Predictive Analytics Lecture 5

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Stat 422/722
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The Scourge of Modeling

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Previously the goal was to fit $f(x_1, \ldots, x_p)$ using $\boldsymbol{X}$ now we only have $\boldsymbol{X}_{obs}$ and $\boldsymbol{M}$.

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2. **Pattern Mixture** Models. The response is not independent of missingness. Same modeling context but here we have the age filled out by a computerized background check which scours public and FBI records. If age goes missing here... that means... the person may have some legal issues going on. It would make sense to fit two models: $f(x, m = 0)$ and $f(x, m = 1)$. Likely, $\hat{p}$ will be higher in the latter!

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By default, when producing a model, JMP will use listwise deletion (don't do this!!). I you are less lazy, you can generate a dummy columns, i.e. $\boldsymbol{m}$, and impute by using $\bar{x}$ (better than nothing). Even better is to create a model to do the imputation by treating the x as the response (meta dude!) and the other $x's$ as the predictors. There are other ideas beyond the scope of the course!

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Let's take missing the age field as an example to explore these three conceptually.

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Also... obvious but must mention it... listwise deletion is not an option for the $\boldsymbol{x}^*$'s! You cannot say, "sorry I don't want to predict for this observation"!! You need to impute — it's your job!

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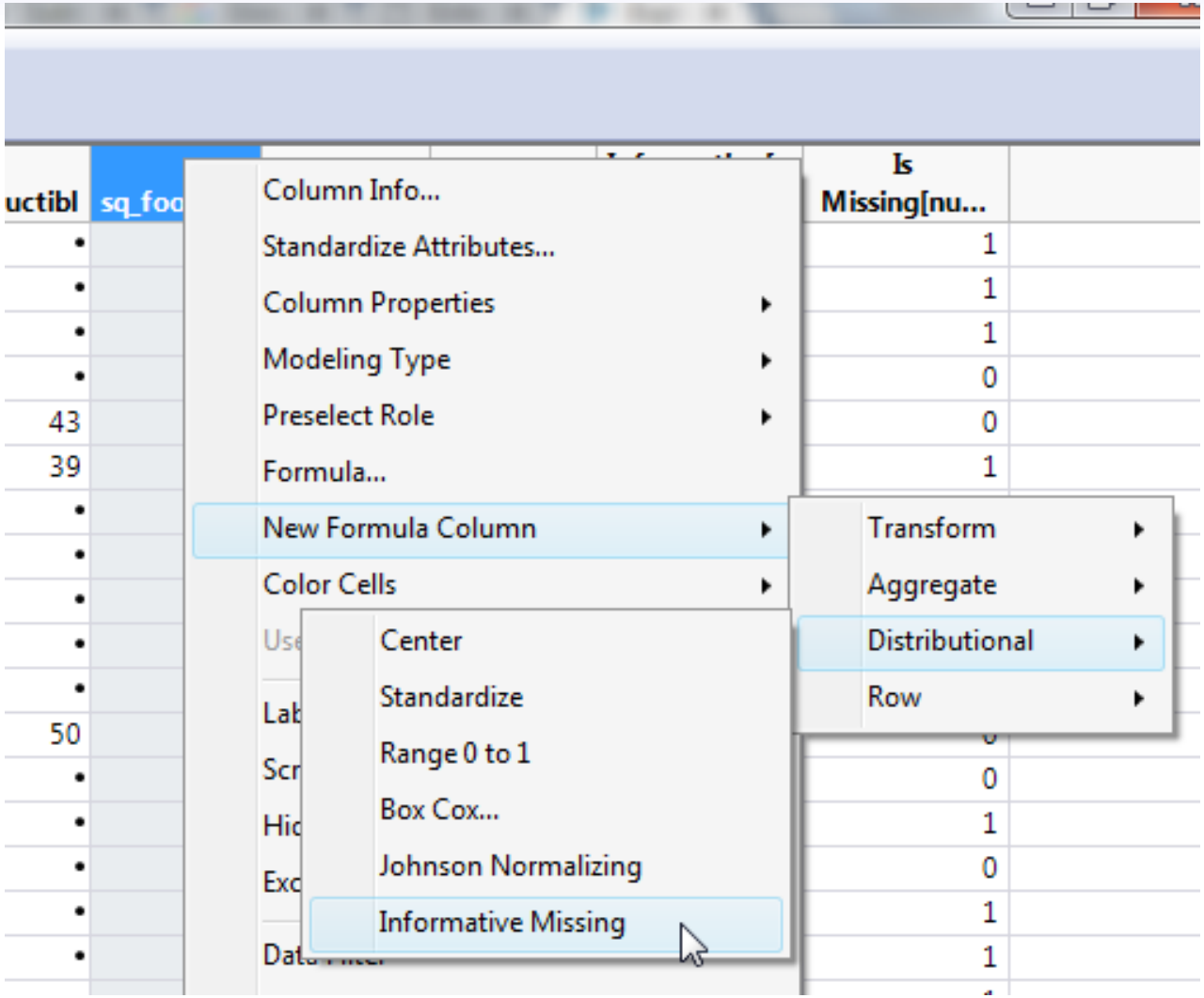
- Attempt to reason through missingness for each measurement separately.
- If MCAR, use $\bar{x}$ to impute holes; if MAR / NMAR, use a prediction model to impute holes (if you are supremely lazy, use $\bar{x}$).
- Delete observations that have missingness at your peril!!

