

STAT540

Lecture 21: March 23th 2020

Supervised learning II: Cross Validation and Regularization

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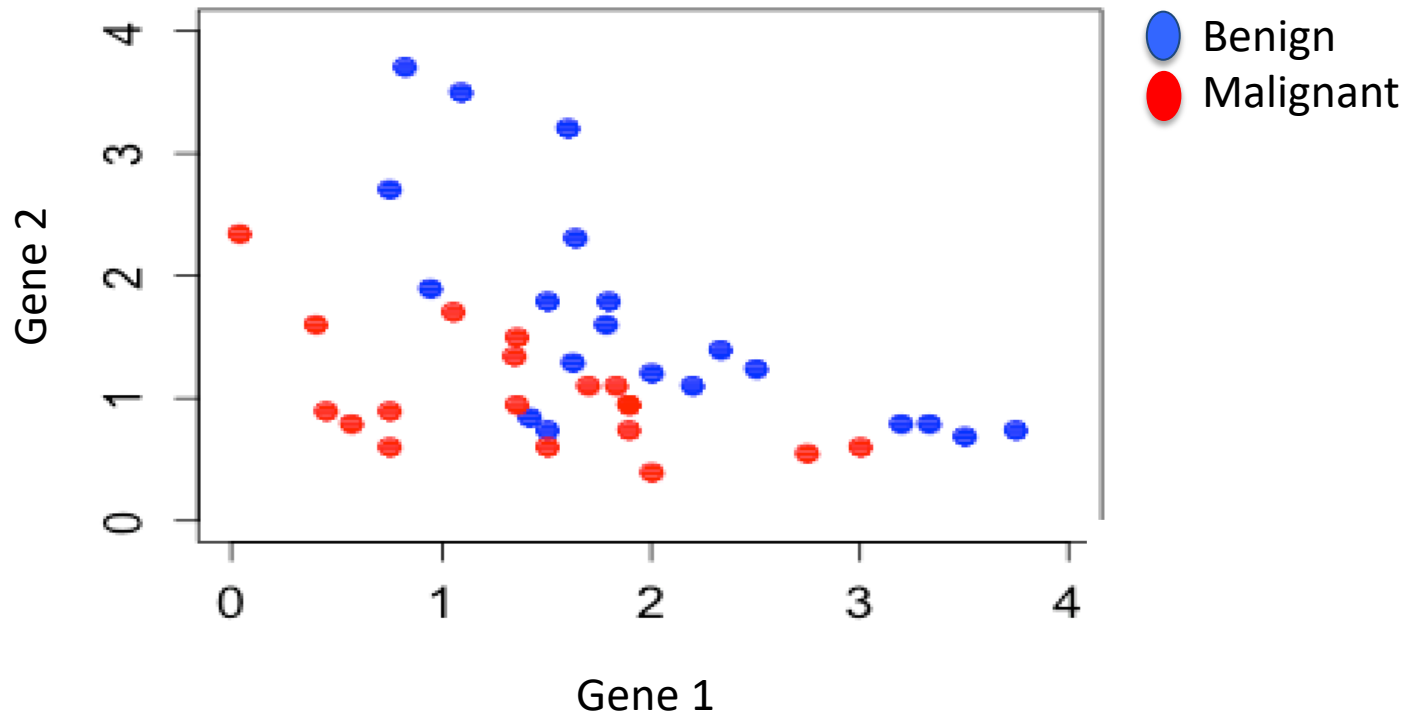
Center for Molecular Medicine and Therapeutics

