Discussion on Regularization

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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)
  - 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**
  - 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)?

1. Yes, especially if we use validation error as the score, because an irrelevant feature that has a tiny effect can improve validation error by chance. It's less likely to happen with ℓ_0 penalty, because each addition feature must improve the loss by at least λ.
2. It will take either or both. The selected features may not be causal. For example, a confounding variable makes irrelevant features look relevant. In general, the effectiveness of a feature must be interpreted in the context of other features.

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?

1. No, the training error always decreases if we increase the complexity of the hypothesis space.

Test error

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

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

- 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

1. No! Now that you've seen the test data, it will influence your model development, and we risk overfitting to the test set. You should only run on the test set at the end.

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 is a random variabl. Why?
- Assume the true model is $y = f(x) + \epsilon$ and $\mathbb{E}\epsilon = 0$ and $\mathrm{Var}(\epsilon) = \sigma^2$
- Consider the expected square loss over *training sets*:

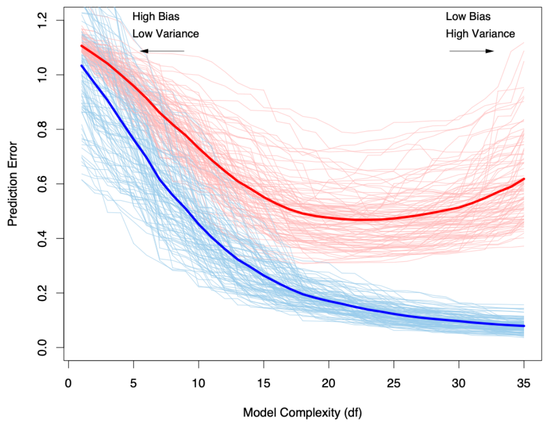
$$\mathrm{err}(x) = \mathbb{E}\left[\left(y - \hat{f}(x)\right)^2\right] \tag{1}$$

$$= \epsilon^2 + \mathbb{E}\left[\hat{f}(x) - \mathbb{E}\hat{f}(x)\right]^2 + \left[f(x) - \mathbb{E}\hat{f}(x)\right]^2 \tag{2}$$

- 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?

1. irreducible error + variance($\hat{f}(x)$) + (bias^2($\hat{f}(x)$))
2. Note that in this case, the irreducible error is the risk of the Bayes predictor.

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



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?

1. L1 and L0. L1 is not as sparse as L0 though.
2. L1 and L2. Descent-based methods.
3. L2. L0 and L1 don't have unique solution given dependent features.

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 $x_2 = x_1$?

1. $\hat{f}(x_1, x_2) = w_1 x_1 + w_2 x_2$ is an ERM iff $w_1 + w_2 = 4$

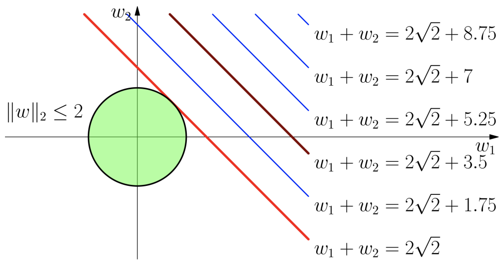
Duplicate Features: ℓ_1 and ℓ_2 norms

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

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

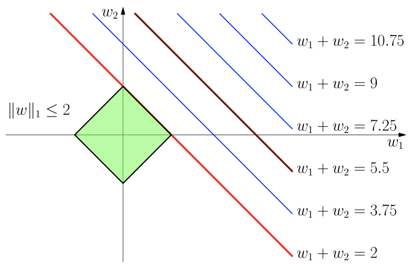
- $\|w\|_1$ doesn't discriminate, as long as all have same sign
- $\|w\|_2^2$ minimized when weight is spread equally
- Picture proof: What does the level sets of ERM look like?

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



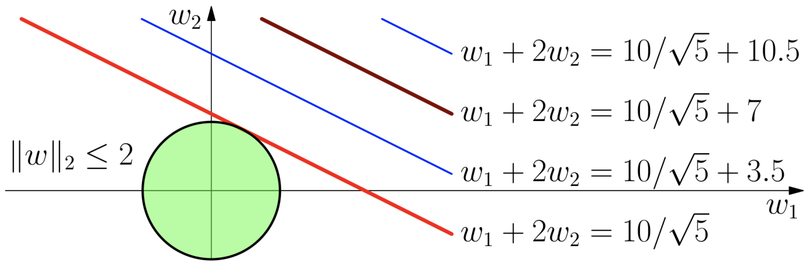
- Suppose the line $w_1 + w_2 = 5.5$ corresponds to the empirical risk minimizers.
- Intersection of $w_1 + w_2 = 2$ and the norm ball $\|w\|_1 \leqslant 2$ is lasso solution.
- Note that the solution set is $\{(w_1, w_2) : w_1 + w_2 = 2, w_1, w_2 \geqslant 0\}$.