How to create m and impute $\bar{x}$ in JMP



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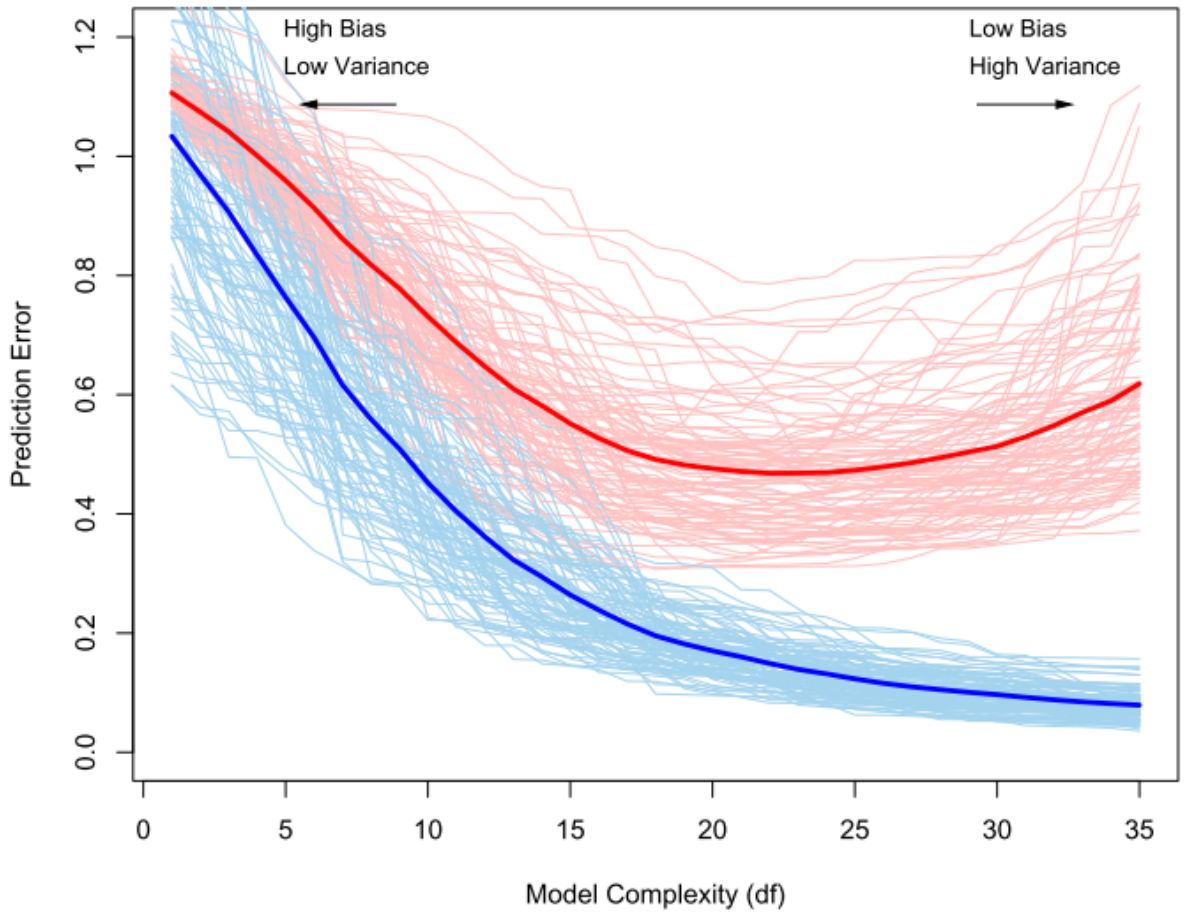
- We fall **short** by underfitting (usually due to too little degrees of freedom and inflexible bases). For example: if the f is a curve and we fit a line, we underfit (recall medicorp sales vs bonus regression).
- We can shoot too **long** by encroaching on and fitting / optimizing to the $\mathcal{E}$. Since $\mathcal{E}$ is independent of $x_1, \ldots, x_p$, this part of $\hat{f}$ is essentially a random fit and it is the opposite of the "data-driven approach".