Recall: Supervise Learning

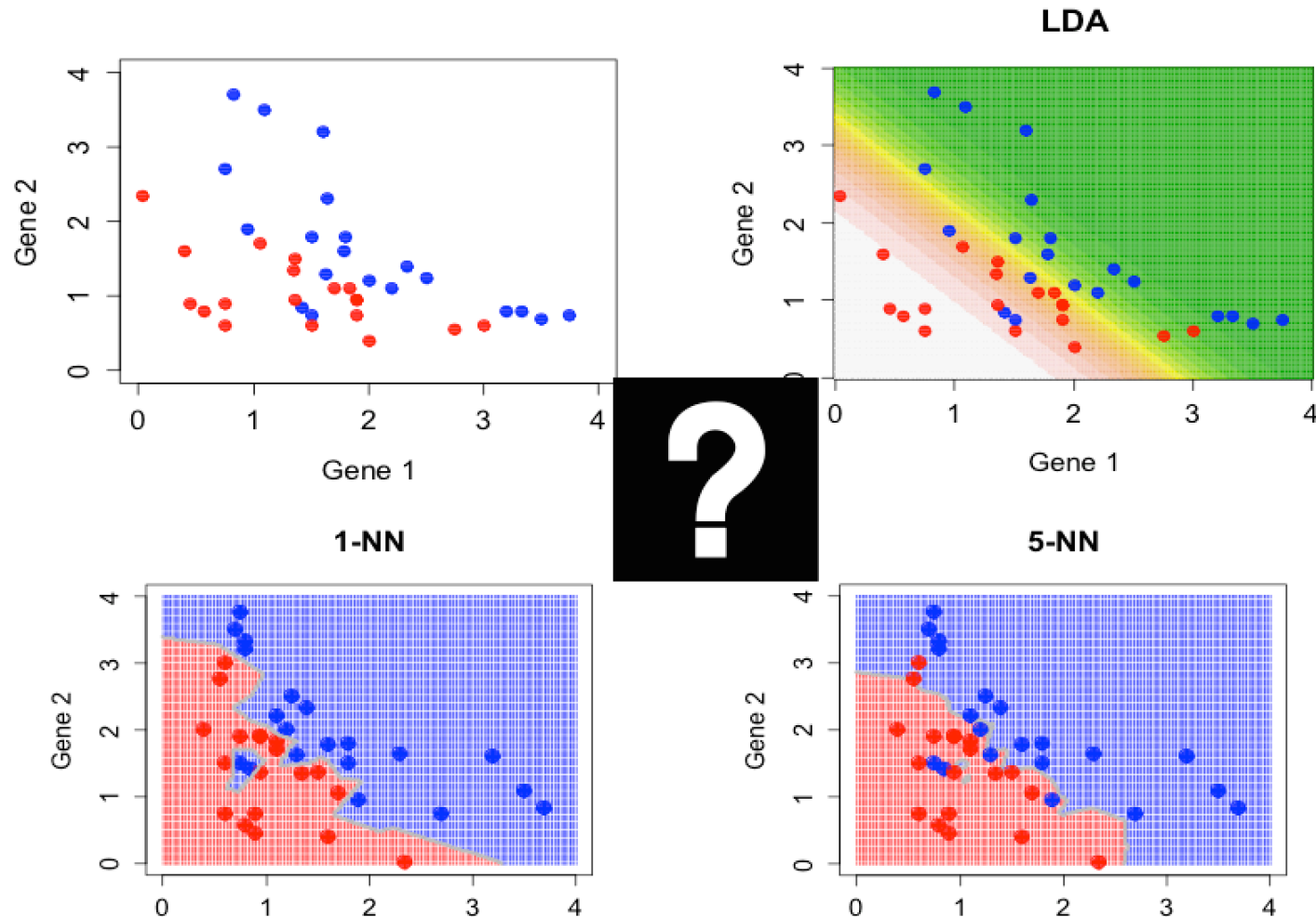
- We have a training data set of n examples in which we know the value of both y and X
- Based on the training data, we will produce a model (function) to predict y . The model can be parametric or non-parametric.
- We want to predict y on new samples of a “test set” for which we only know X .

How can we find the best-trained model?

Assume we'd like to train a classifier to predict tumor type from gene expression data

