Kris Sankaran

Selection

IFT6758, Fall 2019

Reading: ISLR section 5.1 and PDS pg. 359 - 375

Daily Choices for Data Scientists

Knowing how to fit models is not enough, if you want to solve a real-world problem.

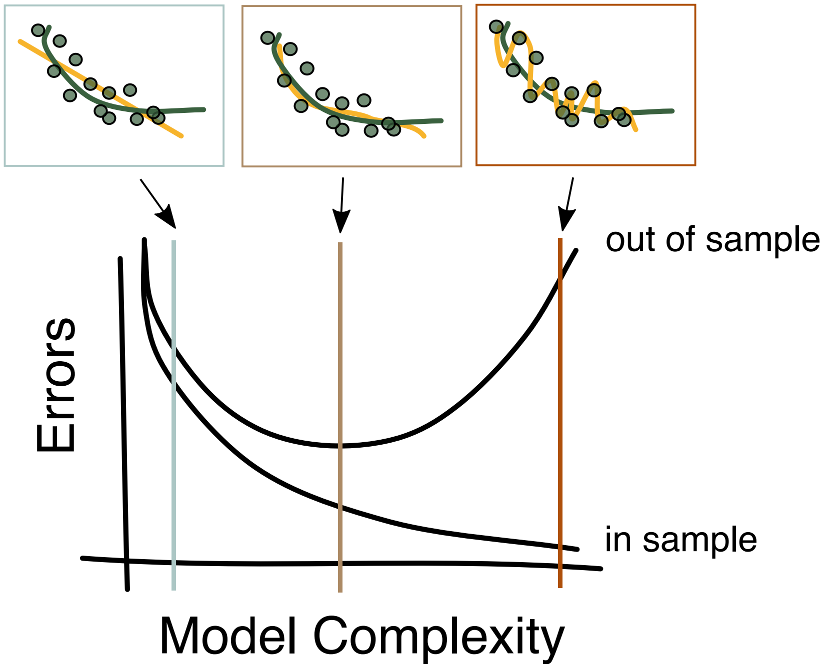
- How should you select between model families?
- Which parameters are best within a model family?
- Should you be trying to improve the data?
  - More samples? Richer features?
  - Less missingness, fewer outliers, ...

Transitioning to Inference

- We'll be more introspective, trying to understand properties of our algorithms
- The heart of inference: Being critical of the processes people use to learn from data

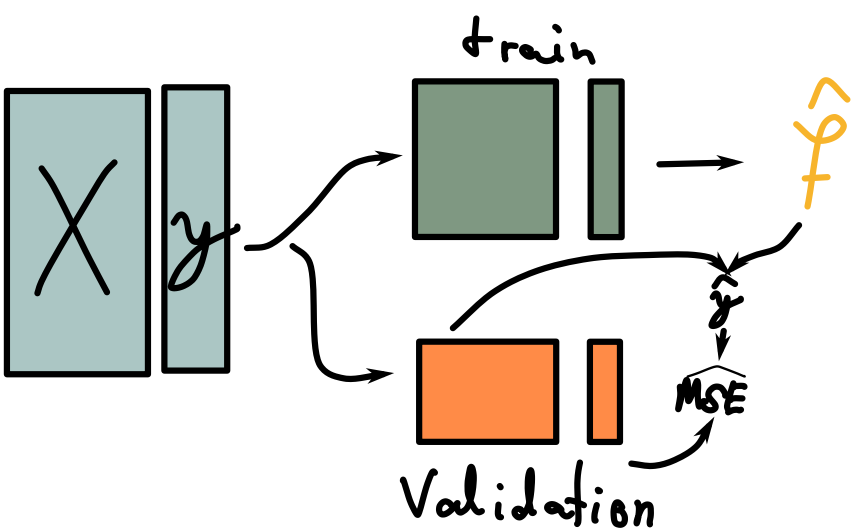
Reminder: Bias-Variance Tradeoff

- If you only evaluate on in-sample data, you will underestimate the out-of-sample error



Validation Sets

- To approximate the out-of-sample error, we can use a validation set.
- Randomly divide your sample into two pieces, one to train and another to validate



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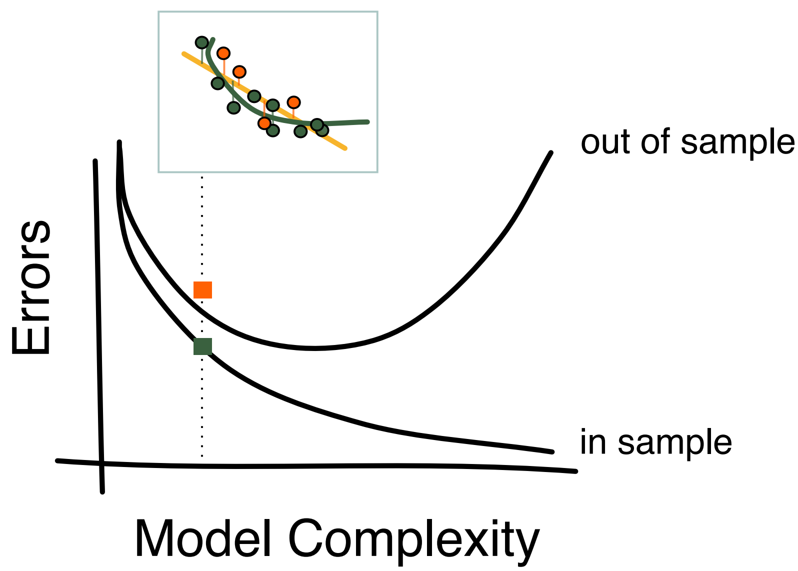
Validation Sets

If you run this over models with different degrees of complexity, you can see the bias-variance tradeoff.