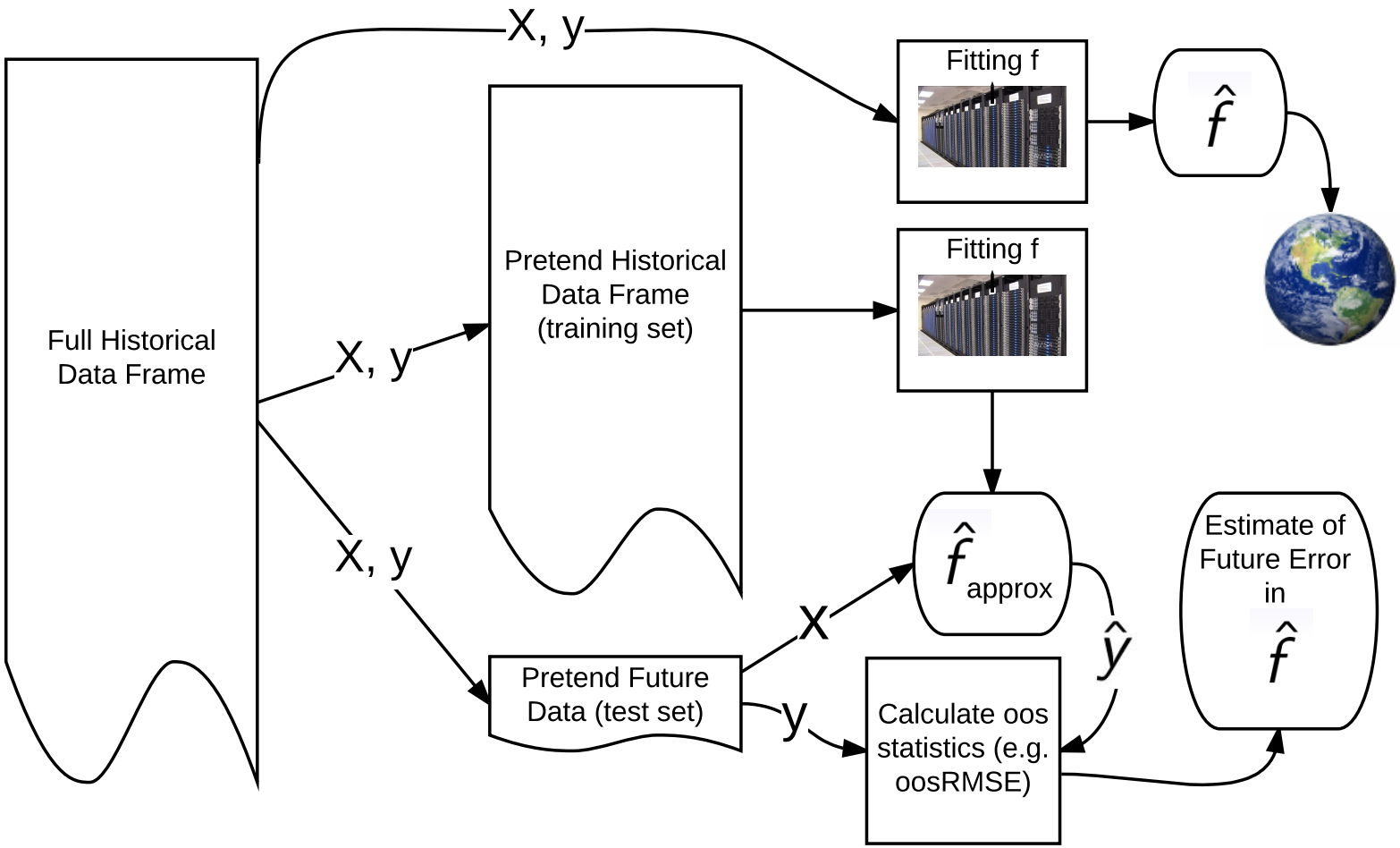
Complexity-Fit Tradeoff



Blue is in-sample fit metric and red is oos fit metric. This is Fig 7.1 from Hastie and Tibsharani (2009).

Assessment: OOS Validation

But knowing where you are on that y-axis would involve knowing the truth. We need to estimate this, so we use oos validation:



Assumptions and Tradeoffs when Splitting

We have a choice to split our dataframe into two pieces. Assuming each data point is independent (the running assumption), you should do this completely randomly. When would this assumption not be true?

Assumptions and Tradeoffs when Splitting

We have a choice to split our dataframe into two pieces. Assuming each data point is independent (the running assumption), you should do this completely randomly. When would this assumption not be true? For example, a time series.

Additionally, we need to assume a non-stationary model relationship. So,

$$Y = f(x_1, \ldots, x_p) + \mathcal{E} \quad \text{and not} \quad Y = f_t(x_1, \ldots, x_p) + \mathcal{E}$$

where f changes with time. In essence non-stationarity is a lack of generalization and when predicting, it is a form of extrapolation.

How large should the test set be? Usual sizes are 10-30%. What's the tradeoff? If the test set is larger, then ...

1. the more accurate the assessment of generalization error would be (less variance) and
2. the less accurate the model will be since it's fitting with less data (more bias)

If the test set is smaller then, vice versa. Note: the in-sample and oos statistics are statistics! Thus, they are random!

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If we change the observations in the training/test splits, we will get different models and different estimates of future error.

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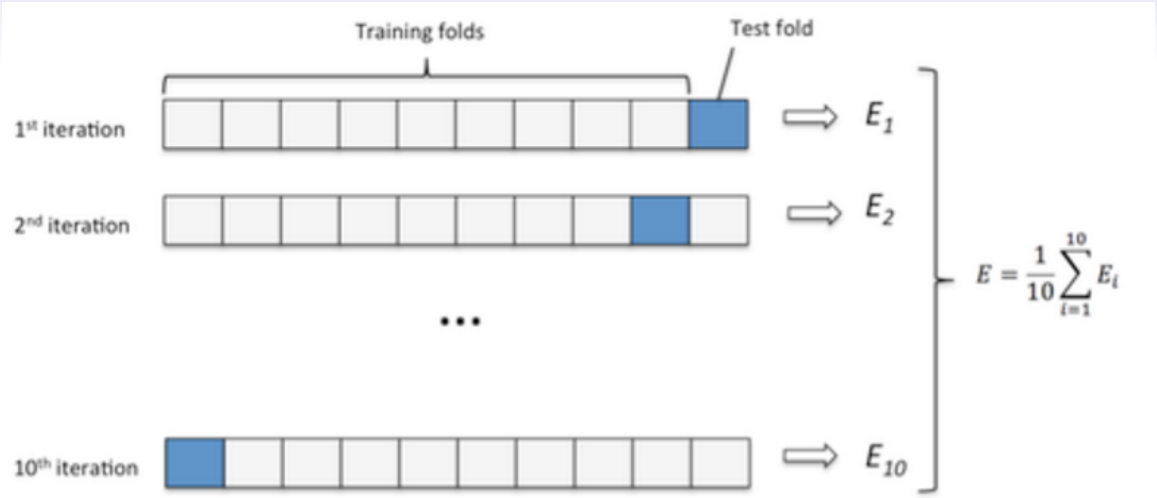
10-fold CV


Training folds
Test fold
1st iteration
2nd iteration
10th iteration
E_1
E_2
E_{10}
$E = \frac{1}{10}\sum_{i=1}^{10} E_i$

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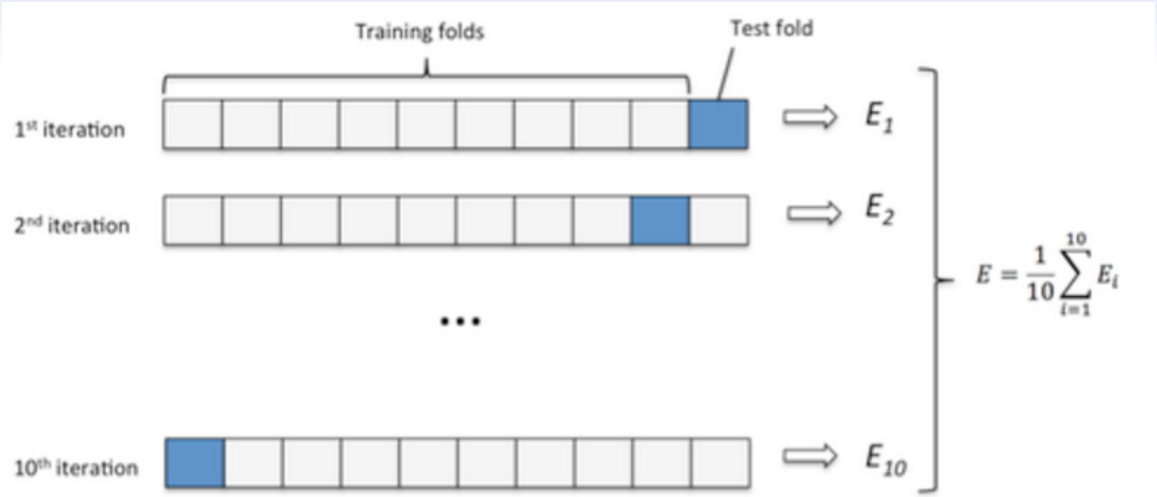