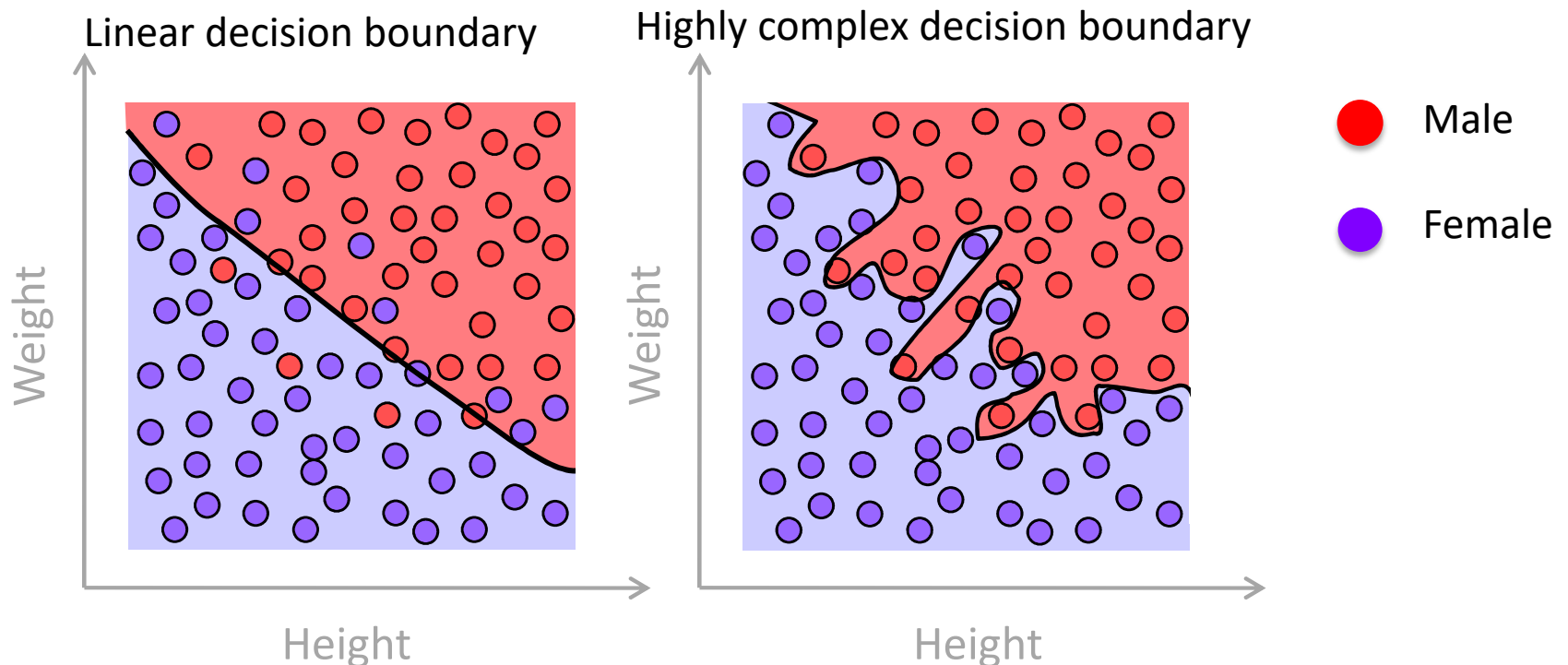


Many methods can be used to build a classifier (ie. define a decision boundary), depending on the exact model and learnt parameters. But which one is better?



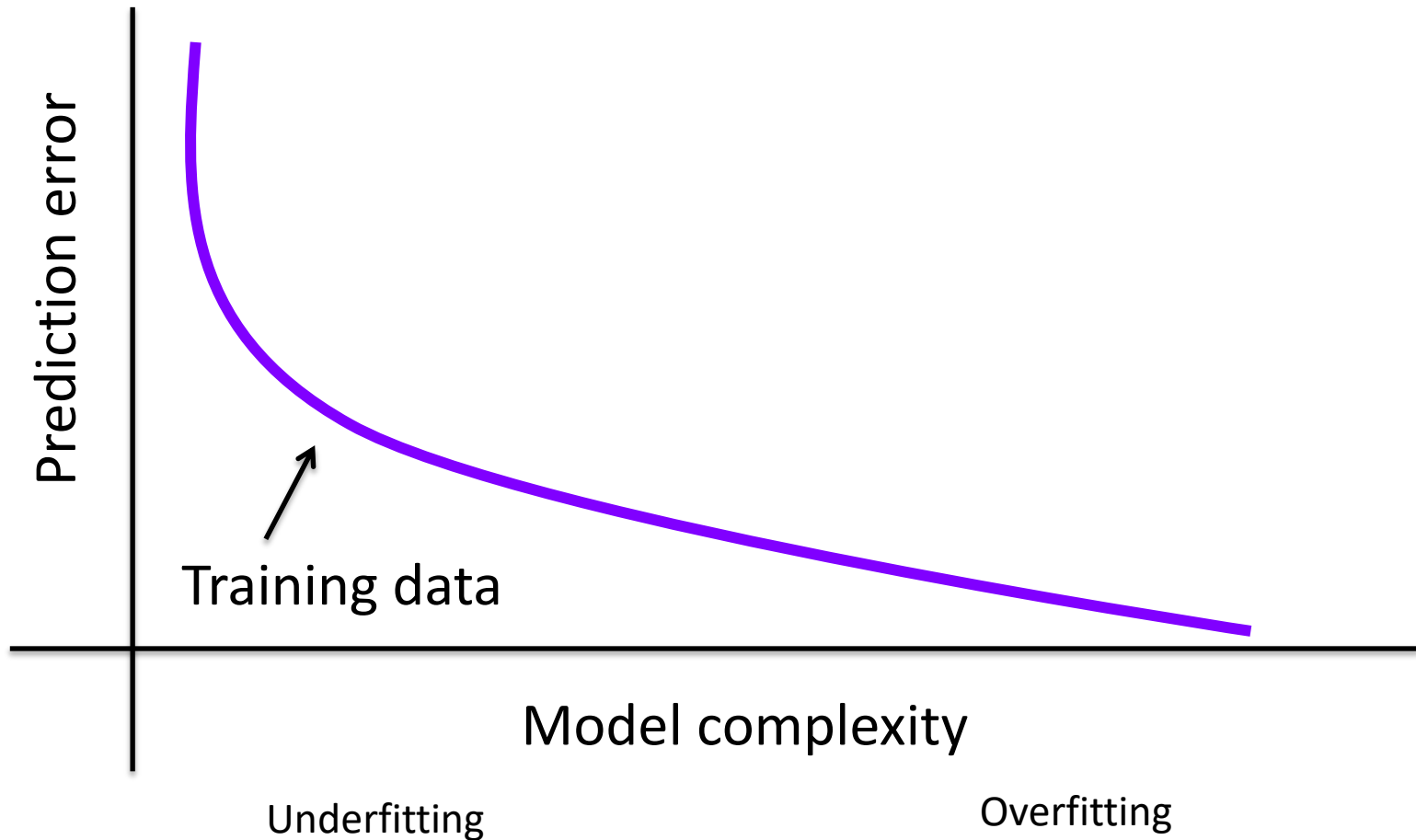
Overfitting

If we allow very complicated predictors, we could overfit the training data:

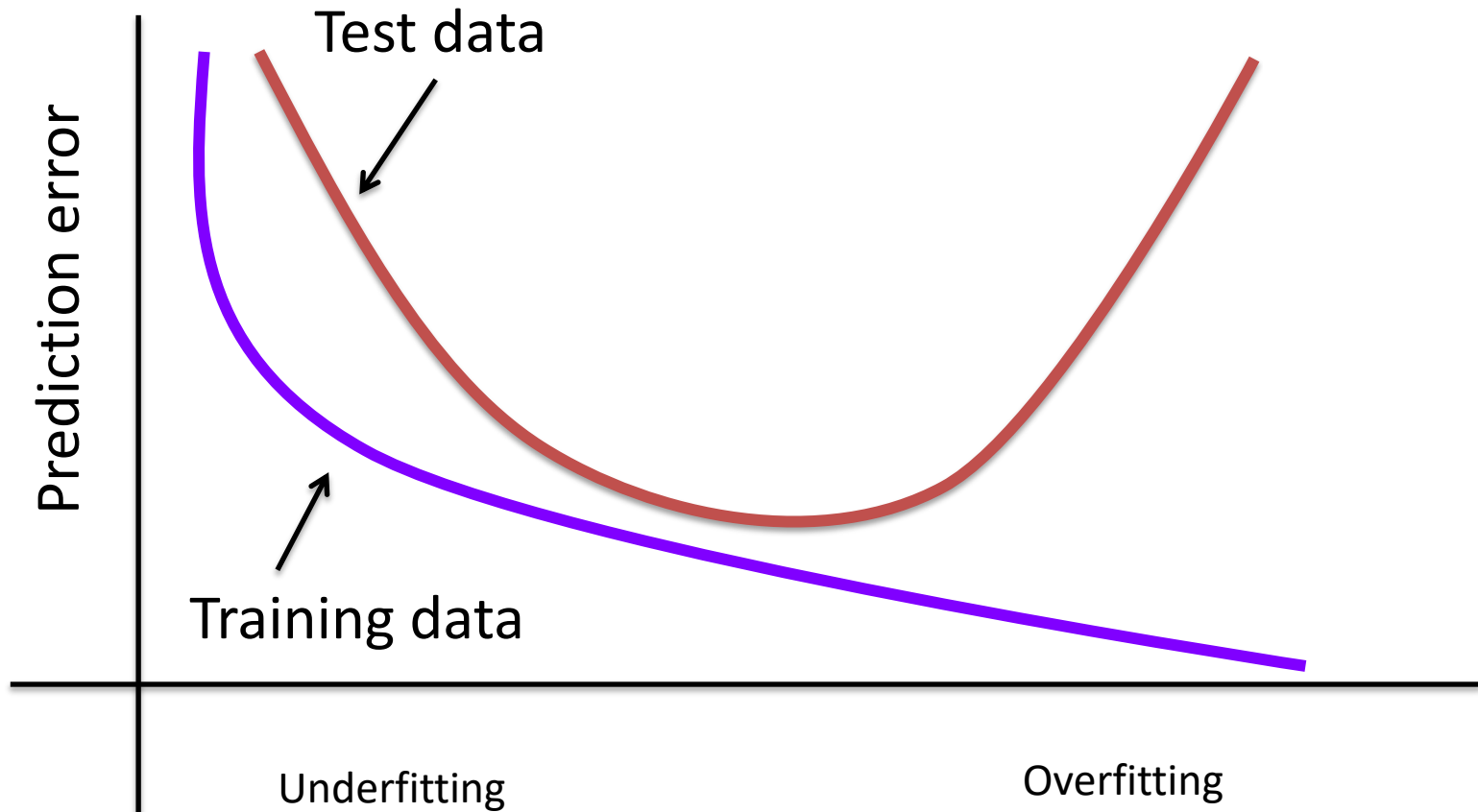


- The best model should predict the class labels of the samples in the *test* set accurately!
- “the model should **generalize**”