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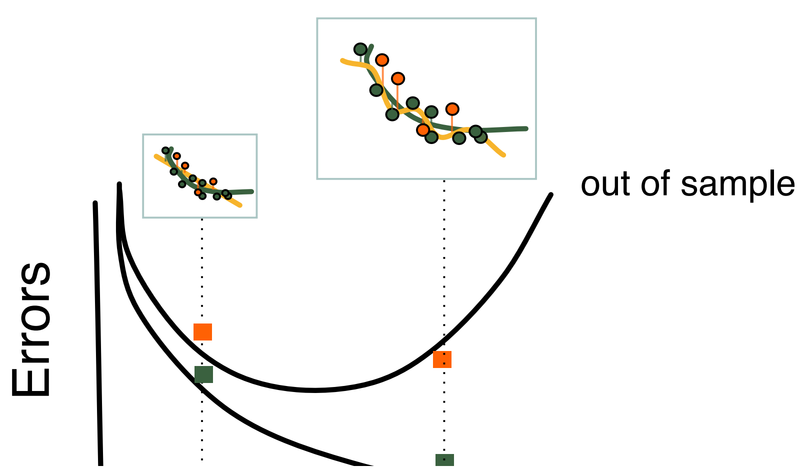


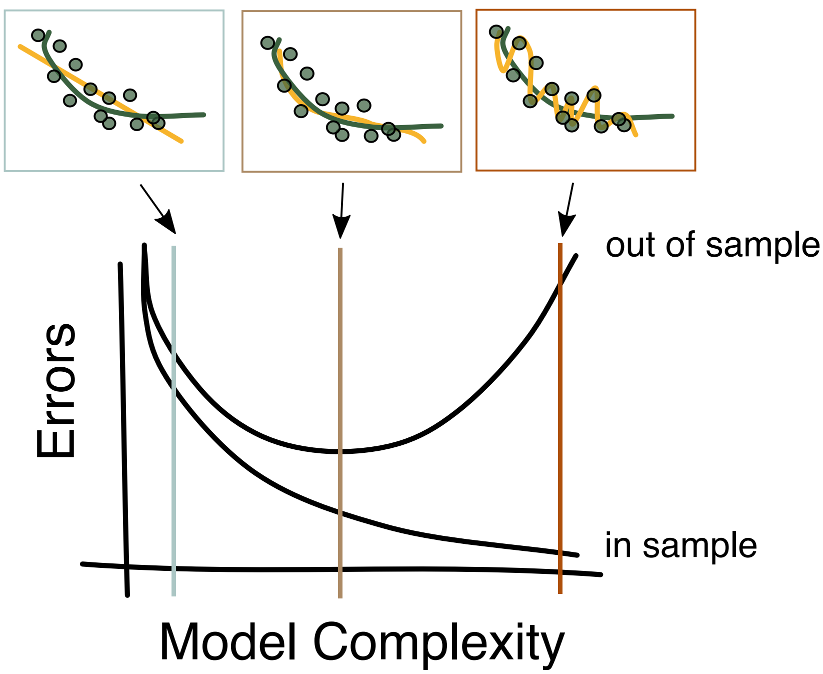
Model Complexity

Complexity Regimes

Even if you only evaluate the train / validation error for a model of a given complexity, you get useful information.

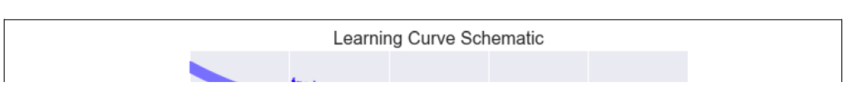
- Training $\ll$ validation error $\rightarrow$ Model is overfit
- Training $\approx$ validation error $\rightarrow$ Model is underfit (or OK)

Common heuristic: Overfit the data first, then regularize.



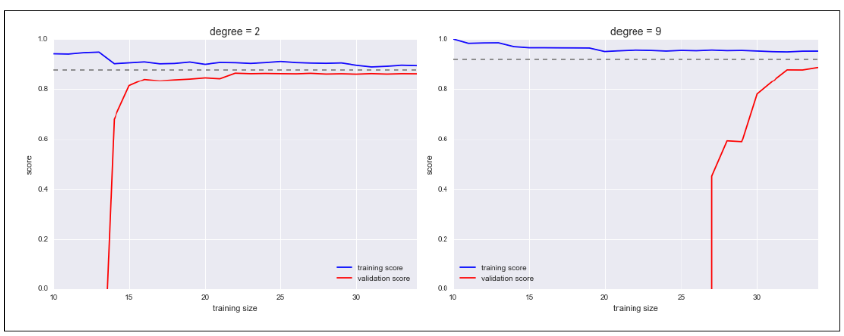
Learning Curves

- As you gather more data, how much better do your models get?
- This can guide the decision to collect more data.