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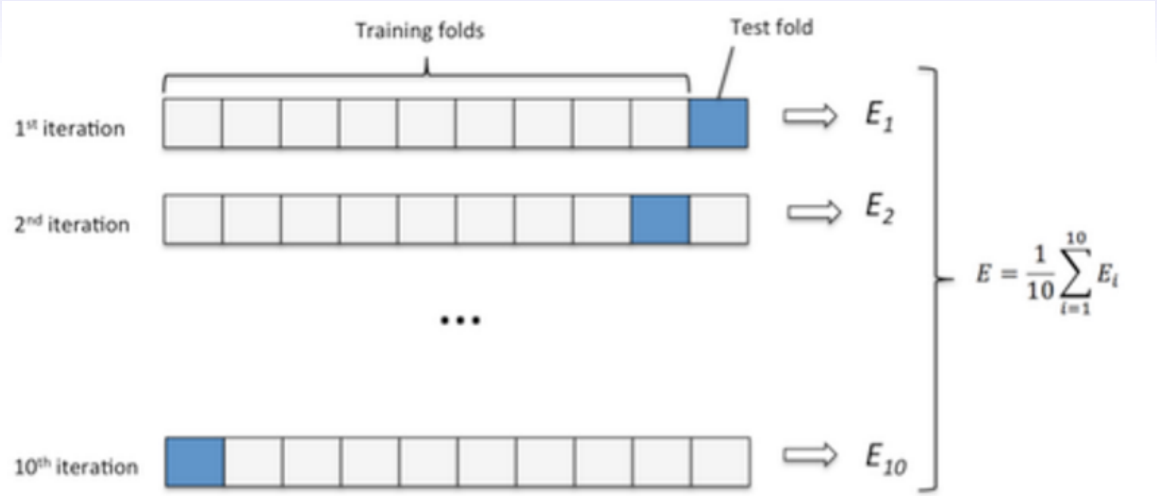

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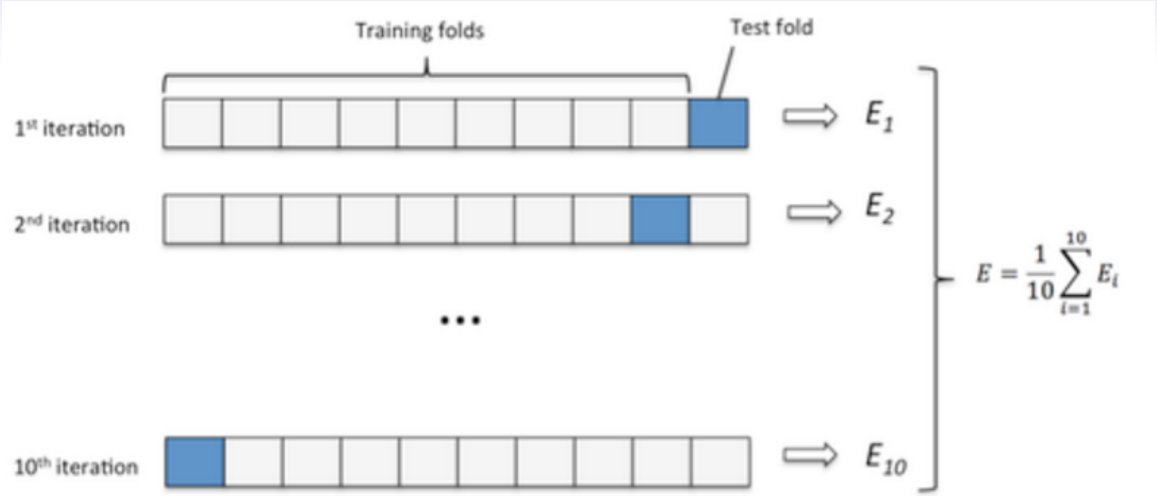

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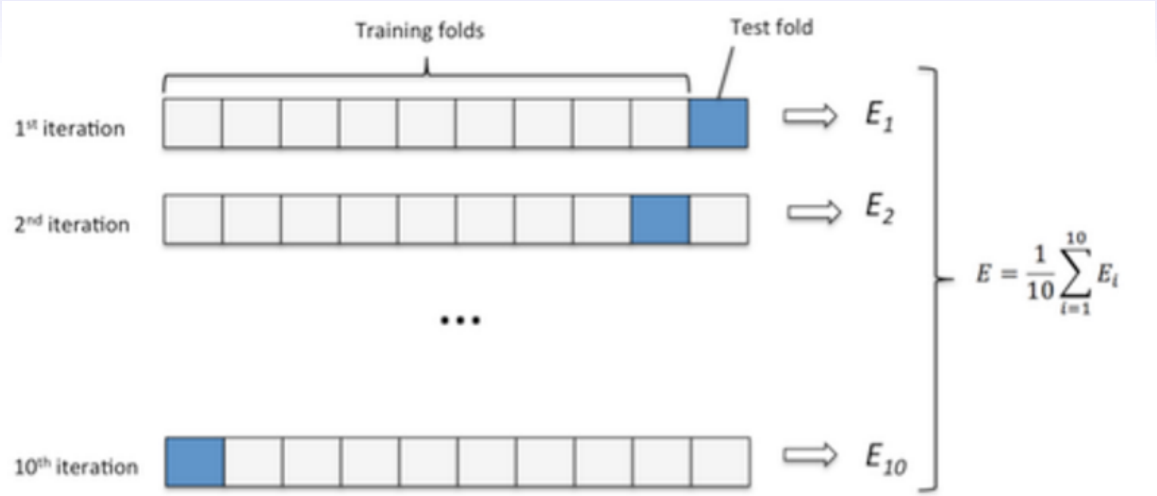

