

# Discussion on Regularization

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- 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

# Feature 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  $\ell_0$  regularization
  - $\ell_0$  “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** (or **generalization error**) of a predictor  $\hat{f}$ :

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

- 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*:

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

$\nearrow$  fixed     $\nearrow$  RV     $\nearrow$  RV

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

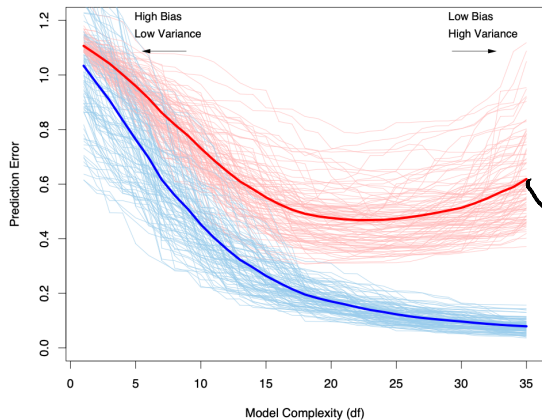
irreducible error  $\leftarrow \sigma^2$

- 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?



# Bias-Variance Trade-off

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



## Regularization and Dependent Features

# $\ell_p$ Regularization

$\ell_0$  regularization (subset selection)

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

$\ell_1$  regularization (Lasso)

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

$\ell_2$  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  $x_1 \in \mathbb{R}$  and response variable  $y \in \mathbb{R}$ .
- 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: $\ell_1$ and $\ell_2$ norms

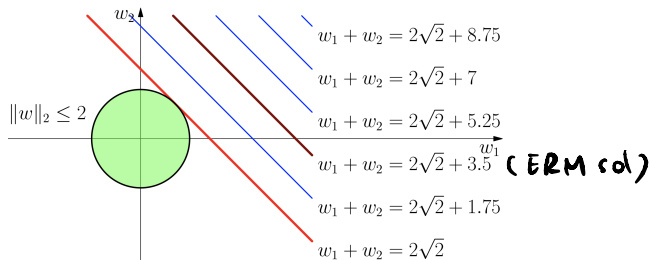
- $\hat{f}(x_1, x_2) = w_1 x_1 + w_2 x_2$  is an ERM iff  $w_1 + w_2 = 4$ .
- What if we introduce the  $\ell_1$  and  $\ell_2$  regularization:

$|w_1| + |w_2|$

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

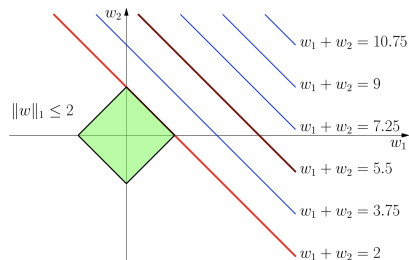
- $\|w\|_1$  doesn't discriminate, as long as all have same sign
- $\|w\|_2^2$  minimized when weight is spread equally
- Picture proof: What does the level sets of ERM look like?

## Equal Features, $\ell_2$ 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  $\|w\|_2 \leq 2$  is ridge solution.
- Note that  $w_1 = w_2$  at the solution

## Equal Features, $\ell_1$ Constraint



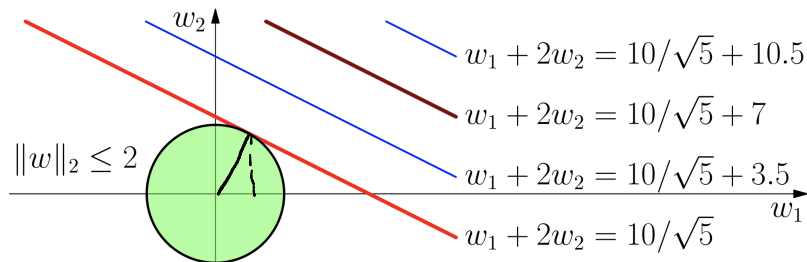
- Suppose the line  $w_1 + w_2 = 5.5$  corresponds to the empirical risk minimizers.
- Intersection of  $w_1 + w_2 = 2$  and the norm ball  $\|w\|_1 \leq 2$  is lasso solution.
- Note that the solution set is  $\{(w_1, w_2) : w_1 + w_2 = 2, w_1, w_2 \geq 0\}$ .

# Linearly Related Features

- Linear prediction functions:  $f(x) = w_1x_1 + w_2x_2 = w_1x_1 + w_2 \cdot 2x_1 = kx_1$ ,  
 $w_1 + 2w_2 = k$
- 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  $\ell_1$  or  $\ell_2$  constraint?