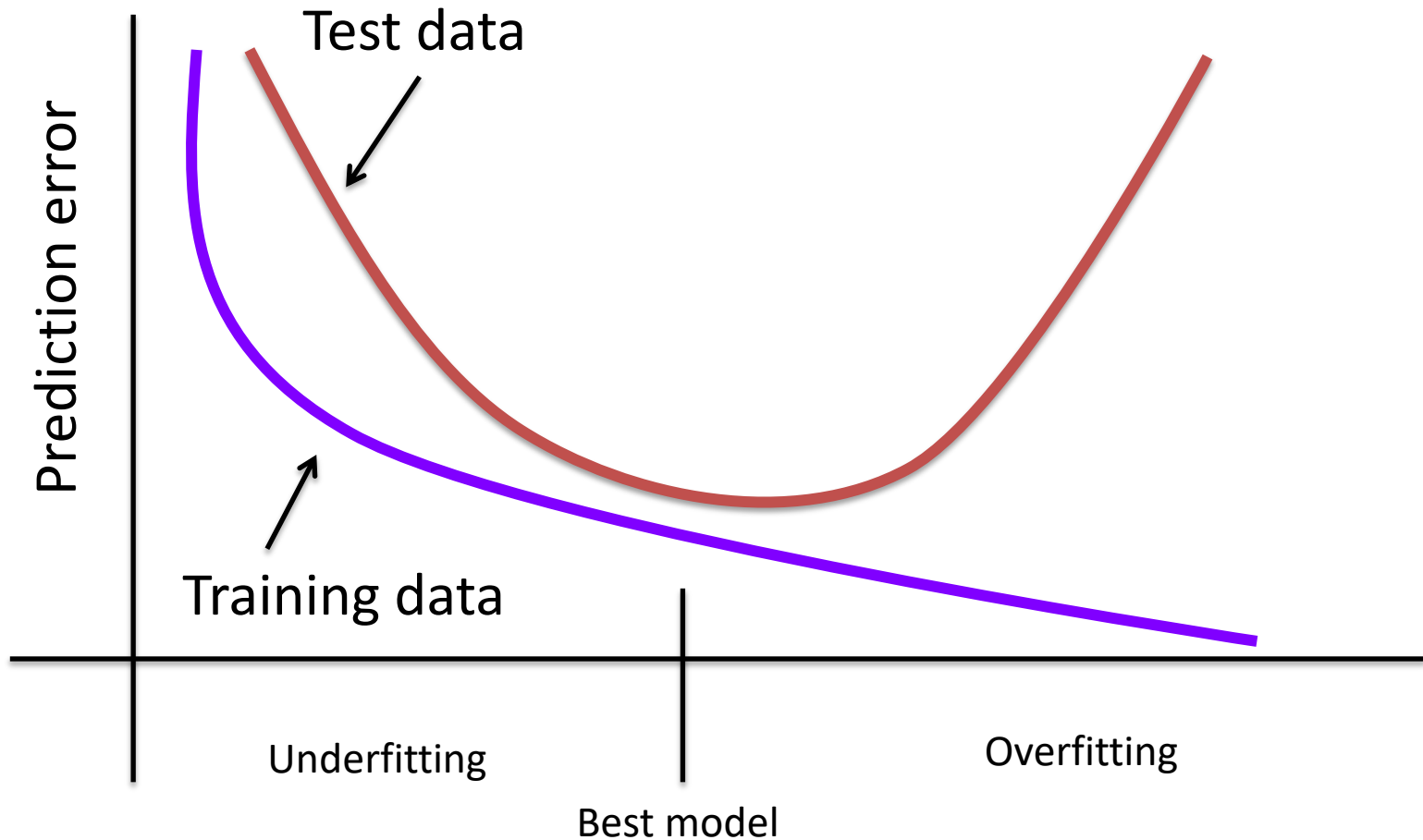
Error and model complexity



Error and model complexity



Error and model complexity



But ...

But ... How do we find a test set? And how do we know what the right prediction is for a test sample?

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- **We can not use the same test set to train a model and test it**
- Ideally, we want to train the model on some samples and use other samples to test the model:
 - Training set
 - Validation set
 - Test set
- If an independent test dataset is not available, we need to use part of our training data to create one. How?

Cross-validation

- General approach for estimating the error of the model in an “unbiased” way.
- Split the data to many sub-sets, use some to train model and others to test the model’s predictions.

Cross-validation (CV)

- K-fold cross-validation:
 1. Create k partition (folds) of input data
 2. Set aside data in one of the partition (fold) for validation
 3. Train model on all but the **held-out** fold
 4. Measure cross-validation (CV) error using data from the left-out fold:

$$\text{CV Error}_i = \frac{1}{n_i} \sum_{j \in T_i} L(y_j, \hat{y}_{j(-i)})$$

5. Repeat leaving out for all folds and measure average error

$$\text{CV Error} = \frac{1}{k} \sum_{i=1}^k \text{CV Error}_i$$

Example: 4-fold cross-validation



Example: 4-fold cross-validation

Fold-1



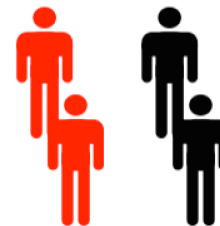
Fold-2



Fold-3

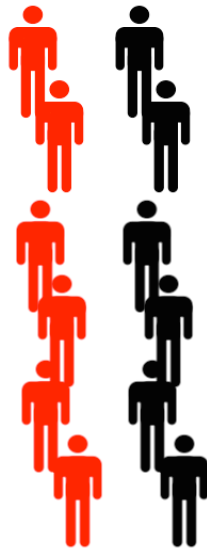


Fold-4

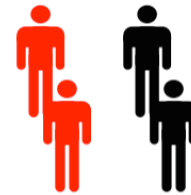


Example: 4-fold cross-validation

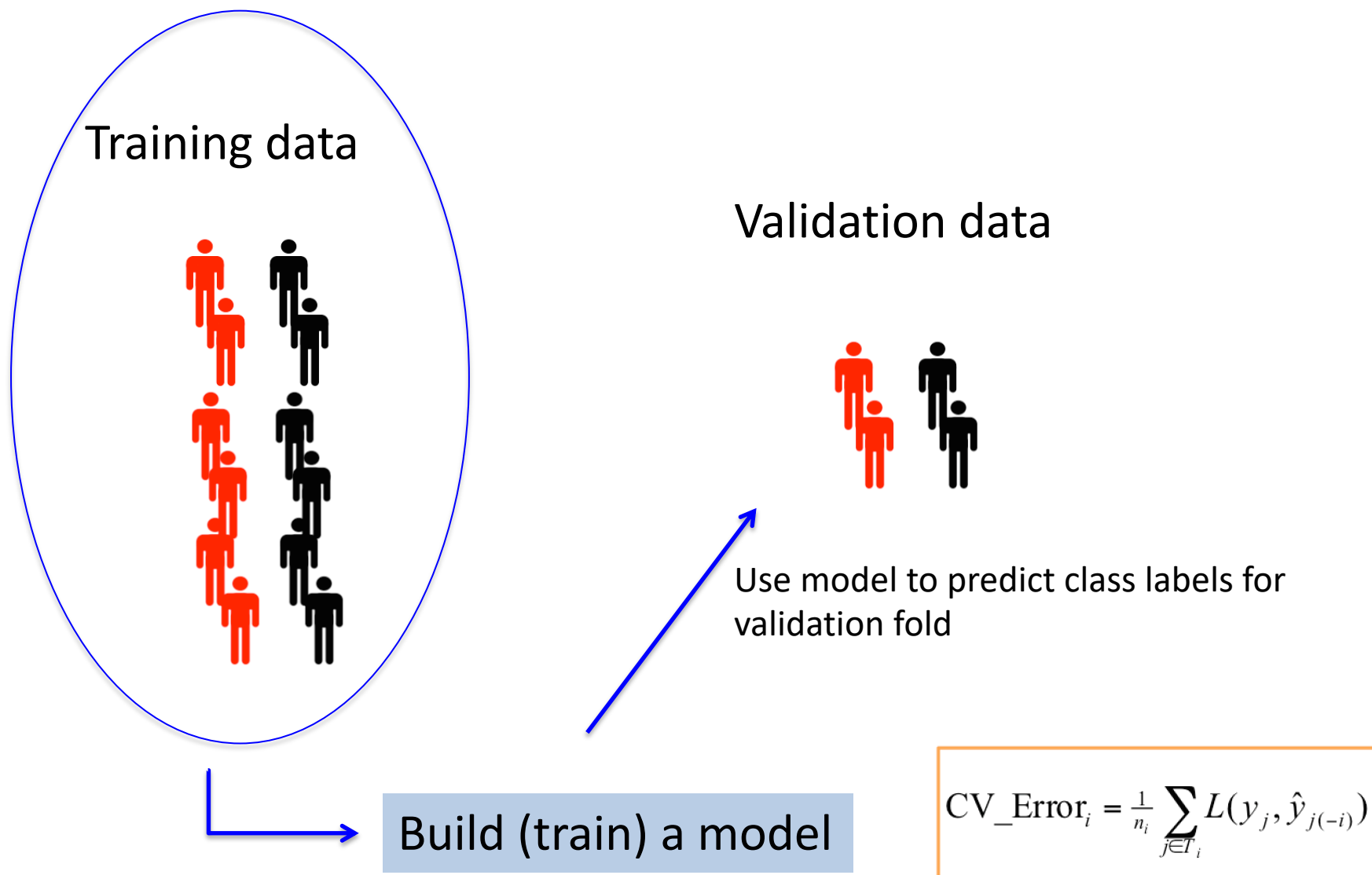
Training data



Validation data



Example: 4-fold cross-validation



K-fold cross-validation

- k can range from 2 to n:
 - Larger k:
 - Variance of true error will be high
 - Computational time will be large
 - Smaller k:
 - + reduced computation time
 - + variance of error estimate is small
- N-fold CV is called “Leave-One-Out” CV
- In practice:
 - Lower k is more reliable, eg., 3-fold CV is standard.

How do we measure error on validation/test set?

continuous response

Examples:

- ▶ Squared error loss

$$L(\mathbf{y}, \hat{\mathbf{y}}) = \|\mathbf{y} - \hat{\mathbf{y}}\|_2^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

- ▶ Absolute error loss

$$L(\mathbf{y}, \hat{\mathbf{y}}) = \|\mathbf{y} - \hat{\mathbf{y}}\|_1 = \sum_{i=1}^n |y_i - \hat{y}_i|$$

Binary response/labels

- ▶ True positive (TP)
- ▶ True negative (TN)
- ▶ False positive (?Type I error?) (FP)
- ▶ False negative (?Type II error?) (FN)

- ▶ Accuracy $(TP + TN)/N$ (=1-error rate)
- ▶ Sensitivity: $TP/(TP+FN)$ (recall)
- ▶ Specificity: $TN/(TN + FP)$

Summary of SL and CV so far ...

- Supervised learning:
 - Write down a model \rightarrow objective function
 - Algebraically simplify model/objective as much as possible
 - Write down the optimization problem: solve for parameters
(highly recommend doing the above, and program your own logistic regression function)
- Overfitting:
 - Constantly think about it!
 - Overfitting can severely delude you about the accuracy of your model
- Cross-validation:
 - Good first-pass solution for tuning parameters, finding the “right” model
 - Assumption: test and training data are independent (this may not always be the case, especially due to systematic artifacts in genomics)
 - Batch effects result in inflated estimate of accuracy

- In high dimensional biology (“omics studies”) we typically have thousands to millions of features/covariates (**p>>n problem**):
 - Gene expression datasets: >20,000 genes
 - Genotyping datasets: > 1M SNPs
 - DNA Methylation datasets: > 200K methylation sites
- A main analysis goal is to identify features/covariates that important in predicting a trait/disease/outcome
- **Complexity regularization through feature selection and penalization**