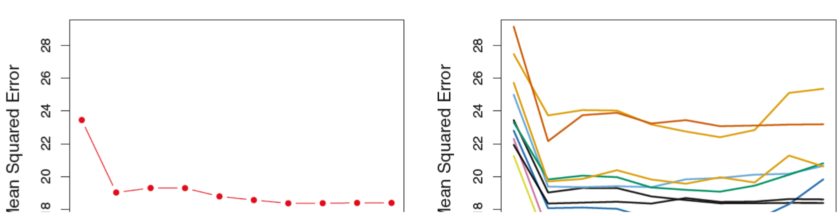
Learning Curves

- Models of different complexities have different learning curves
- Larger models don't saturate as quickly. They are,
  - worse than small models on small datasets
  - better than small models on large datasets



Evaluation and Randomness

- We are only *estimating* out-of-sample error
- These estimates might be good or bad
  - Have randomness from choice of validation set
  - Have randomness from dataset collection



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Degree of Polynomial

Degree of Polynomial

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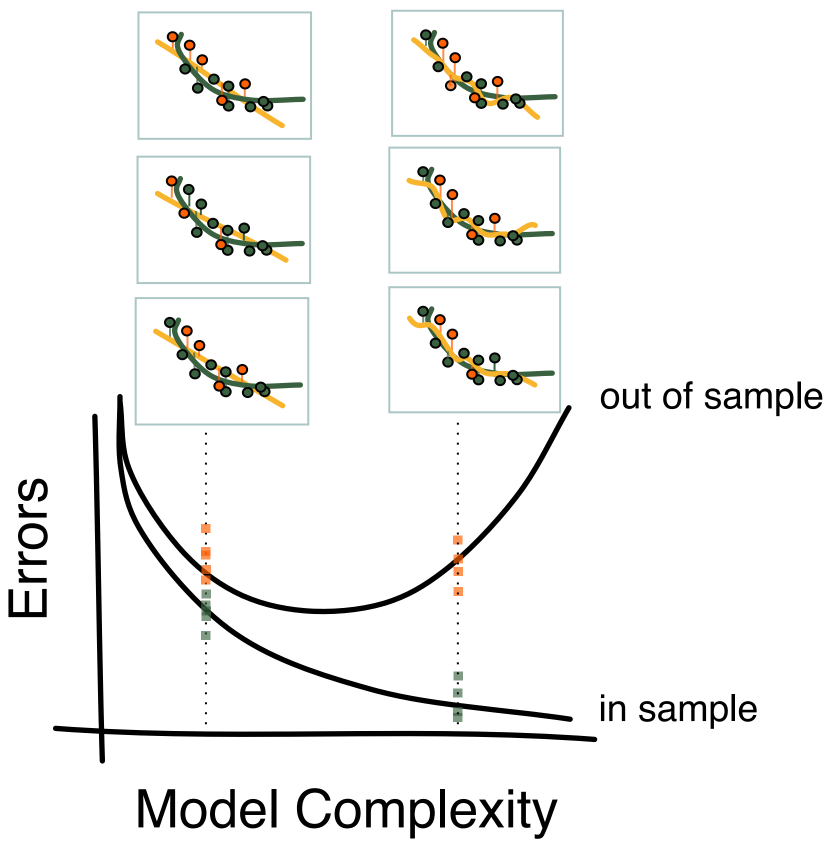


Bias and Variance in Validation Error

- Variance: Different validation sets give different estimates
- Bias: Training on subset leads to worse expected performance (remember learning curves)

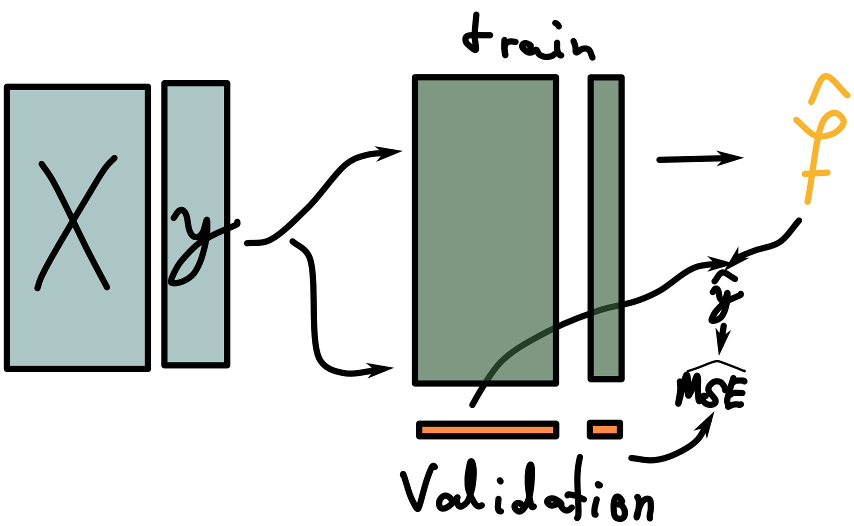
There are a few alternatives to validation sets. We'll talk about,

- Leave-One-Out Cross Validation [LOOCV]
- K-Fold Cross Validation.