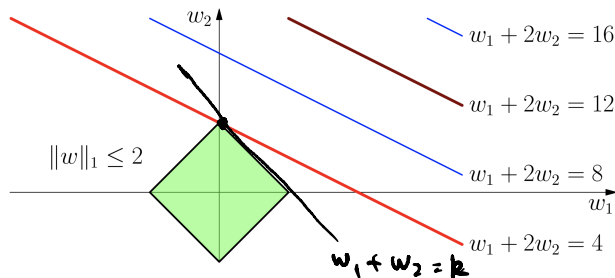


## Linearly Related Features, $\ell_2$ Constraint



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

## Linearly Related Features, $\ell_1$ Constraint



- Intersection of  $w_1 + 2w_2 = 4$  and the norm ball  $\|w\|_1 \leq 2$  is lasso solution.
- Solution is now a corner of the  $\ell_1$  ball, corresponding to a sparse solution.

## Linearly Dependent Features: Take Away

- For identical features
  - $\ell_1$  regularization spreads weight arbitrarily (all weights same sign)
  - $\ell_2$  regularization spreads weight evenly
- Linearly related features
  - $\ell_1$  regularization chooses variable with **larger scale**, 0 weight to others
  - $\ell_2$  prefers variables with larger scale, spreads weight **proportional to scale**
- In practice, **feature standardization** is important.
- How to standardize the test set?

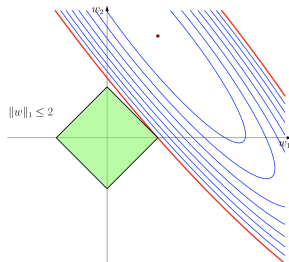
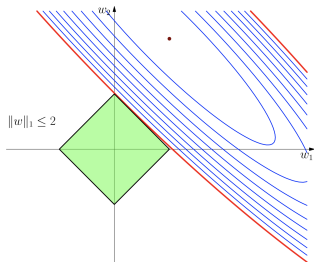
## Correlated Features on Same Scale

- 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, $\ell_1$ Regularization



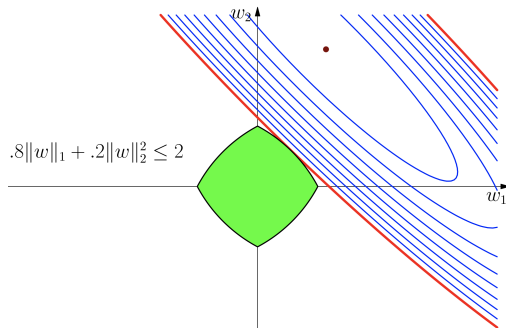
- Intersection could be anywhere on the top right edge.
- Minor perturbations (in data) can drastically change intersection point – very unstable solution.
- Makes division of weight among highly correlated features (of same scale) seem arbitrary.
  - If  $x_1 \approx 2x_2$ , ellipse changes orientation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

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

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

What are the coefficients for correlated variables?

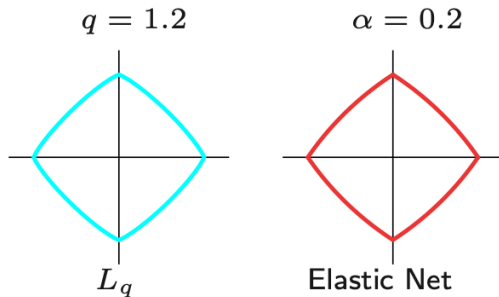
# Highly Correlated Features, Elastic Net Constraint



- 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 variables like Ridge

# Elastic Net vs $\ell_q$ Constraints

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





# Sparsity

## Why doesn't $\ell_2$ give sparsity

Consider  $\ell_2$  regularized least squares:

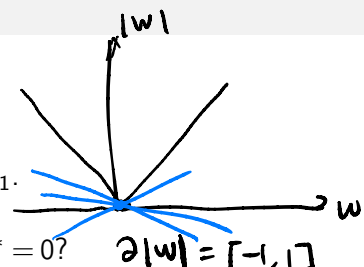
$$L(w) = \frac{1}{2} \|Xw - y\|^2 + \underbrace{\frac{1}{2} \|w\|^2}_{w_j} \quad (3)$$

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

$$\left. \frac{\partial}{\partial w_j} L(w) \right|_{w_j=0} = \underbrace{x_j^\top}_{j\text{-th col of } X} \underbrace{(Xw - y)}_{\text{if } w_j = 0, \text{ residual w/o using the } j\text{-th feature}} = 0$$

## Why does $\ell_1$ give sparsity

Consider  $\ell_1$  regularized least squares:

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


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

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

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: approximation/estimation error trade-off
- No free lunch theorem

