Lecture 5: Evaluation

How do I choose among the various models?

e.g. choose k for kNN

e.g. choose design for OLS

We need some way to evaluate which model building process is going to perform better.

→ use OLS w/ 5 vars

→ use kNN w/ $k=5$

→ use kNN and optimize over possible values of k

A (maybe not always great) way of doing this!

Calculate some performance metric on $\hat{f}$ from the training data

e.g.

1. training residual sums of squares

$$RSS_{train} = \sum_{n=1}^{N} (y_n - \hat{y}_n)^2$$

2. training mean sq. error

$$MSE_{train} = \frac{RSS_{train}}{N}$$

3. traing root mean sq. err: $RMSE_{train} = \sqrt{MSE_{train}}$

④ training $R^2_{train} = 1 - \frac{RSS_{train}}{TSS_{train}}$

↑ % of var. explained by $\hat{f}$

$TSS_{train} = \sum_n (y_n - \bar{y})^2$

Why isn't a training metric always a good measure of performance?

→ I don't actually care about performance on my training data
(I already know the answer)

→ I actually care about is performance of $\hat{f}$ on new/unseen data.
(generalization performance)

ERM:

$$\underbrace{\frac{1}{N}\sum_{n=1}^{N} L(y_n, f(x_n))}_{\text{avg. loss over training data}} \approx \mathbb{E}[\underbrace{L(Y, f(X))}_{\text{actual loss}}]$$

Similarly:

$$\underbrace{\text{Metric}(\{y_n, f(x_n)\})}_{\text{training metric/perf.}} \approx \mathbb{E}[\underbrace{\text{Metric}(\{Y, f(X)\})}_{\text{generalization performance}}]$$

Focusing too much on training metric can be misleading.

This happens b/c when I evaluate $\hat{f}$ on my training data I am evaluating it on the same data used to build $\hat{f}$.

So my model building process has already seen the training data - its not a fair evaluation.

Analogy: Test 1: I give you 10 practice problems and a week from now I give exam w/ exactly those 10 problems.

eval. on training data →

Test 2: I give you 10 practice problem and a week from now I give exam w/ 10 related but not exactly the same questions.

generalization perf. →

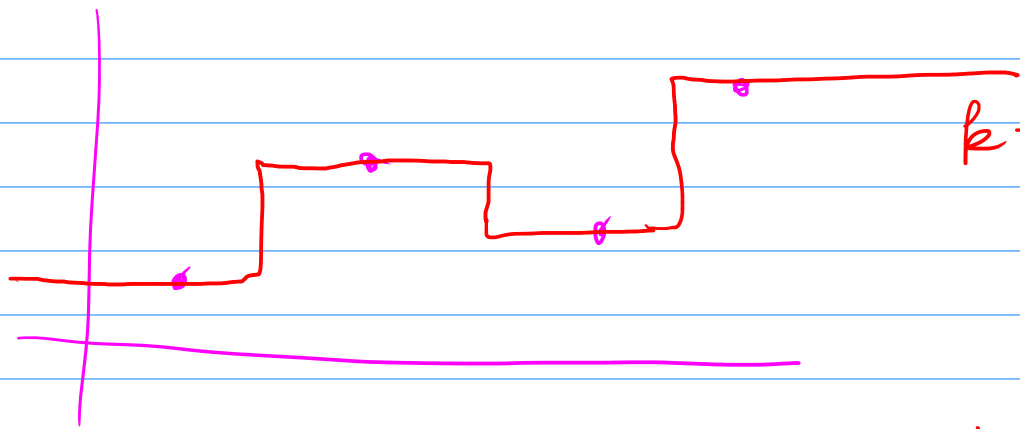
Ex. This can happen in SML too.

Consider optimizing the value of k for kNN by choosing the value of k that minimizes RSS_{train}.