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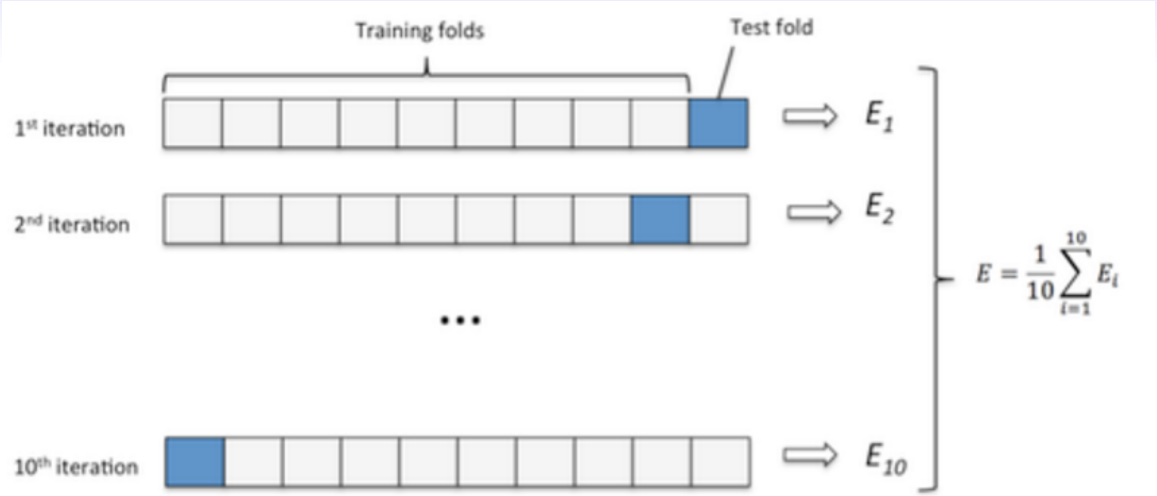

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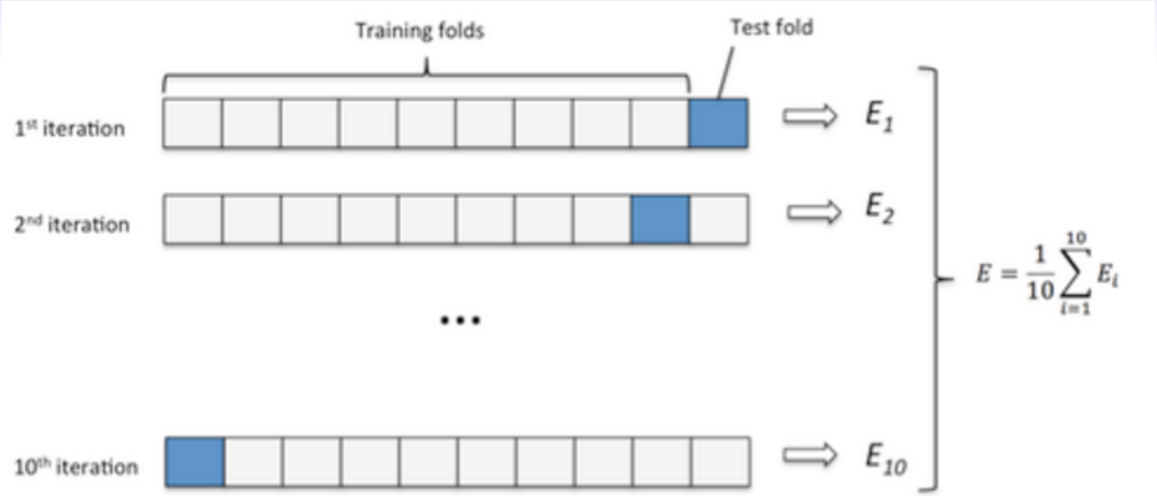

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Note 1: If $K = n$ then we the test set as one sample; this is known as "leave on out CV" (LOOCV) and it not recommended — high variance and computational cost! Note 2: bleeding edge of stats — find CI's for generalization error. Note 3: this is not the only way to reduce the variance in oos statistics but it's the one we will use in this class.

What does K-fold CV estimate?

Remember... there will be different models built on each training set. So ...

- without K-fold CV, you are estimating the generalization of a model defined as the functional form and specific parameter estimates (the model and the fit).

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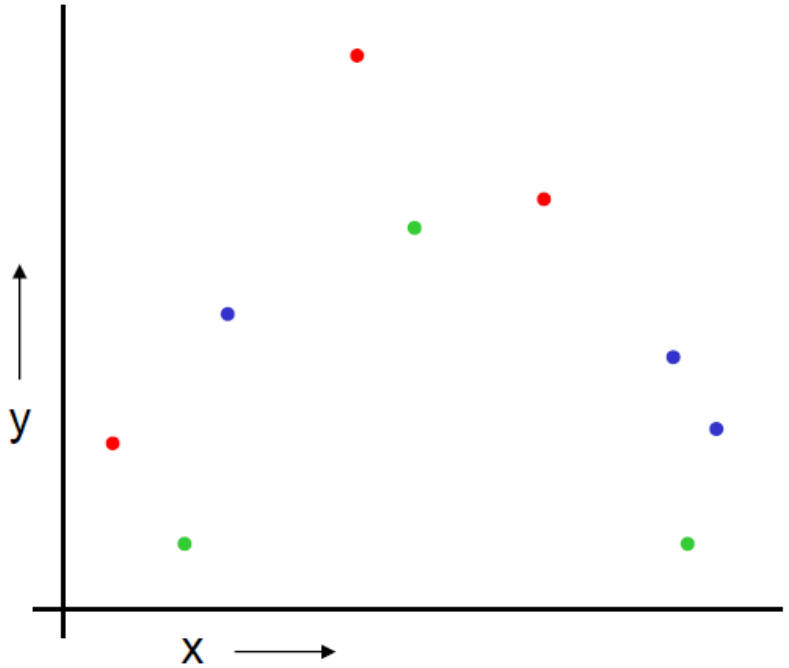
- with K-fold CV, you are estimating the generalization of a model defined as just the functional form (the model).

I guess it depends on how you define "model". Usually, it's the latter... this is frequently ill-defined. This is a subtle point... and I won't be testing you on it!

