STAT 215A Fall 2023 Week 10

Chengzhong Ye

Announcements

- Congrats on completing the midterm!
- We'll go over midterm solutions next Tuesday
- Lab 4 will be released Today
    - due 11/09 at 11:59pm
    - Reach out to your group members (will be announced on bcourse)!

Outline for today

- Regularization Pt. 2
- Data splitting and statistical learning pipeline
- Introduction to Lab 4

Regularization Part II: Lasso

Lasso motivation

Feature selection

- Want to find best subset of size s of variables for prediction (typically $s << p$)
    - Best for our purposes = smallest MSE
- Ridge doesn't perform *automatic* feature selection
    - Can use to order the importance of features via magnitude of their coefficients
    - Typically there are no exact 0's among the coefficients estimates
- Methods that provide more direct feature selection:
    - Best subsets (L^0) regression
    - Lasso

Best subsets regression

Goal: Find the best (smallest MSE) subset of size s of the features.

$$\tilde{\beta} = \underset{\beta}{\operatorname{argmin}} \left\{ \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2 + \lambda \underbrace{\sum_{j=1}^{p} |\beta_j|^0}_{\text{Number of non-zero coefficients}} \right\}$$

Problem:

- Computationally infeasible for moderate-sized problems[1]
- Have to do an exhaustive search over $\binom{p}{s}$ regressions

1. E.g. the R package `best-subset` can find solutions for p = 100 in a reasonable amount of time (but much slower than e.g. lasso)

Lasso

Uses an $\boldsymbol{L^1}$ penalty (rather than the L^2 penalty that ridge uses).

$$\hat{\beta}^{\text{lasso}} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{N} \Big(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j \Big)^2 \quad \text{subject to} \quad \sum_{j=1}^{p} |\beta_j| \le t.$$

Equivalently: $$\hat{\beta}^{\text{lasso}} = \underset{\beta}{\operatorname{argmin}} \Big\{ \frac{1}{2} \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \Big\}$$

- Lasso is the "best convex relaxation" of the best subsets problem
- The L^1 penalty results in **sparse** solutions (many coefficients zero)
- More interpretable than ridge, but if the true data-generating process is not sparse then can result in worse prediction accuracy

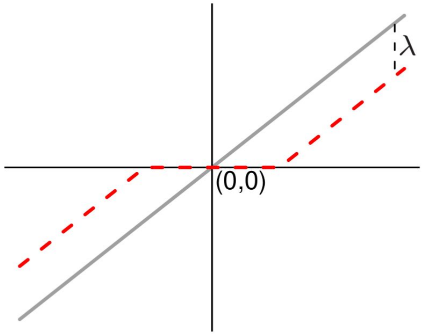
Lasso with orthonormal design matrix

If the columns of the design matrix predictors X are orthonormal, then the lasso estimate is related to the OLS estimate by

$$\hat{\beta}_j^{\text{lasso}} = \text{sign}(\hat{\beta}_j)(|\hat{\beta}_j| - \lambda)_+$$

OLS estimate

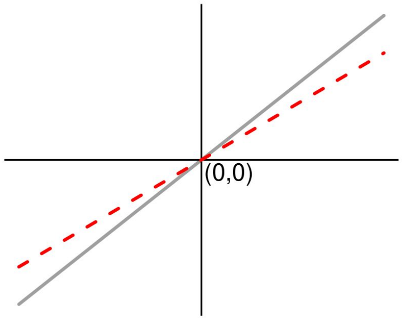
Lasso



Compare that to what happens in the case of ridge:

$$\hat{\beta}_j^{\text{ridge}} = \hat{\beta}_j/(1+\lambda)$$

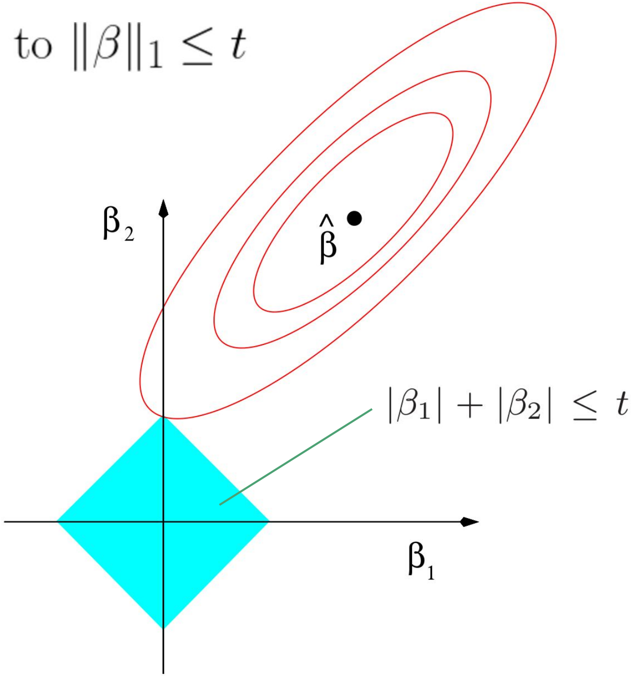
Ridge



Lasso vs. ridge, non-orthogonal case

$$\hat{\beta}^{\text{lasso}} = \arg\min_{\beta} \|y - X\beta\|_2^2$$

subject to $\|\beta\|_1 \leq t$



$$\hat{\beta}^{\text{ridge}} = \arg\min_{\beta} \|y - X\beta\|_2^2$$

subject to $\|\beta\|_2^2 \leq t$

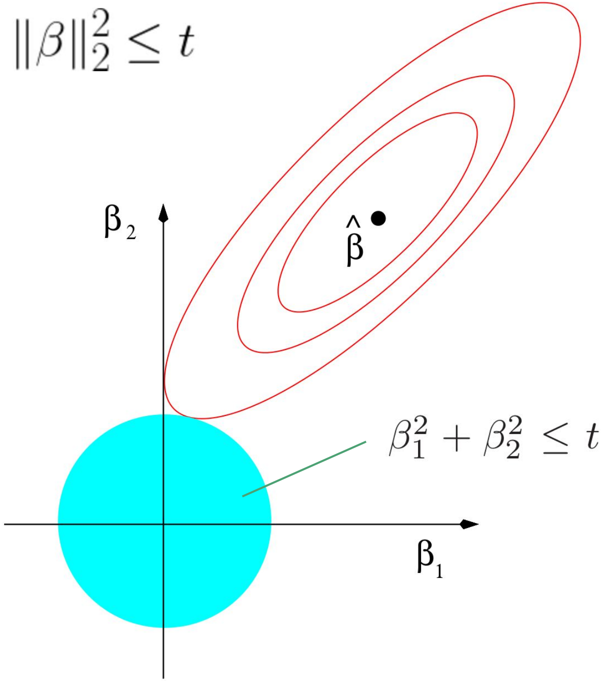
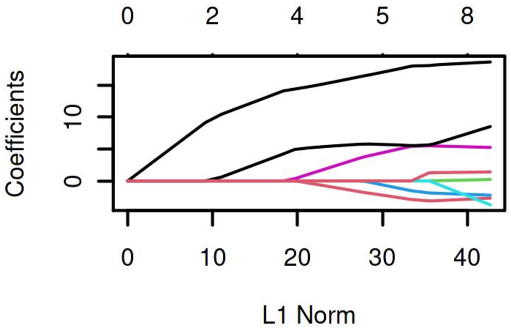


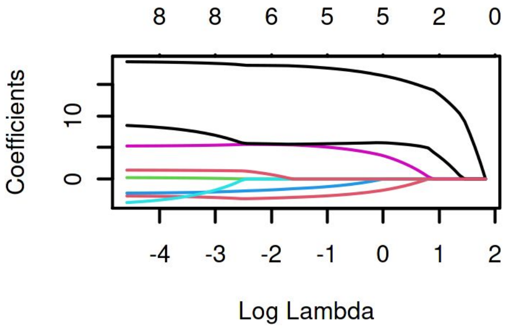
Image source: *The Elements of Statistical Learning*, p. 71

Lasso shrinkage profiles

$$\hat{\beta}^{\text{lasso}} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{N}\Big(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j\Big)^2 \text{ subject to } \sum_{j=1}^{p}|\beta_j| \le t.$$

- If t is larger than $t_0 = \sum_1^p |\hat{\beta}_j|$ then the lasso solution is the same as the OLS solution.
- If $t = t_0/2$ then lasso shrinks the OLS coefficients by about 50% on average
- By default, the R package `glmnet` plots the coefficients vs. their L^1 norm, but you can have it plot λ on the x-axis instead.