Alternatives: LOOCV

1. Fit your model without sample (x_i, y_i). Call the fit $\hat{f}_{-i}$.
2. Compute holdout $\widehat{MSE}_i := \left(y_i - \hat{f}_{-i}\left(x_i\right)\right)^2$
3. Estimate the out-of-sample error by averaging this over all possible holdouts coming from (1) and (2),

$$\widehat{MSE} = \frac{1}{n}\sum_{i=1}^{n}\widehat{MSE}_i$$



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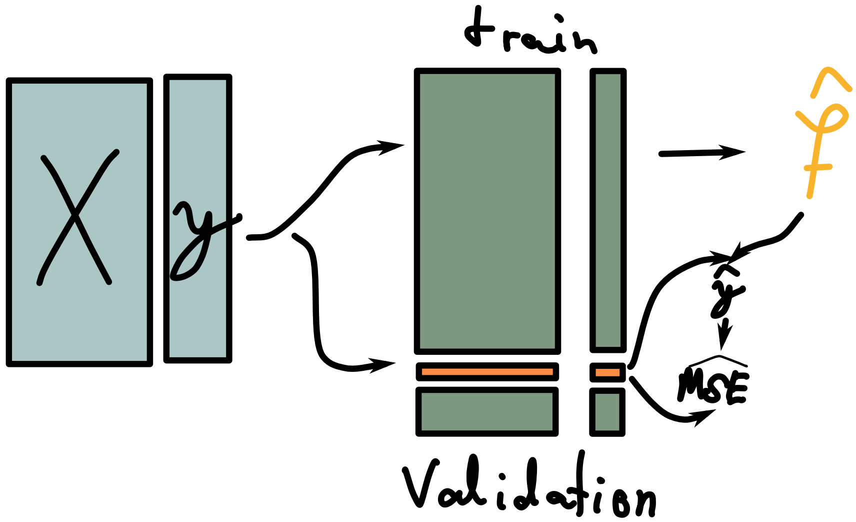
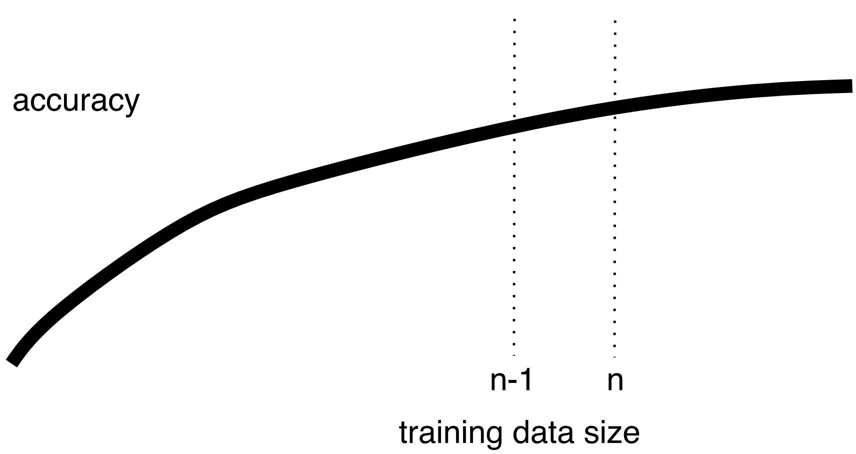


LOOCV

Advantages

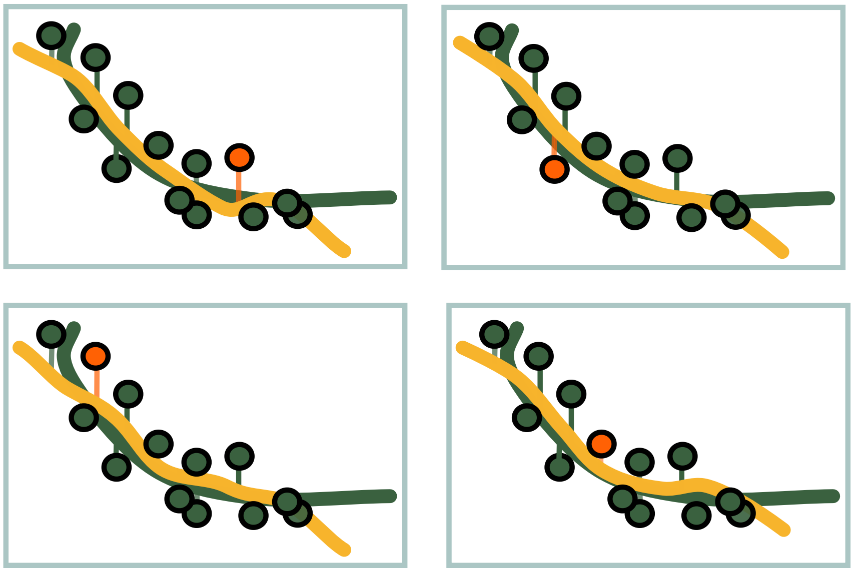
- Lower bias. We use almost all the training data, so we don't underestimate performance.