$K = 3$-fold CV on a Linear Model Ex. 1/5

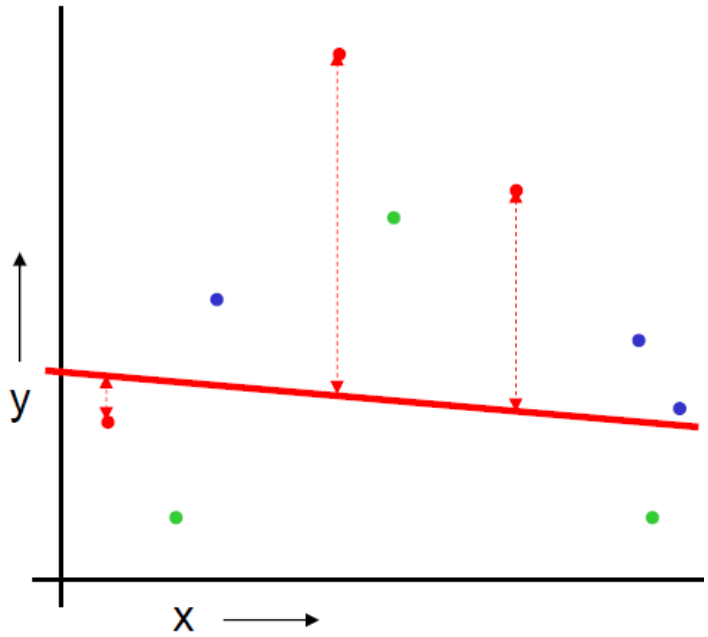
Imagine the following data $n = 9$ where we are fitting a response by one feature (ignore the colors):



Imagine we choose a linear model.

$K = 3$-fold CV on a Linear Model Ex. 2/5

In the first fold, the red is left out and thus we fit a line to the blue and green points:

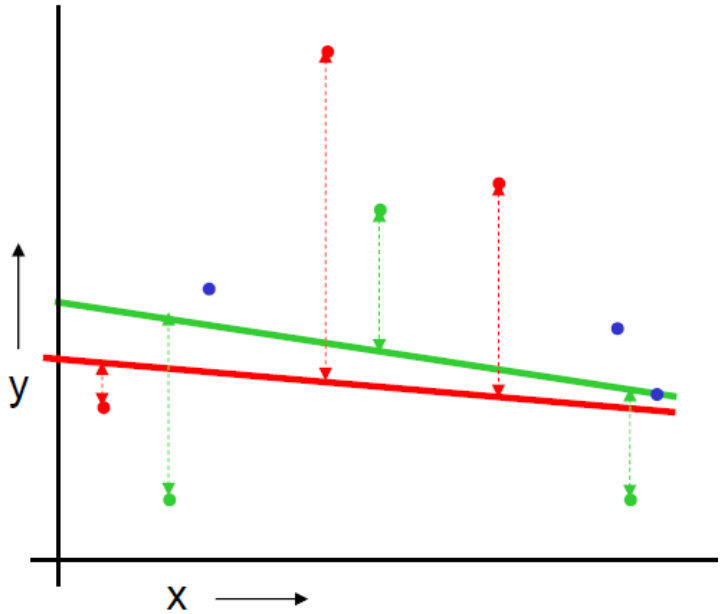


Then we calculate the residuals to the red points (the test set in this fold) and calculate

$$SSE = (2 - 2.2)^2 + (3.8 - 2.1)^2 + (3.5 - 2.05)^2 = 5.03$$

$K = 3$-fold CV on a Linear Model Ex. 3/5

In the second fold, the green is left out and thus we fit a line to the blue and red points:

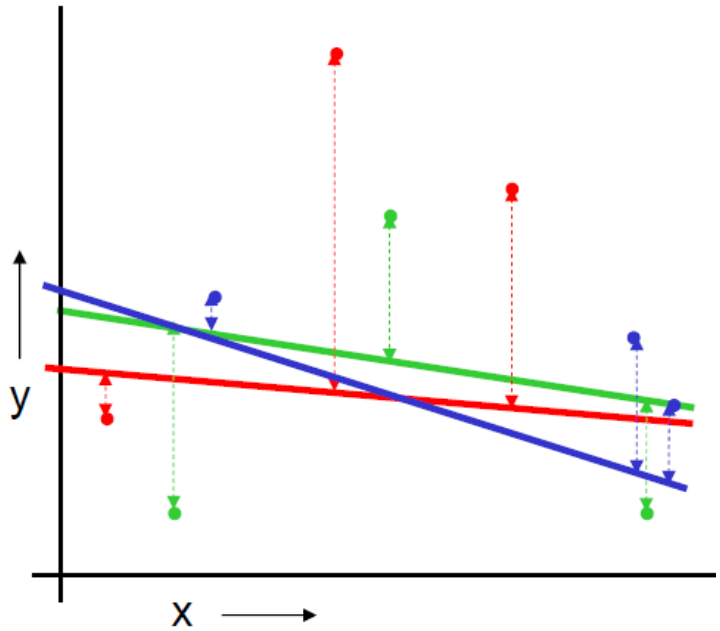


Then we calculate the residuals to the red points (the test set in this fold) and calculate

$$SSE = (1.2 - 2.3)^2 + (3.4 - 2.25)^2 + (1.3 - 2.2)^2 = 3.34$$

$K = 3$-fold CV on a Linear Model Ex. 4/5

In the third (last) fold, the blue is left out and thus we fit a line to the green and red points:



Then we calculate the residuals to the red points (the test set in this fold) and calculate

$$SSE = (2.35 - 2.3)^2 + (2.4 - 1.5)^2 + (2.2 - 1.4)^2 = 1.45$$

$K = 3$-fold CV on a Linear Model Ex. 1/5

Then we aggregate all oos results together (SSE's are additive) and we can compute a final oos statistics e.g. the oosRMSE:

$$oosRMSE = \sqrt{\frac{5.03 + 3.34 + 1.45}{9}} = 1.045$$

Limits of JMP / Intro to R's MLR Package

And...

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And... JMP can't do K-fold CV! (Except in one limited case which doesn't help us right now). But of course R can do it... [R Demo with MLR]

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Let's look at a few models for the White Wine data with no validation (but no cross-validation). Here the response is wine quality as measured by professional raters and features are 11 features (e.g. acidity, sugar, pH and alcohol content).