non-zero coefficients

Lasso in practice

- Great for feature selection and interpretability
- Tends to select one representative from a group of correlated features
  - Good if goal is a parsimonious model
  - Bad for data-driven discoveries
- Like ridge, don't forget to center and scale data
  - `glmnet()` does this by default, but returns results on original scale
- For large λ, the coefficients are heavily biased
  - Eventually the variance goes to zero (all 0 coefficients)
- **Warnings**:
  - Non-zero lasso coefficients ≠ statistically significant
  - Don't fit OLS after doing lasso and interpret the p-values the same way; OLS inference no longer valid after model model selection

Other alternatives / modifications to lasso

- **Weighted lasso**: use the weighted penalty $\lambda \sum_{j=1}^{p} w_j |\beta_j|$
  - If true β_j is large (small), want to penalize less (more) so w_j should be small (large)
- **Adaptive lasso** (Zou, 2006): $w_j = \left(\frac{1}{\left| \hat{\boldsymbol{\beta}}_j^{OLS/ridge} \right|} \right)^{\gamma} \quad (\gamma \in \{0.5, 1, 2\})$
- Non-convex penalties:
  - **SCAD** (Fan, 2001)
  - **MCP** (Zhang, 2009)
- **Randomized lasso** (Meinshausen, 2010): combines stability via bootstrapping and randomized weights to handle correlated variables

Elastic net

$$\hat{\beta}^{\text{enet}} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{N}\Big(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j\Big)^2 + \lambda \sum_{j=1}^{p}(\alpha|\beta_j| + (1-\alpha)\beta_j^2)$$

- Compromise between ridge and lasso depending on choice of $\alpha \in [0, 1]$
  - Lasso: $\alpha = 1$
  - Ridge: $\alpha = 0$
- Can handle correlated features better than lasso, but enforces more sparsity than ridge
- Difficult to tune both α and λ in practice

Summary: OLS + Regularized Regression

	OLS	Ridge	Lasso	Elastic Net
Advantages	• Simple • Can do inference (with all the caveats)	• Good with correlated features • MSE Existence Theorem (good for prediction)	• Feature selection and sparsity • Interpretability	• Compromise between ridge and Lasso
Disadvantages	• Major problems when p>n	• Dense model is not interpretable • No automatic feature selection	• Tends to choose 1 feature from correlated group • Can give worse prediction results if truth is not sparse	• Difficult to tune two parameters in practice

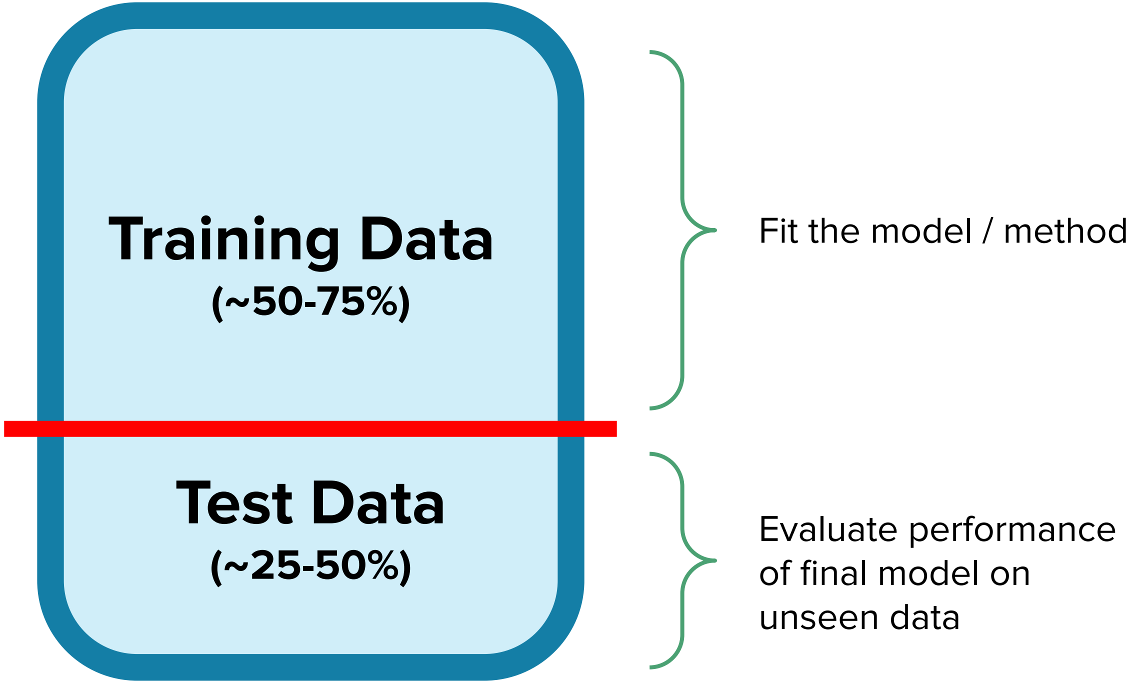
Statistical learning

Goal: Learn insights about the current data that are *generalizable* to future data