LOOCV

regression)

- The trained models are correlated
  - The $\widehat{MSE}_i$ are correlated
  - The average of correlated variables has larger variance than the average of independent ones
  - The out-of-sample estimate has higher variance

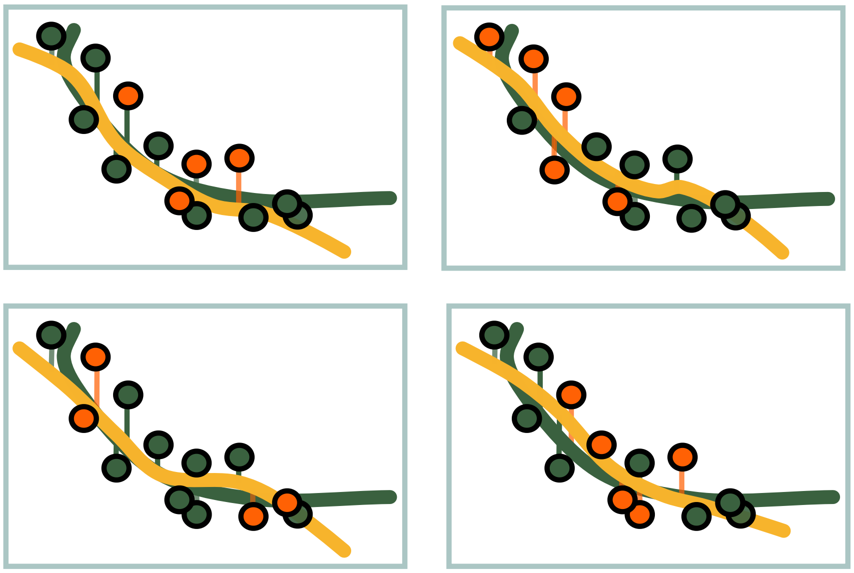


Alternatives: K-Fold CV

1. Randomly partition samples into one of K folds, $\{S_1, \ldots, S_K\}$.
2. Fit your model without fold S_k. Call the fit $\hat{f}_{-k}$.
3. Compute holdout $\widehat{MSE}_k := \sum_{i \in S_k} \left(y_i - \hat{f}_{-k}\left(x_i\right)\right)^2$
4. Estimate the out-of-sample error by averaging over folds,

$$\widehat{MSE} = \frac{1}{K} \sum_{k=1}^{K} \widehat{MSE}_k$$

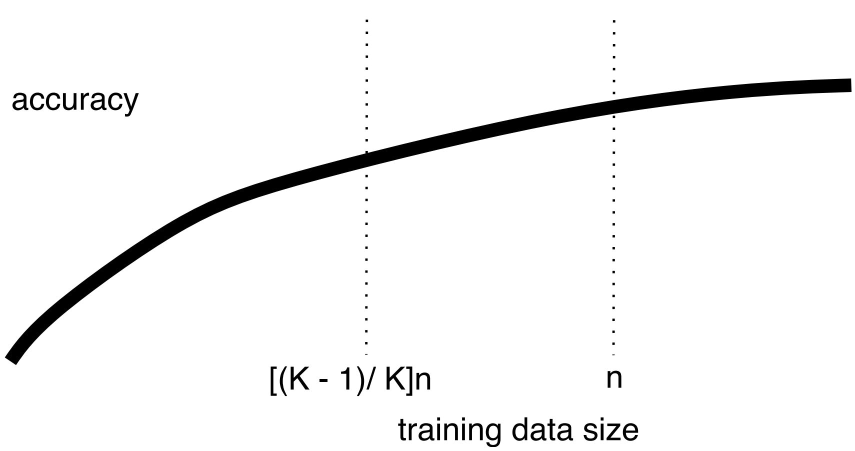
- More computationally tractable
- Learns less correlated models
  - The estimates $\widehat{MSE}_k$ are less correlated
  - The estimate $\widehat{MSE}$ has lower variance



K-Fold CV

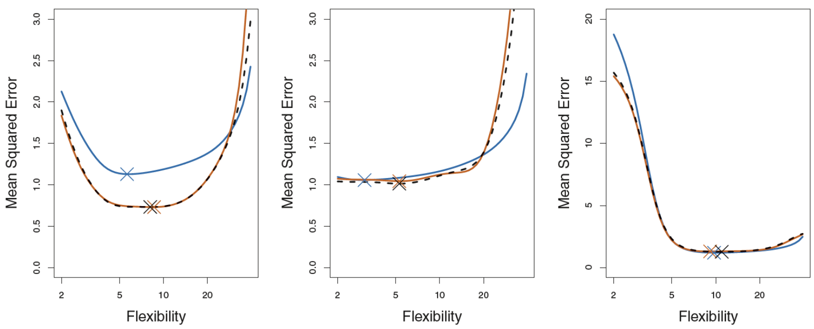
Disadvantages

- We don't train using the full training set
- We bias our estimates upwards
  - Model on full dataset is actually better than estimated



Estimation Quality: LOOCV and K-Fold

- The blue curves are known out-of-sample MSE's from a simulation experiment
- Black and orange are LOOCV and K-Fold estimates, respectively
- Note: Even when estimates of out-of-sample MSE is poor, the estimate of the minimum might be good