What value of k do I choose?

$$k = 1$$

When $k=1$ I interpolate my training data



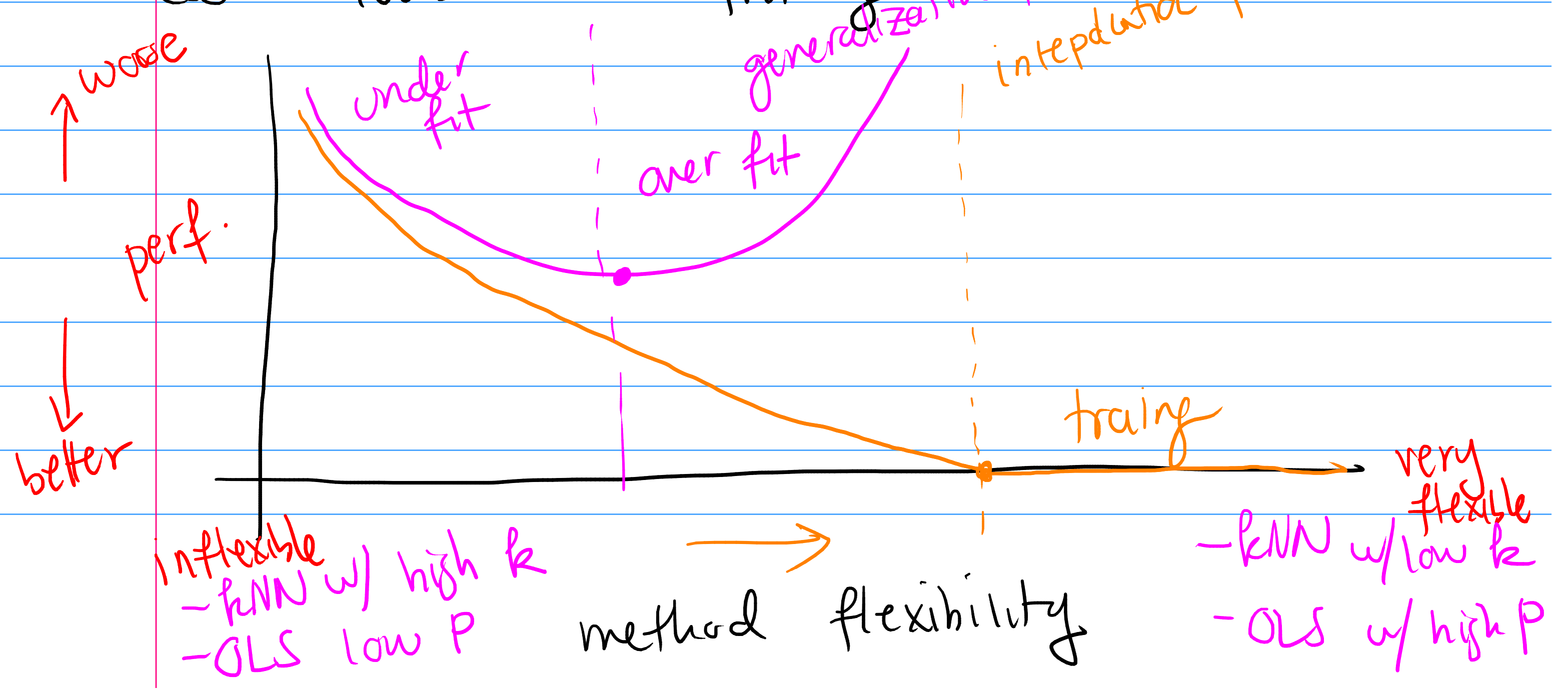
So $\hat{y}_n = y_n$ for training data $n=1,\dots,N$

hence $RSS_{train} = \sum_n (\underbrace{y_n - \hat{y}_n}_{0})^2 = 0$

A similar story is true for OLS when choosing what terms to include in the design.

as $p \to N$ I will interpolate my training data

We call this "over-fitting"



How do we solve this?

Let's estimate generalization perf.

Need independent set of (unseen) data to evaluate our model on.