- Typically, one of the following tasks in mind:
    - **Prediction**: outcome of interest
    - **Data-driven discoveries**: pattern recognition, feature selection, etc.
- Two main branches of statistical learning:
    - **Unsupervised**: no outcomes / response data
        - Clustering, dimension reduction, pattern recognition
    - **Supervised**: have the outcome / response
        - **Classification** - categorical response
        - **Regression** - continuous response

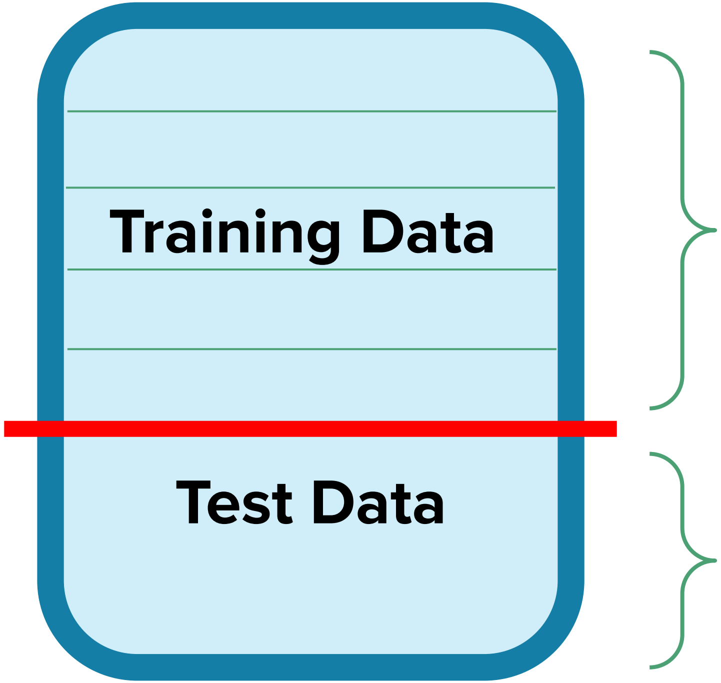
Data splitting: a way to assess generalizability

Simplest case:



Data splitting: a way to assess generalizability

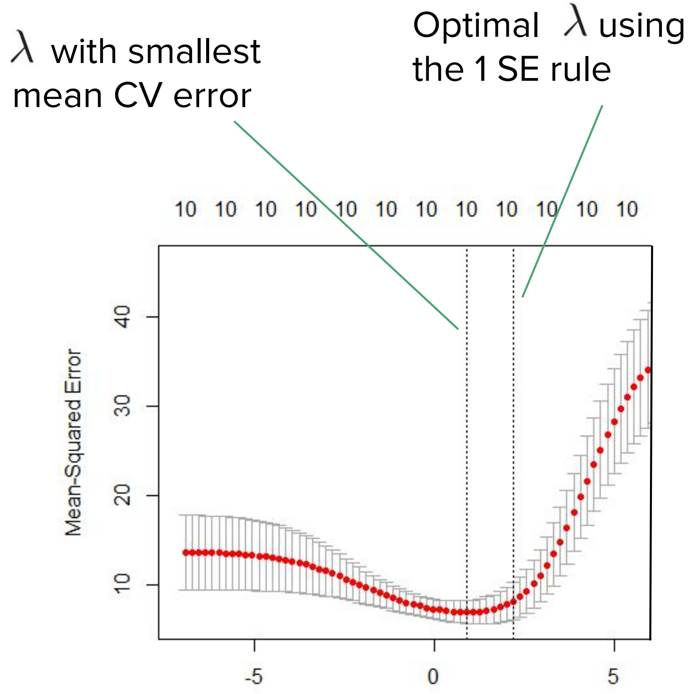
With cross validation:



Do 5-fold or 10-fold CV to choose hyperparameters and fit tuned model

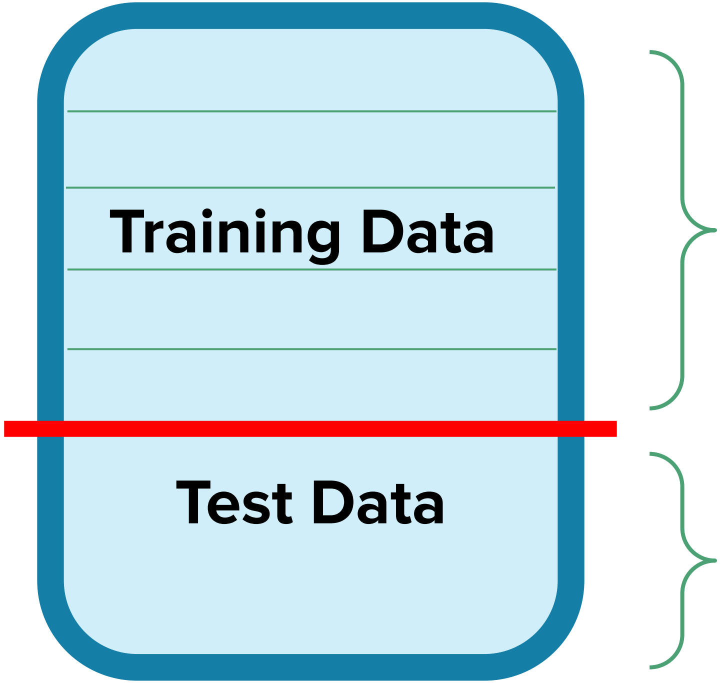
Evaluate performance of final model on unseen data

K-fold cross validation for choosing hyperparameters



Data splitting: a way to assess generalizability

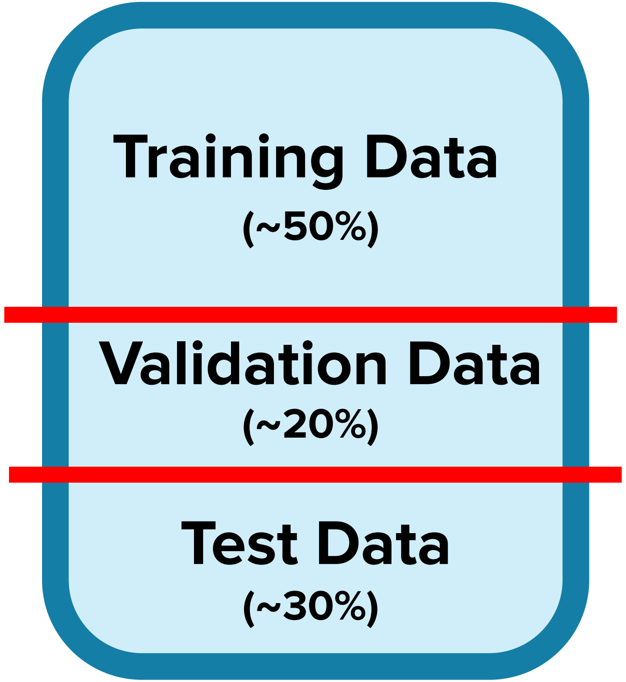
With cross validation:



Do 5-fold or 10-fold CV to choose hyperparameters and fit tuned model

Evaluate performance of final model on unseen data

Data splitting + tuning hyperparameters + multiple methods



E.g., use CV on this split to pick best λ for both lasso and ridge

Evaluate trained lasso and ridge models and pick the model with lower error

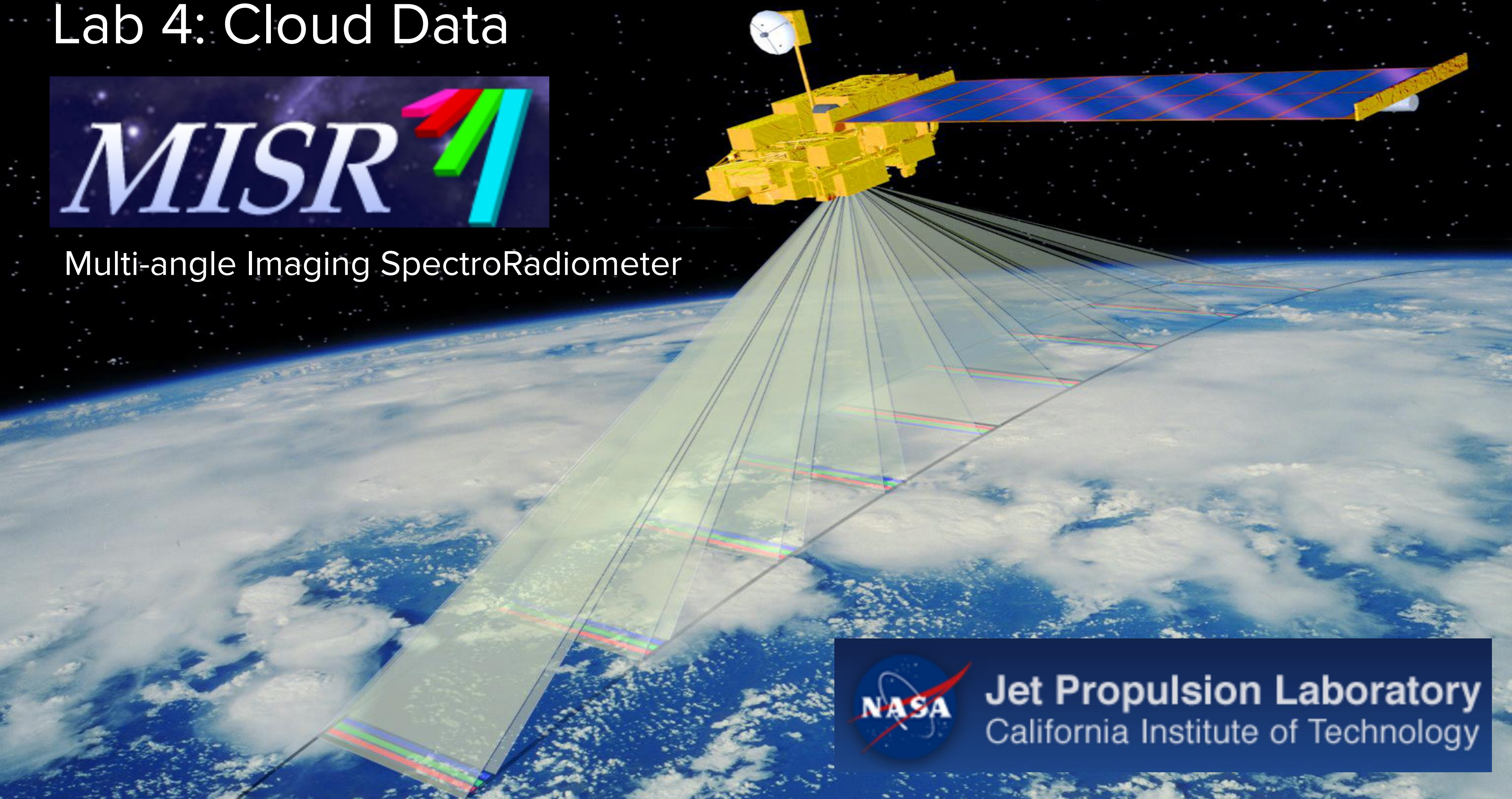
Evaluate performance of final model on unseen data

- Can repeat this data splitting B times to get a variance estimate of the test error
- This gives you an unbiased estimate of the prediction error for the *statistical learning process*, NOT a specific model