Hyperparameter Search

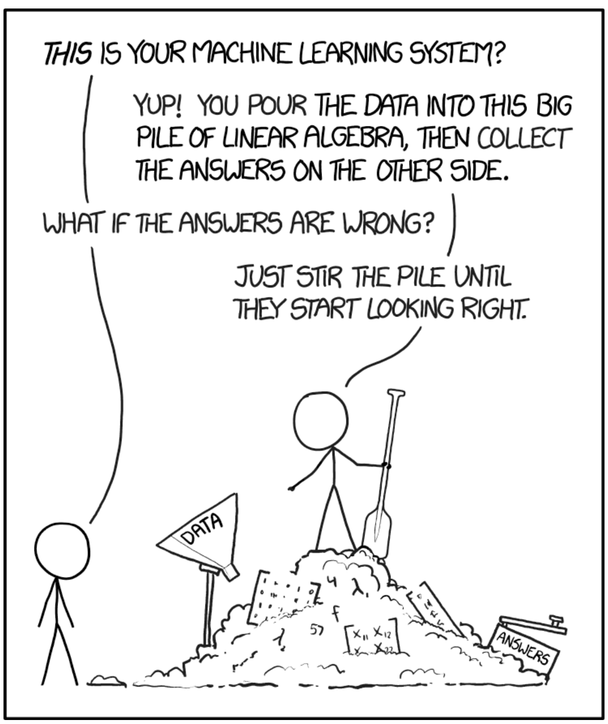
- We will often have many parameters to tune simultaneously
  - Model parameters: Polynomial degree, # trees, ...
  - Training parameters: Learning rate, subsampling, ...
  - Preprocessing: Normalization, outlier removal, ...
- No single "model complexity" parameter

Search Options

- Grid search
- Random search
- Combinations of these

Manual Search

- Relate all the parameters to overall model complexity
  - e.g., more iterations $\rightarrow$ higher complexity
- Guide your choice of parameters by which regime (over vs. underfitting) you are in
- Advantage: Uses bias-variance tradeoff information
- Disadvantage: Tedious, not fully reproducible



Grid Search

- Compute out-of-sample error on all combinations of

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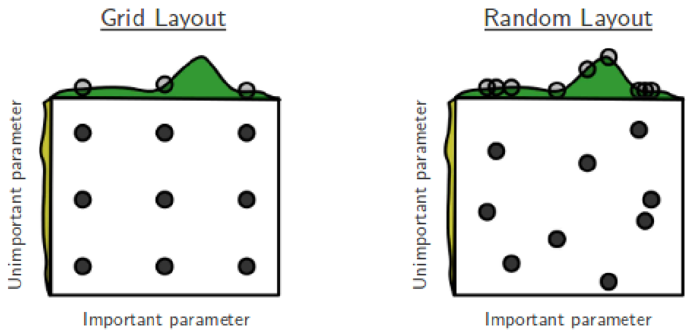
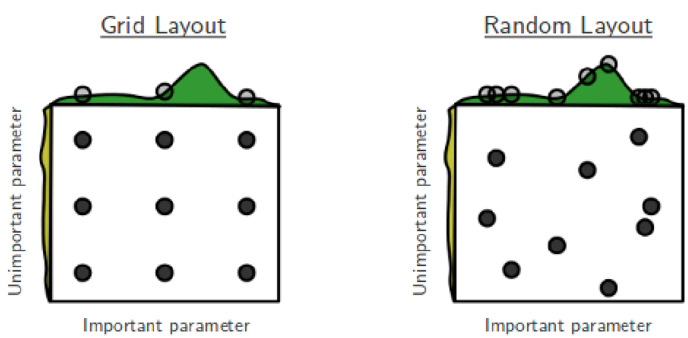
- Disadvantage: Exponentially many parameter configurations



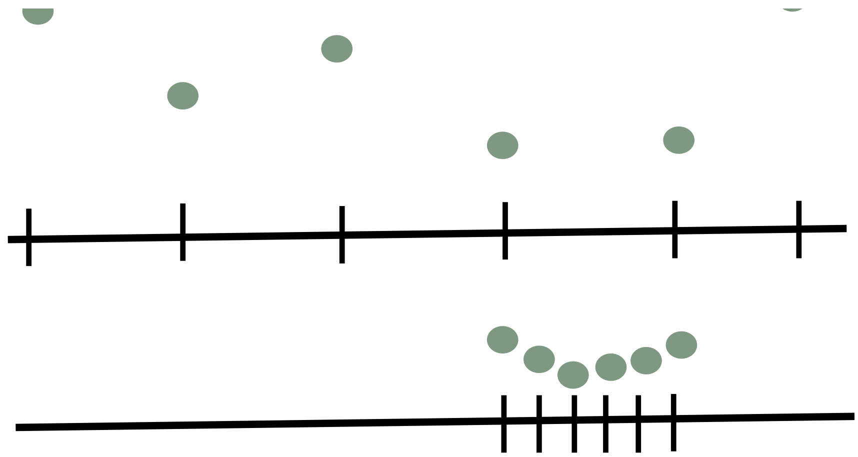
Random Search

- Compute out-of-sample error on random samples of parameters
- Advantage: Automatic, easy to implement. Relevant parameters become clear quickly.
- Disadvantage: Still suffers when very many parameters.



