g. colinearity)?

Model Selection

- Feature selection is a special case of **model selection**:
  - Degree of the polynomial function
  - Decision tree vs kNN
  - More broadly, hyperparameters of learning algorithms
- We need to assess the performance of the model in order to select the "best" one
  - Can we use the training error?
  - What is the ideal performance measure?

Test error

- **Test error** (or **generalization error**) of a predictor $\hat{f}$:

$$\mathbb{E}_{P_{\mathcal{X}\times\mathcal{Y}}}\left[\ell(\hat{f}(x), y)\right]. \quad R(\hat{f})$$

- Note that this is just the risk of $\hat{f}$.
- What we really care about is the test error, not the error on the test set!
- But we can use the test set error to estimate the test error.
- Important: the test set cannot influence training in *any* way.
    - Is it okay to look at the test set as long as the label is hidden?
- For model selection, our goal is to estimate the test error of each model

Estimate Test Error for Model Selection

In order to do model selection,

- We need to estimate test error, but we cannot use the true test set.
- Best approach is to use a **validation set** (if we have enough data).

Other methods to estimate test error:

- Re-use training samples: create multiple train/test sets
  - Cross validation, bootstrap
- Training error + penalty
  - AIC, BIC, MDL

Bias-Variance Decomposition

- Note that the test error is a random variable. Why?

$\hat{f}(x) = \hat{w}^T x + b$

- Assume the true model is $y = f(x) + \epsilon$ and $\mathbb{E}\epsilon = 0$ and $\text{Var}(\epsilon) = \sigma^2$

- Consider the expected square loss over *training sets*:

fixed RV RV

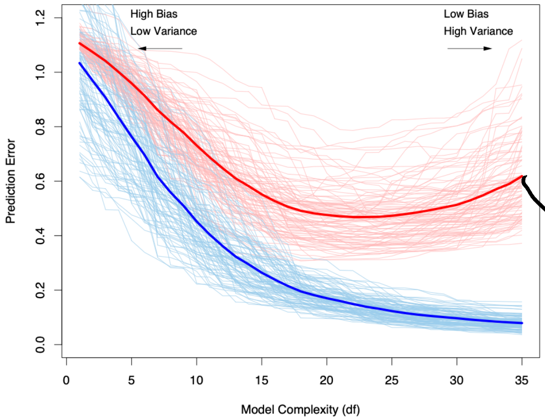
$$\text{err}(x) = \mathbb{E}\left[\left(y - \hat{f}(x)\right)^2\right] \quad \text{test example} \tag{1}$$

$$= \underbrace{\sigma^2}_{\text{irreducible error}} + \underbrace{\mathbb{E}\left[\hat{f}(x) - \mathbb{E}\hat{f}(x)\right]^2}_{\text{variance of } \hat{f}} + \underbrace{\left[f(x) - \mathbb{E}\hat{f}(x)\right]^2}_{(\text{bias of } \hat{f})^2} \tag{2}$$

- Both excess risk decomposition and bias-variance decomposition analyze different sources of the test error and they lead to similar conclusions.

- What's the relation between complexity and bias/variance?

Training set error (blue) and test set error (red)



double descent

Regularization and Dependent Features

ℓ_p Regularization

ℓ_0 regularization (subset selection)

$$f(w) = \|Xw - y\|^2 + \lambda \|w\|_0$$

ℓ_1 regularization (Lasso)

$$f(w) = \|Xw - y\|^2 + \lambda \|w\|_1$$

ℓ_2 regularization (Ridge)

$$f(w) = \|Xw - y\|^2 + \lambda \|w\|^2$$

- Which one(s) can be used for feature selection?
- Which one(s) is fast to solve?
- Which one(s) gives unique solution?

Repeated features

- Suppose we have one feature $x_1 \in \mathrm{R}$ and response variable $y \in \mathrm{R}$.
- Got some data and ran least squares linear regression. The ERM is

$$\hat{f}(x_1) = 4x_1.$$

- What is the ERM solution if we get a new feature x_2, but we always have $x_2 = x_1$?

$$3x_1 + x_2$$
$$2x_1 + x_2$$

Duplicate Features: ℓ_1 and ℓ_2 norms

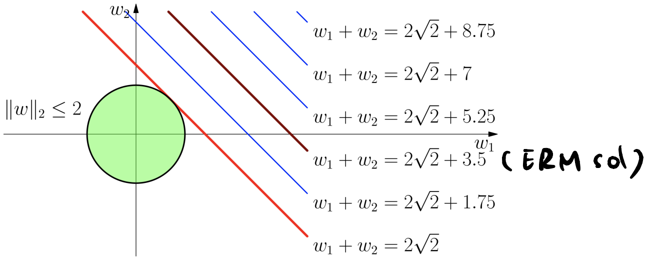
- $\hat{f}(x_1, x_2) = w_1 x_1 + w_2 x_2$ is an ERM iff $w_1 + w_2 = 4$.
- What if we introduce the ℓ_1 and ℓ_2 regularization:

$|w_1| + |w_2|$

w_1	w_2	$\|w\|_1$	$\|w\|_2^2$
4	0	4	16
2	2	4	8
1	3	4	10
-1	5	6	26

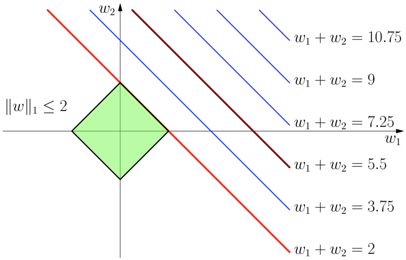
- $\|w\|_1$ doesn't discriminate, as long as all have same sign
- $\|w\|_2^2$ minimized when weight is spread equally
- Picture proof: What does the level sets of ERM look like?

Equal Features, ℓ_2 Constraint



- Suppose the line $w_1 + w_2 = 2\sqrt{2} + 3.5$ corresponds to the empirical risk minimizers.
- Empirical risk increase as we move away from these parameter settings
- Intersection of $w_1 + w_2 = 2\sqrt{2}$ and the norm ball $\|w\|_2 \leqslant 2$ is ridge solution.
- Note that $w_1 = w_2$ at the solution

Equal Features, ℓ_1 Constraint



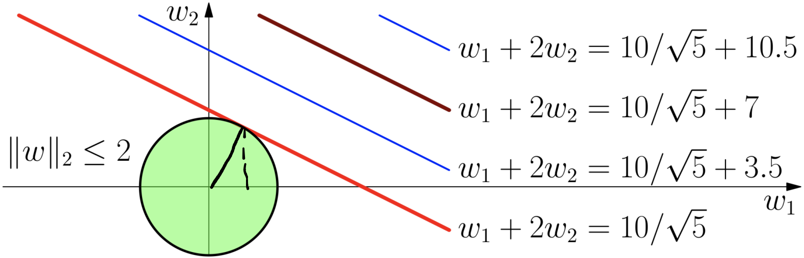
- Suppose the line $w_1 + w_2 = 5.5$ corresponds to the empirical risk minimizers.
- Intersection of $w_1 + w_2 = 2$ and the norm ball $\|w\|_1 \leqslant 2$ is lasso solution.
- Note that the solution set is $\{(w_1, w_2) : w_1 + w_2 = 2, w_1, w_2 \geqslant 0\}$.

Linearly Related Features

- Linear prediction functions: $f(x) = w_1x_1 + w_2x_2$ $= w_1 x_1 + w_2 \cdot 2x_1 = kx_1$

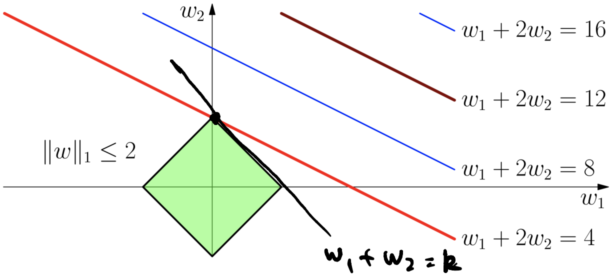
  $w_1 + 2w_2 = k$
- Same setup, now suppose $x_2 = 2x_1$.
- Then all functions with $w_1 + 2w_2 = k$ have the same empirical risk.
- What function will we select if we do ERM with ℓ_1 or ℓ_2 constraint?

Linearly Related Features, ℓ_2 Constraint



- $w_1 + 2w_2 = 10/\sqrt{5} + 7$ corresponds to the empirical risk minimizers.
- Intersection of $w_1 + 2w_2 = 10\sqrt{5}$ and the norm ball $\|w\|_2 \leqslant 2$ is ridge solution.
- At solution, $w_2 = 2w_1$.

Linearly Related Features, ℓ_1 Constraint



- Intersection of $w_1 + 2w_2 = 4$ and the norm ball $\|w\|_1 \leqslant 2$ is lasso solution.
- Solution is now a corner of the ℓ_1 ball, corresonding to a sparse solution.