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A Possible Spin on Validation

Recall the proposal from last class:

1. Split dataframe into training and test.
2. Build model A on training.
3. Predict using the test set.
4. Calculate estimate of future generalization error of model 1.
5. Build a different model B on training.
6. Predict using the test set.
7. Calculate estimate of future generalization error of model 2.
8. ... steps 5-7 for model 3
9. ... steps 5-7 for model 4
10. ...
11. ... steps 5-7 for model M
12. Pick whichever model has better generalization error.

This is a form of **Model Selection**. What was wrong with it?

Looking into the Future is Not Legal

The oos validation is only valid if...

you treat the test set as a lockbox. Once you open it up, that's it! And we opened it up M times!

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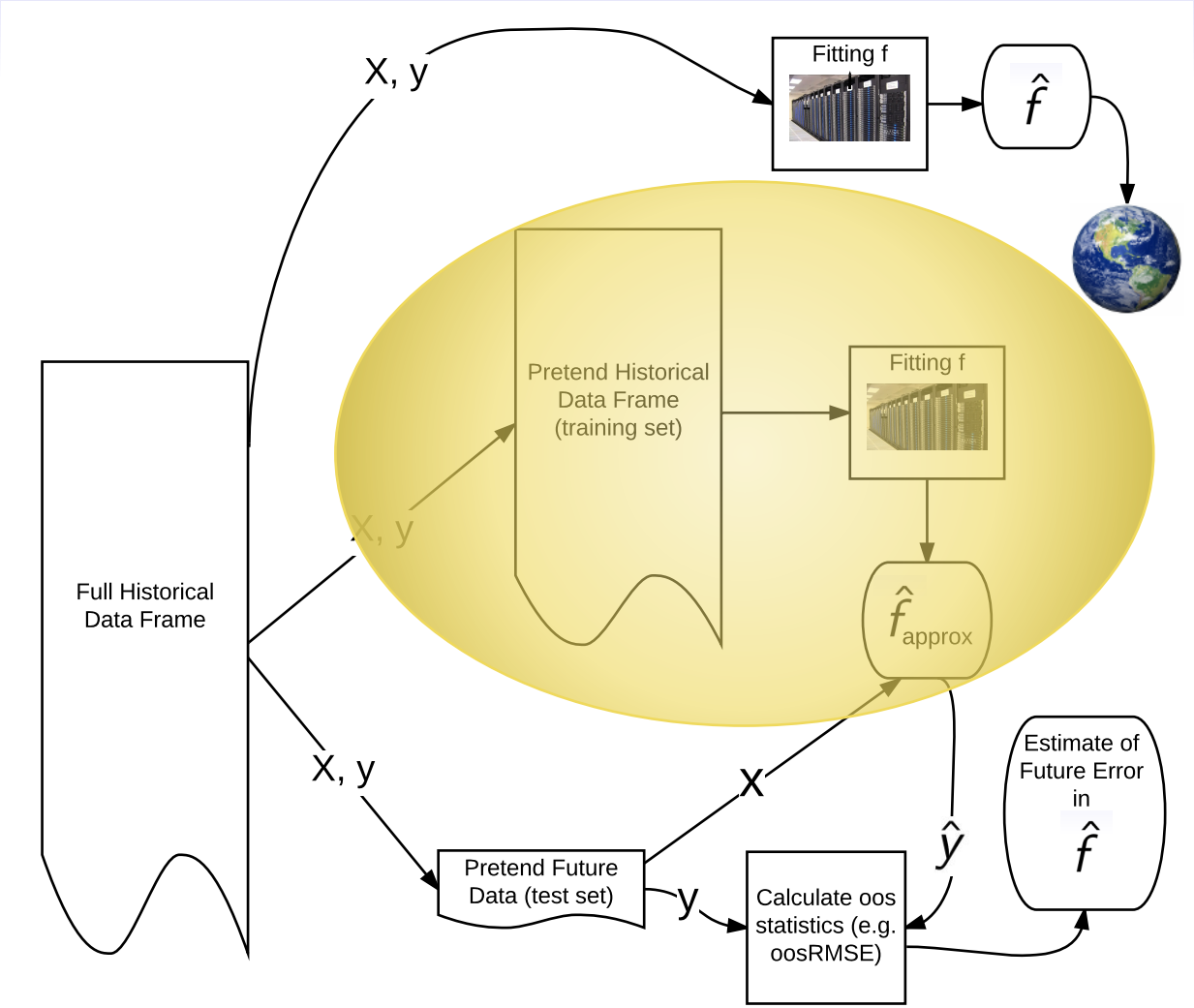
This is indeed a **Model Selection** procedure but ... our estimate of future generalization error is invalid. How can we do both?