Testing Data: $\{(x_{test,n}, y_{test,n})\}_{n=1}^{N_{test}}$

Procedure: (1) use training data to build $\hat{f}$

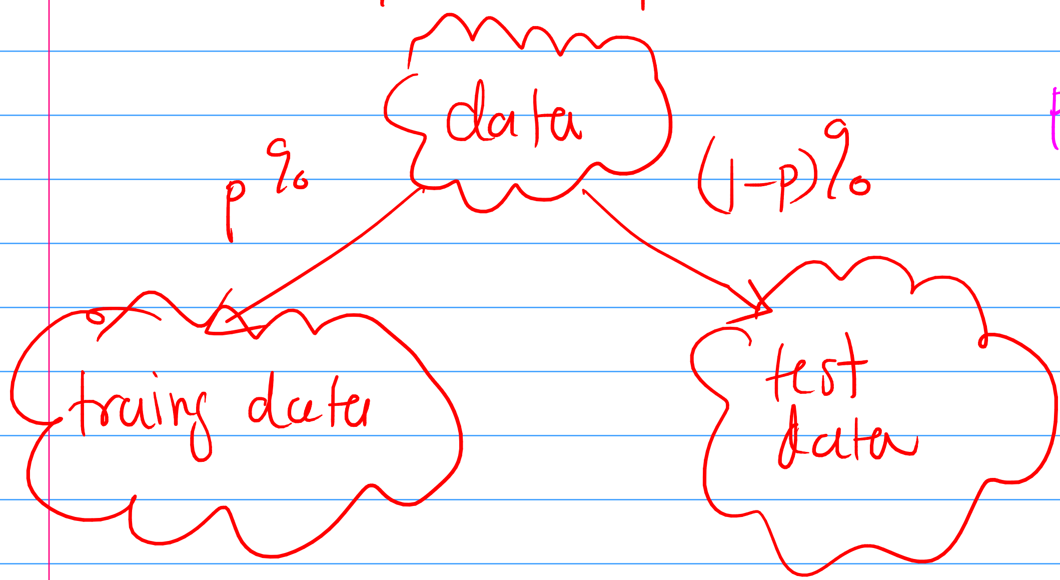
(2) eval. perf. of $\hat{f}$ on testing data

$\hookrightarrow$ an estimate of generalization perf. of my model building process.

RSS_{test}, MSE_{test}, $RMSE_{test}$, R^2_{test}

How do I get testing data?

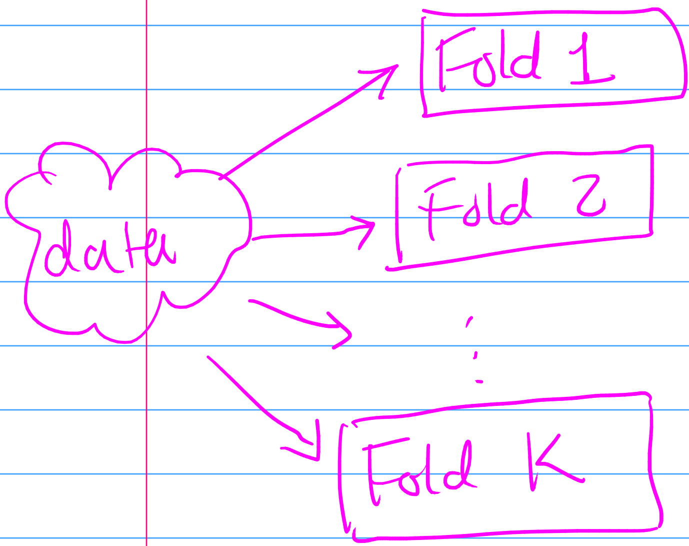
Do a test/train split.



p = 90, 80, 50

One can do this split multiple times which is called <u>cross-validation</u>

K-Fold Cross Validation



Cycle through folds

For $k = 1, \dots, K$

1. train model on all but fold k
2. test model on fold k

call this test metric m_k

So at the end of loop I have

$$m_1, m_2, \dots, m_K$$

can combine to get overall perf. metric

$$m = \text{median}(m_1, \dots, m_K)$$

But wait! If I train K different models which do I use?

None. I train a model using <u>all</u> of my data.

We want to evaluate performance generally for two reasons:

(1) I want to know how good this MBP might be

(2) I want to choose among various models.

We can use a test/train split or X-validation to choose among models - but we need to be very careful.