Feature selection

- The “filter” approach:
 - Don’t look at the labels/response: e.g., only keep genes with STD/mean > threshold
 - Consider the labels/response: e.g., only keep genes significantly correlated with response (note: must be careful to do this in a proper, nested, CV framework)
- The “wrapper” approach:
 - Identifying features that lead to good performance by the specific classifier
 - Cross-validation
- The “embedded” approach:
 - Modify the objective function to identify a reduced feature set intrinsically
 - Regularization/penalization

Feature selection in linear regression

- **Best subset regression:**
 - Finds subset of size k with smallest error (e.g., mean squared error).
 - Unfeasible for omics studies, because $p\text{-choose-}k$ is huge!! (e.g., $>10^{10}$)
- **Forward/backward stepwise regression**
 - Sequentially add the best covariate that most improves the fit (e.g., minimizes prediction error)
- **Regularization methods (shrinkage/penalization)**
 - Modify the objective function, to explicitly penalize “magnitude” of coefficients

Regularized regression

$$\operatorname{argmin}_{\boldsymbol{\beta}} \underbrace{(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})}_{\text{Squared error}} + \underbrace{\lambda P(\boldsymbol{\beta})}_{\text{Penalization function}}$$

Squared error

Penalization function

Penalization (tuning) parameter

** Note change in notation: use bold lower case letters for vectors, upper case letters for matrices, lower case letters for scalars **

Regularized regression: ridge

$$\operatorname{argmin}_{\boldsymbol{\beta}} \underbrace{(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})}_{\text{Squared error}} + \underbrace{\lambda P(\boldsymbol{\beta})}_{\text{Penalization function}}$$

$$P(\boldsymbol{\beta}) = \|\boldsymbol{\beta}\|_2^2 = \sum_{i=1}^p \beta_i^2$$

Ridge regression: L2 norm
("squared") penalty function

(Hoerl and Kennard, *Technometrics*, 1970)

Regularized regression: ridge

$$\underset{\beta}{\operatorname{argmin}} \underbrace{(\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta)}_{\text{Squared error}} + \underbrace{\lambda P(\beta)}_{\text{Penalization function}}$$

$$P(\beta) = \|\beta\|_2^2 = \sum_{i=1}^p \beta_i^2$$

Ridge regression: L2 norm
("squared") penalty function

$\lambda \geq 0$ is the penalization parameter that we can "tune"

- When $\lambda = 0$ we get the linear regression estimate
- When $\lambda = \infty$ what happens?
- For λ in between 0 and infinity we are balancing error term vs penalty

Regularized regression: ridge

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \underbrace{(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})}_{\text{Squared error}} + \underbrace{\lambda \|\boldsymbol{\beta}\|_2^2}_{\text{Penalization function}}$$

$$\boldsymbol{\beta}^{\text{ridge}} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y}$$

Regularized regression: ridge

$$\underset{\beta}{\operatorname{argmin}} \underbrace{(\mathbf{y}-\mathbf{X}\boldsymbol{\beta})^T (\mathbf{y}-\mathbf{X}\boldsymbol{\beta})}_{\text{Squared error}} + \underbrace{\lambda P(\boldsymbol{\beta})}_{\text{Penalization function}}$$

$$P(\boldsymbol{\beta}) = \|\boldsymbol{\beta}\|_2^2 = \sum_{i=1}^p \beta_i^2$$

Ridge regression: L2 norm
("squared") penalty function

Important details:

- How do you choose λ ? Need nested CV to tune parameter and estimate test error.
- Requires standardization of the covariates (columns of X) :
 - the covariates need to be on the same "scale"
- Since columns standardized no intercept required

Regularized regression: ridge

$$\operatorname{argmin}_{\boldsymbol{\beta}} \underbrace{(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})}_{\text{Squared error}} + \underbrace{\lambda P(\boldsymbol{\beta})}_{\text{Penalization function}}$$