Lab 4: Cloud Data

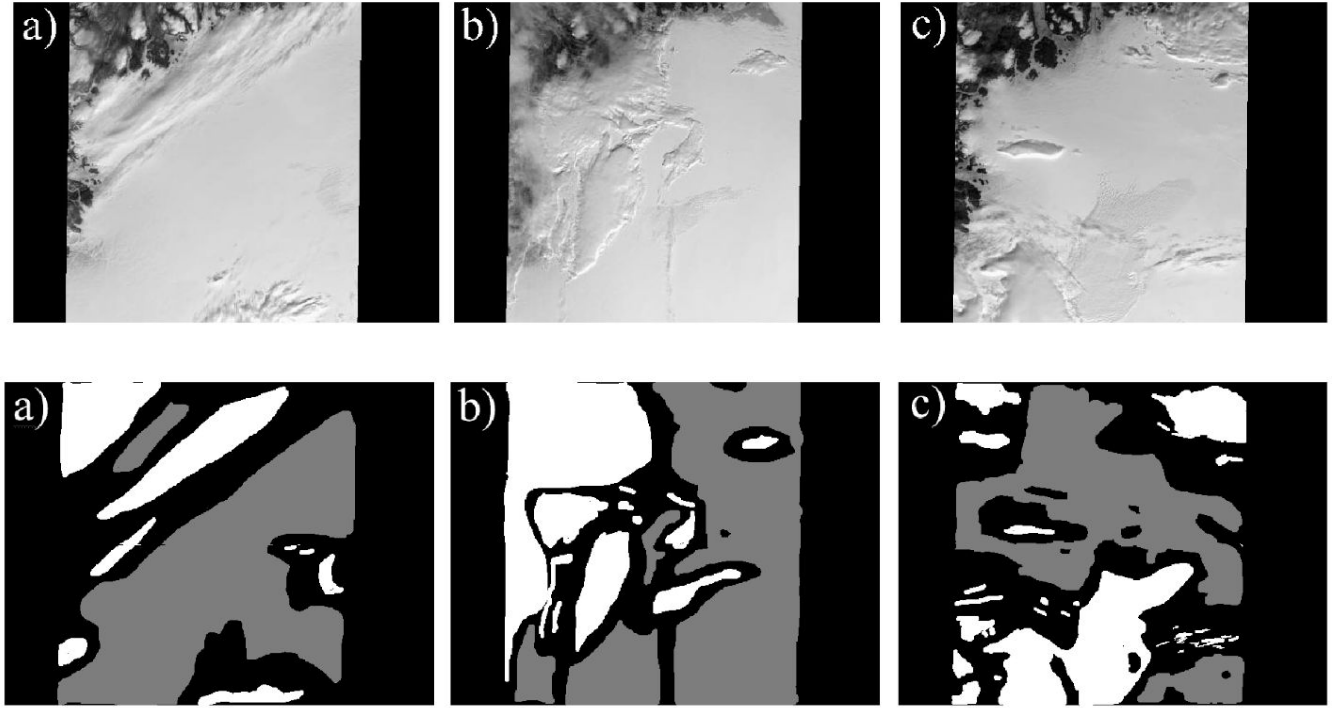
MISR

Multi-angle Imaging SpectroRadiometer

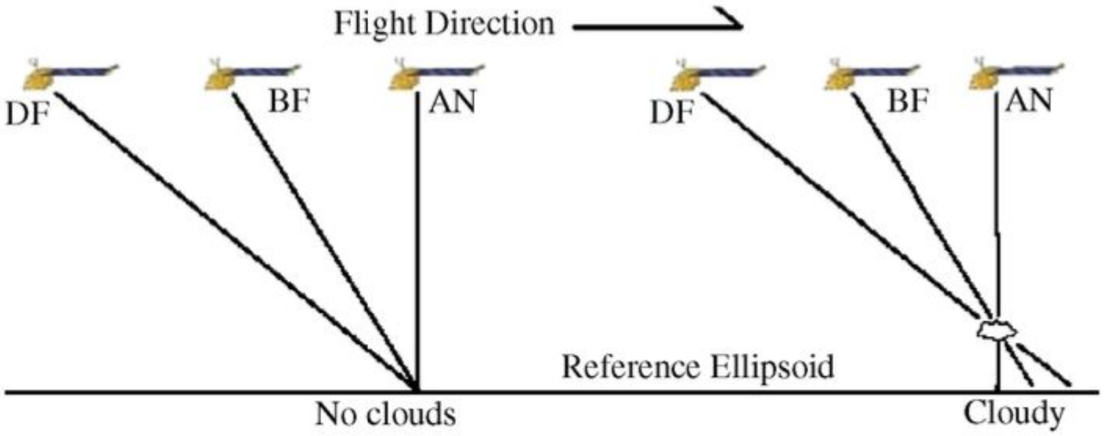


Jet Propulsion Laboratory
California Institute of Technology

Lab 4: Remote sensing / cloud data



Lab 4: Remote sensing / cloud data



Feature engineering:
CORR, SD, NDAI

Lab 4: Things to think about carefully

- Which methods/models?
    - Are they well-suited for this data? Why or why not?
    - What are the advantages/disadvantages and assumptions of the method(s) that you chose?
    - This can help you better identify the limitations of your prediction algorithm
- Data splitting scheme? Very important for generalizability
- Post-hoc EDA? Can provide insights into how to improve your prediction