Linearly Dependent Features: Take Away

- For identical features
  - ℓ_1 regularization spreads weight arbitrarily (all weights same sign)
  - ℓ_2 regularization spreads weight evenly
- Linearly related features
  - ℓ_1 regularization chooses variable with larger scale, 0 weight to others
  - ℓ_2 prefers variables with larger scale, spreads weight proportional to scale
- In practice, **feature standardization** is important.
- How to standardize the test set?

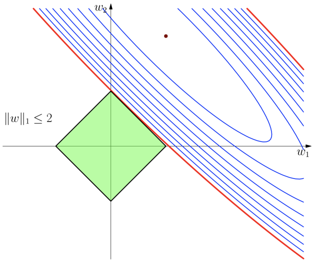
Correlated Features on Same Scale

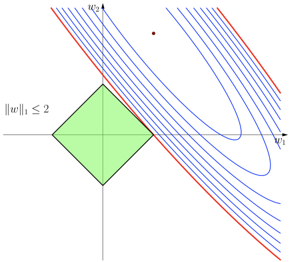
- Suppose x_1 and x_2 are highly correlated and the same scale.
- This is quite typical in real data, after normalizing data.

What do the level sets look like?

- Nothing degenerate here, so level sets are ellipsoids.
- But, the higher the correlation, the closer to degenerate we get.
- That is, ellipsoids keep stretching out, getting closer to two parallel lines.

Correlated Features, ℓ_1 Regularization





- Intersection could be anywhere on the top right edge.
- Minor perturbations (in data) can drastically change intersection point – very unstable solution.
- Makes division of weight among highly correlated features (of same scale) seem arbitrary.
  - If $x_1 \approx 2x_2$, ellipse changes orientation and we hit a corner. (Which one?)

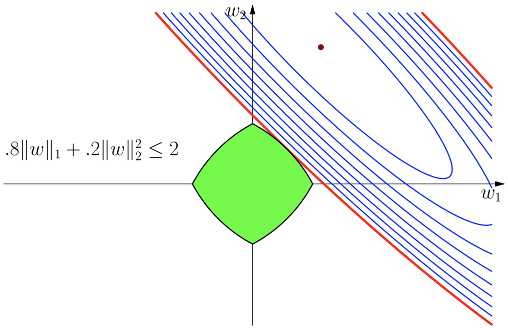
Elastic Net

The **elastic net** combines lasso and ridge penalties:

$$\hat{w} = \underset{w \in \mathbf{R}^d}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 + \lambda_1 \|w\|_1 + \lambda_2 \|w\|_2^2$$

What are the coefficients for correlated variables?

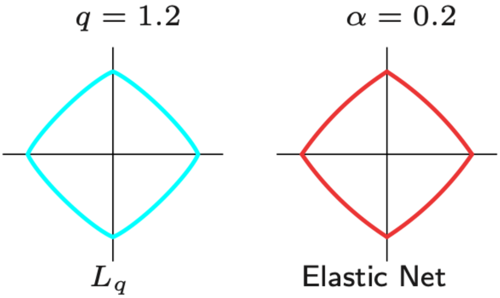
Highly Correlated Features, Elastic Net Constraint



- Elastic net solution is closer to $w_2 = w_1$ line, despite high correlation.
- Elastic net selects variables like Lasso
- And shrinks coefficients of correlated varialbes like Ridge

Elastic Net vs ℓ_q Constraints

What if we use ℓ_q penalty where $q \in (1, 2)$?



Sparsity

Why doesn't ℓ_2 give sparsity

Consider ℓ_2 regularized least squares:

$$L(w) = \frac{1}{2}\|Xw - y\|^2 + \underbrace{\frac{1}{2}\|w\|^2}_{w_j}. \tag{3}$$

Let w^* be the optimal solution. What's the condition for $w_j^* = 0$?

$$\left.\frac{\partial}{\partial w_j} L(w)\right|_{w_j=0} = x_j^T \underbrace{(Xw - y)} = 0$$

x_j: j-th col of X

$(Xw - y)$: If $w_j = 0$, residual w/o using the j-th feature.

Why does ℓ_1 give sparsity

Consider ℓ_1 regularized least squares:

$$L(w) = \frac{1}{2}\|Xw - y\|^2 + \lambda\|w\|_1. \tag{4}$$

Let w^* be the optimal solution. What's the condition for $w_j^* = 0$?

$\partial|w| = [-1, 1]$

$$\frac{\partial}{\partial w_j} L(w)\Big|_{w_j=0} = x_j^T(Xw - y) + \lambda[-1, 1] = 0$$

Do we always want sparsity or simpler models?

Do we always want sparsity or simpler models?

- Subjective desire for parsimony: Occam's razor
- Avoid overfit: approximatin/estimation error trade-off
- No free lunch theorem