Squared error

Penalization function

$$P(\boldsymbol{\beta}) = \|\boldsymbol{\beta}\|_2^2 = \sum_{i=1}^p \beta_i^2$$

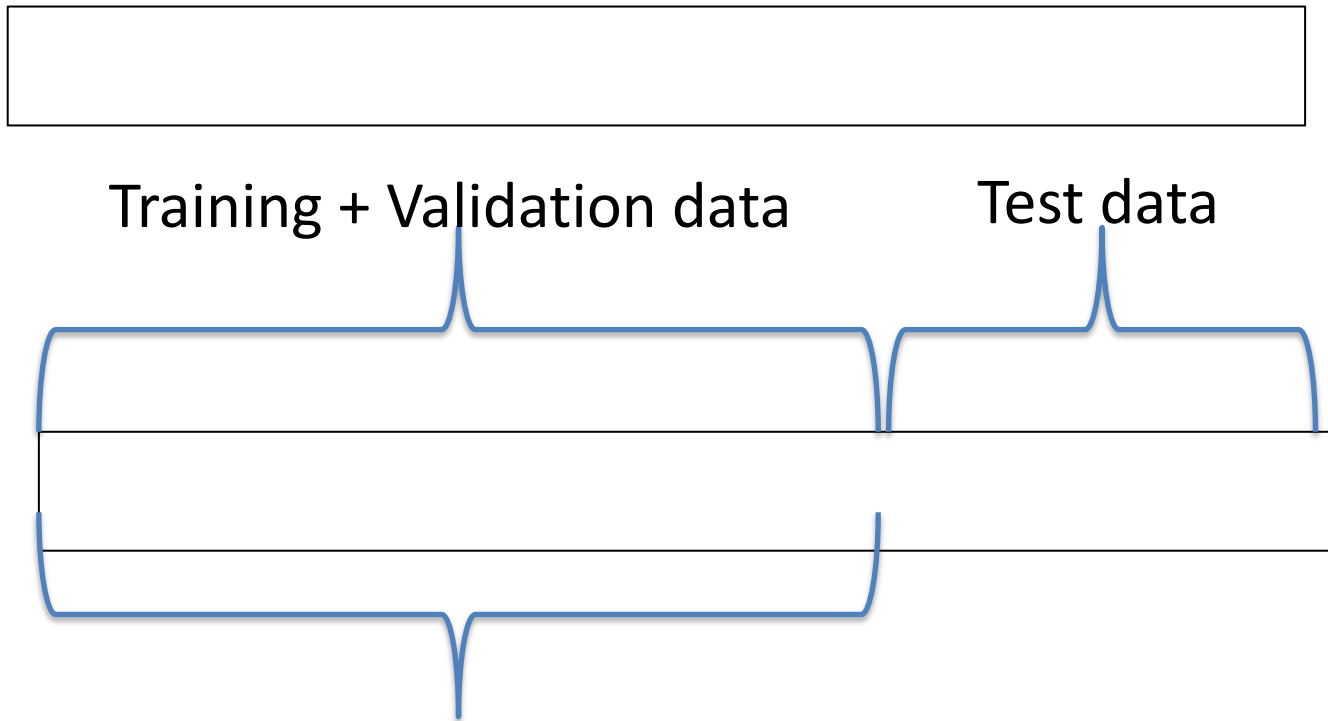
Ridge regression: L2 norm
("squared") penalty function

Choosing the penalization parameter:

To choose the parameter and assess testing error we need to do nested cross-validation. Why?

Nested cross-validation

Full data



Do k-fold CV here to find tuning
parameter, report results on test data

Regularized regression: ridge

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \underbrace{(y - X\beta)^T (y - X\beta)}_{\text{Squared error}} + \underbrace{\lambda \|\beta\|_2^2}_{\text{Penalization function}}$$

Squared error

Penalization function

Probabilistic interpretation:

$$L(\theta \mid \text{Data}) = L(\theta \mid X, y)$$

$$= p(y \mid X, \theta) p(\theta) = \underbrace{N(y \mid X\beta, \sigma)}_{\text{Likelihood}} \underbrace{N(\beta \mid 0, \nu)}_{\text{Prior}}$$

Regularized regression: lasso

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \quad (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) + \lambda \|\boldsymbol{\beta}\|_1$$

$$\|\boldsymbol{\beta}\|_1 = \sum_{i=1}^p |\beta_i| \quad \longrightarrow \quad \text{L1 norm penalty}$$

- Proposed by Tibshirani (1996)
- Lasso is an acronym: Least Absolute Selection and Shrinkage Operator
- The only difference between ridge and lasso regularization is that ridge uses L2 norm vs lasso uses L1 norm. But turns out that the solutions to lasso and ridge behaves very differently.

$$\hat{\beta}_{lasso} = \underset{\beta}{\operatorname{argmin}} \quad (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) + \lambda \|\beta\|_1$$

As before:

- The tuning parameter $\lambda \geq 0$ controls the strength of the penalty. What happens at the 0 and infinity?

But now:

- For $\lambda \geq 0$ between the two extreme setting, we are balancing two ideas: minimizing the squared error, and penalizing the magnitude of the coefficient. But the L1 penalty causes some coefficients to be set to **zero exactly**.
- Because some coefficients are set to zero exactly, lasso performs variable selection.
- No closed form solution: requires numerical optimization.
 - LARS algorithm
 - ADMM algorithm **

Comparing lasso and ridge

- Predictive performance: lasso and ridge are typically comparable
- Interpretation: lasso has a big advantage because it leads to variable selection

Some limitations and considerations

- If $p \gg n$, the lasso can select at most n features (rest of the coefficients will be set to 0).
- If there is a group of highly correlated features, the lasso will choose only one among them (arbitrarily).
- Sensitivity to the choice of penalization parameter.

The elastic net: combined L2 and L1 penalty

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \quad (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) + \lambda((1 - \alpha)\|\boldsymbol{\beta}\|_1 + \alpha\|\boldsymbol{\beta}\|_2^2)$$

- Convex combination of the L1 and L2 penalty
- Addresses the shortcoming of the lasso in the presence of correlated features.
- But now we have to set 2 parameters.

Discussion

- Regularization methods can be extended to other models beyond linear regression (e.g., logistic regression)
- Designing variable penalization functions is an active area of research (e.g., fused lasso, group lasso, etc)
- How do we choose the regularization/penalty parameter?
 - Cross-validation

Two common mistakes when applying supervised learning

1. Do “feature” selection on entire data, and then build classifier
2. Make sure you use nested CV:
 - If you are learning parameters and reporting error, you should have training, validation, and test data splits.