Combinations

- Can fix a few parameters manually, and use random search for others
- Can use "multiscale" search. Automatically search over predefined grids, but manually set the grids to more



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import {mtex} from "@krisrs1128/function-fitting"
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import {mtex_block} from "@krisrs1128/function-fitting"
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More from Observable creators

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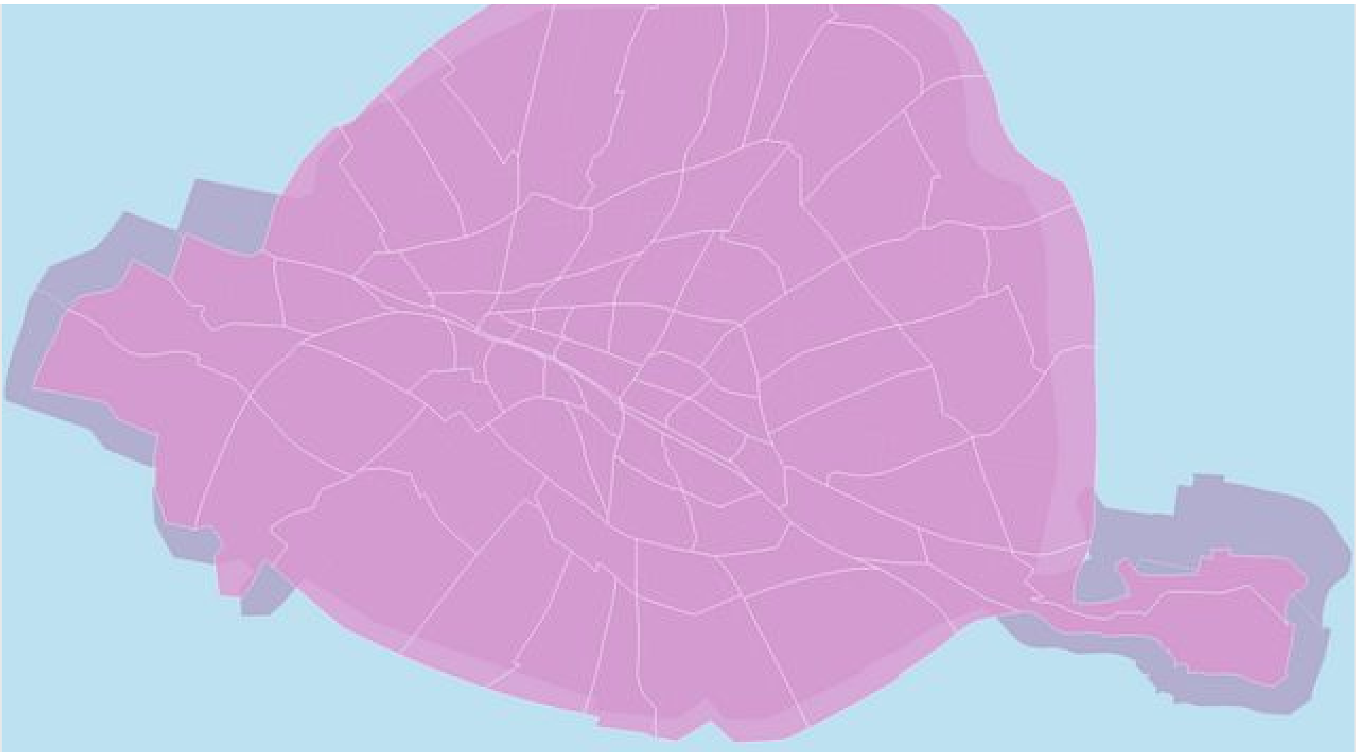