Linearly Related Features

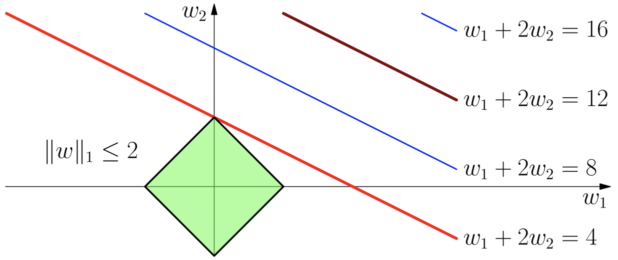
- Linear prediction functions: $f(x) = w_1x_2 + w_2x_2$
- Same setup, now suppose $x_2 = 2x_1$.
- Then all functions with $w_1 + 2w_2 = k$ have the same empirical risk.
- What function will we select if we do ERM with ℓ_1 or ℓ_2 constraint?

1. So $f(x) = w_1x_1 + w_2x_2 = w_1x_1 + 2w_2x_1 = (w_1 + 2w_2)x_1$. So all functions with $w_1 + 2w_2 = k$ are the same.

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, $w_2 = 2w_1$.



- 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?

1. Use the training set statistics.

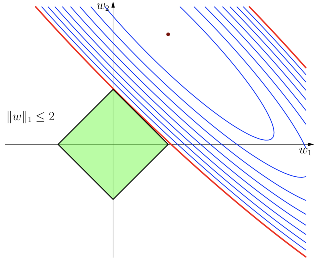
Correlated Features on Same Scale

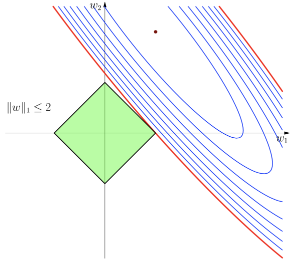
- Suppose x_1 and x_2 are highly correlated and the same scale.
- This is quite typical in real data, after normalizing data.

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

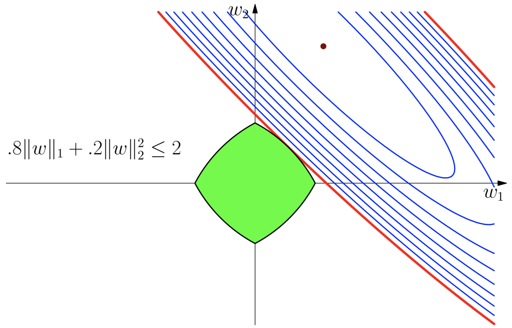
The **elastic net** combines lasso and ridge penalties:

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

What are the coefficients for correlated variables?

1. We expect correlated random variables to have similar coefficients.

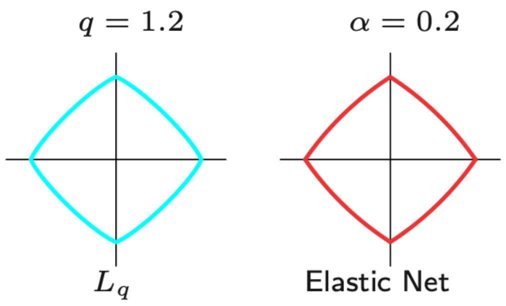
Highly Correlated Features, Elastic Net Constraint



- 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 $q \in (1,2)$?



1. Although they look very similar, ℓ_q does not have sharp/non-differentiable corners thus cannot push weights to exactly zero.

Sparsity

Why doesn't ℓ_2 give sparsity

Consider ℓ_2 regularized least squares:

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

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

1. We need

$$\left.\frac{\partial}{\partial w_j} L(w)\right|_{w_j=0} = x_{\cdot j}^T (Xw - y) = 0 \tag{4}$$

when w_{-j} takes the optimal value. This requires the j-th features, $x_{\cdot j}$, to be orthogonal to the residual without using feature j, $X_{-j}w_{-j}^* - y$.

2. Note that the condition does not depend on λ.

Why does ℓ_1 give sparsity

Consider ℓ_1 regularized least squares:

$$L(w) = \frac{1}{2}\|Xw - y\|^2 + \|w\|_1. \tag{5}$$

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

1. We need

$$\frac{\partial}{\partial w_j} L(w)\Big|_{w_j=0} = x_{\cdot j}^T(Xw - y) + \lambda[-1, 1] = 0 \tag{6}$$

   because subderivative $\partial|w_j|$ at $w_j = 0$ is $[-1, 1]$. This only requires the $j-th$ features to be close to orthogonal to the residual, specifically the inner product is within $[-\lambda, \lambda]$.
2. Thus increasing λ sets more weights to zero.

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