Flow-based cartograms (Gastner, Seguy & More, 2018) in the browser

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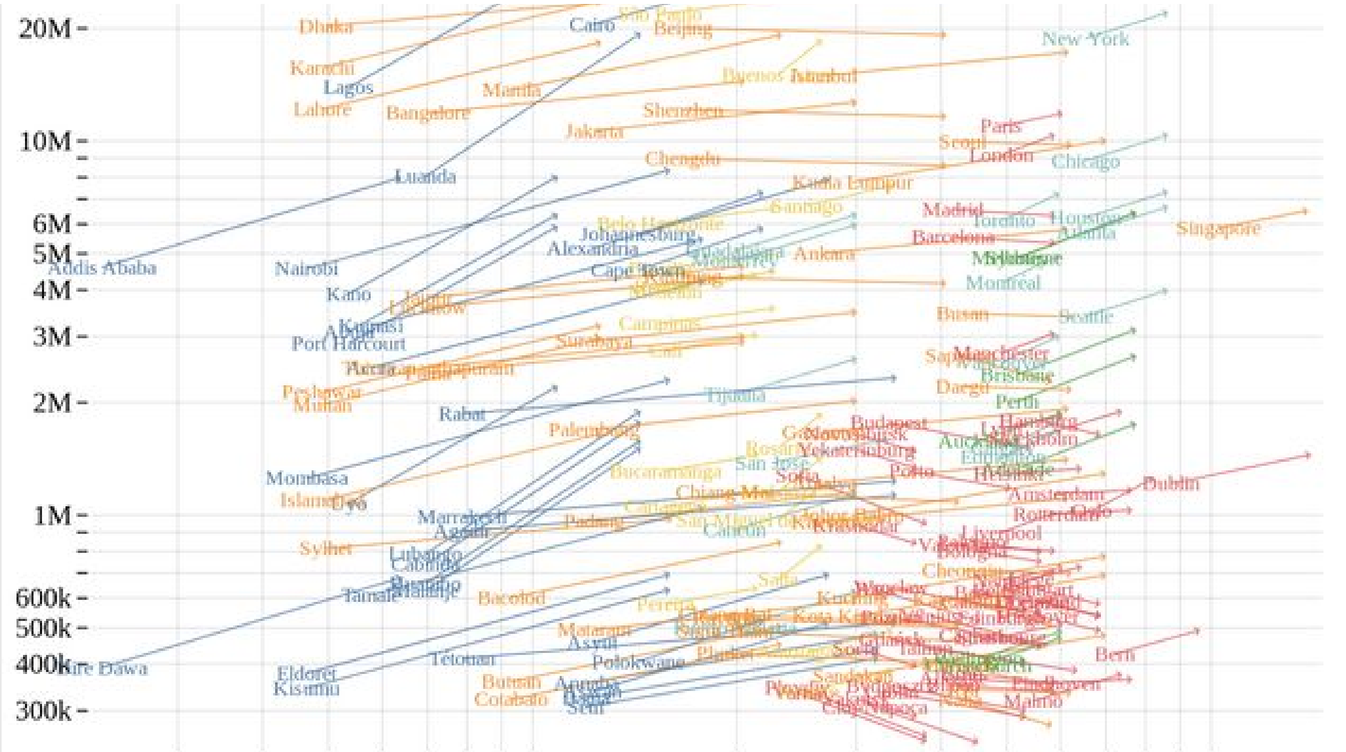

Plot Scatterplot

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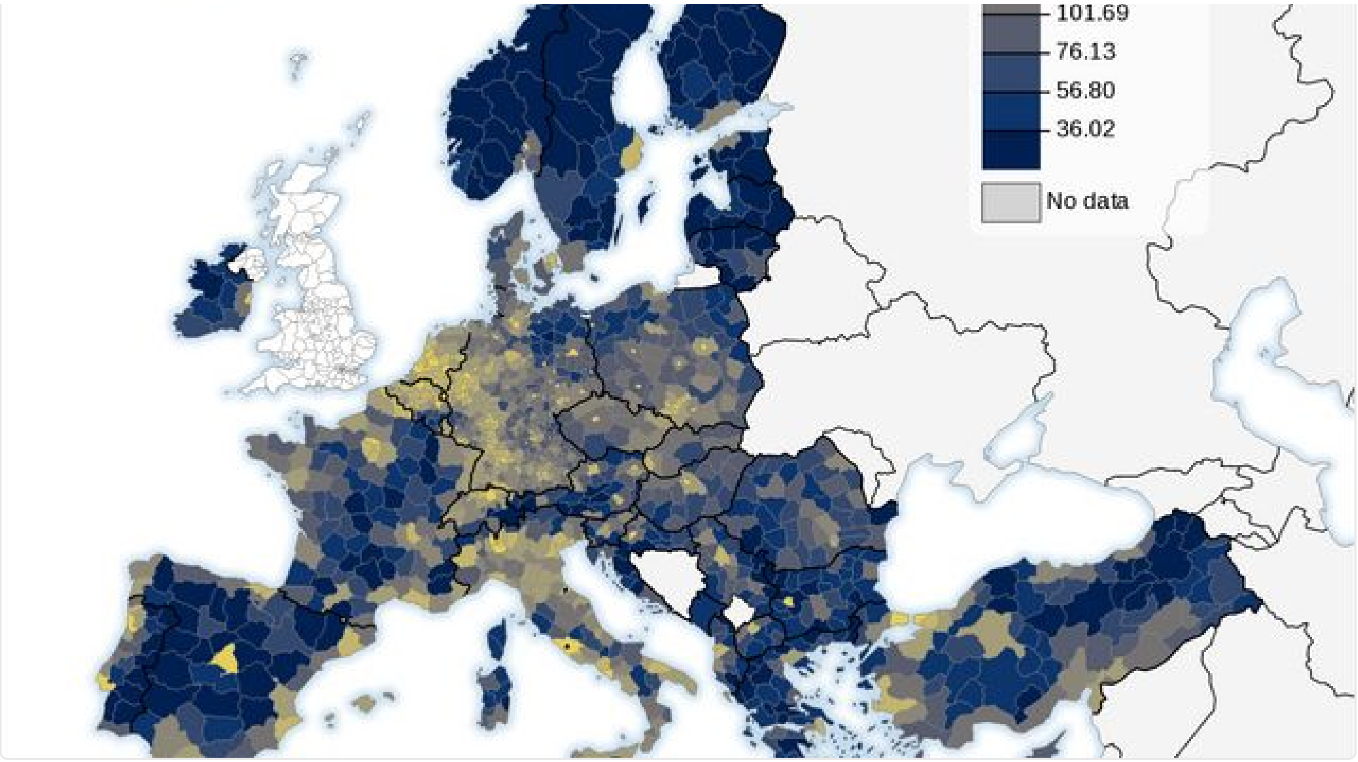

Colours for maps

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