In One Fold Let's Focus on the Training Set



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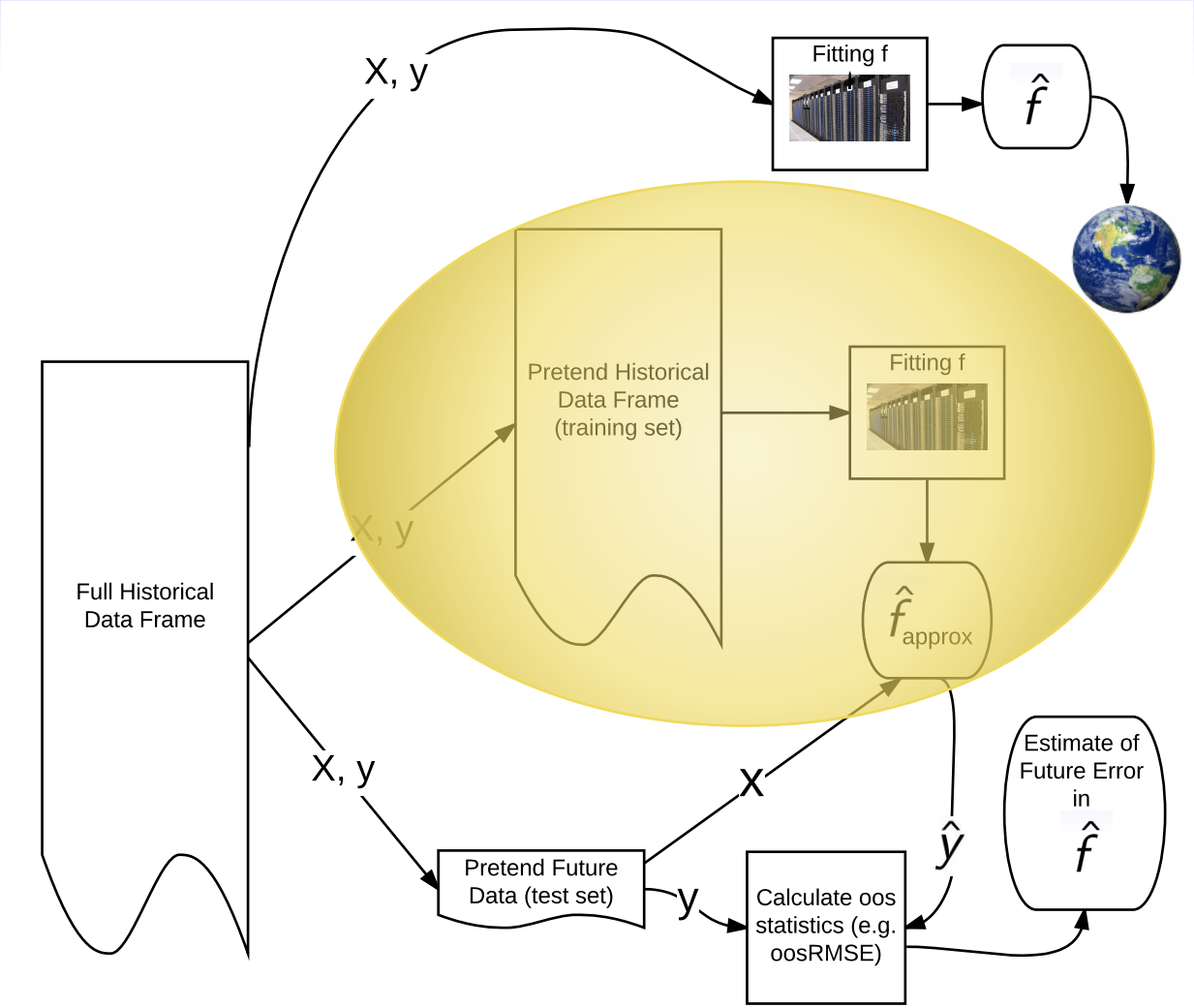

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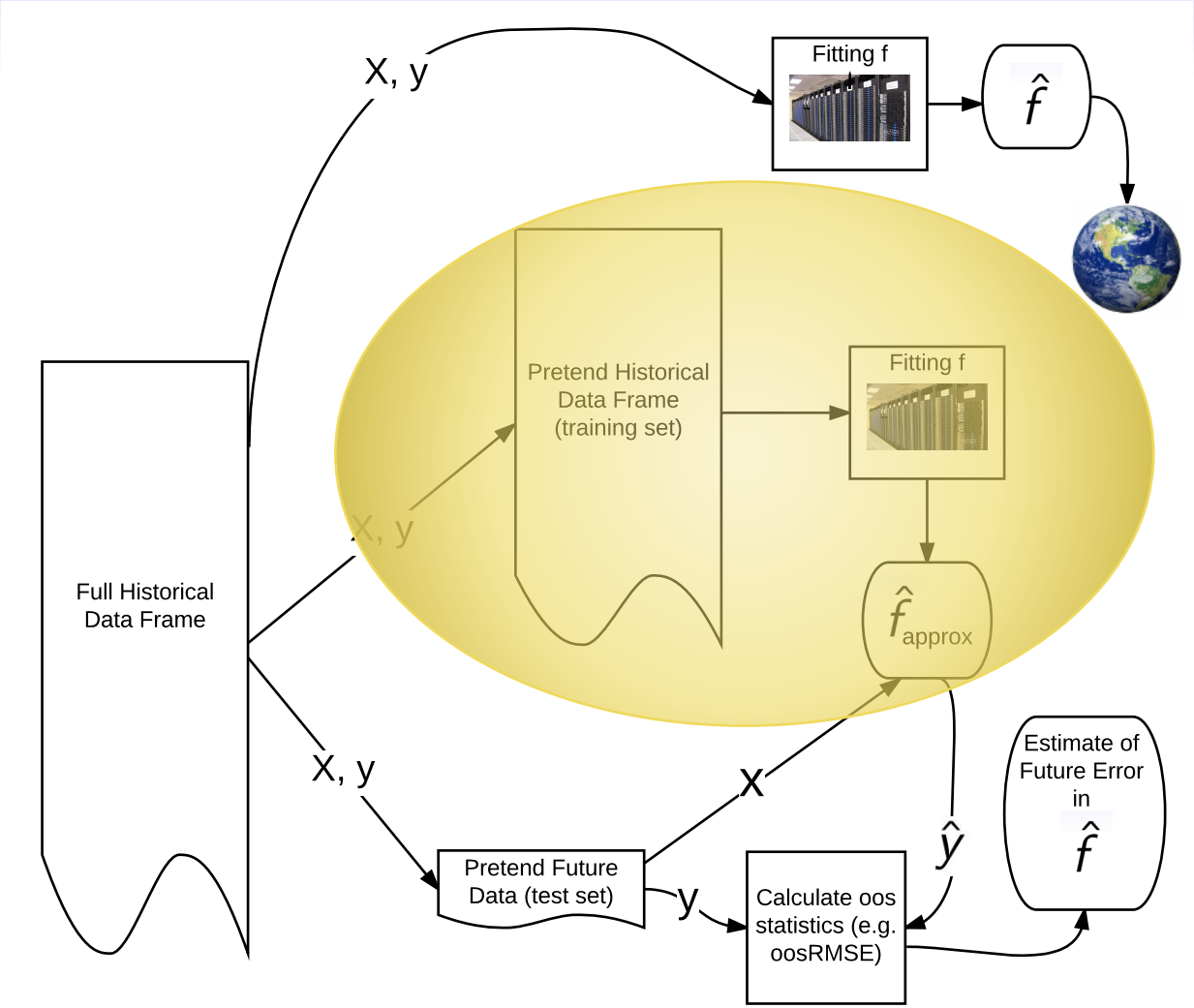
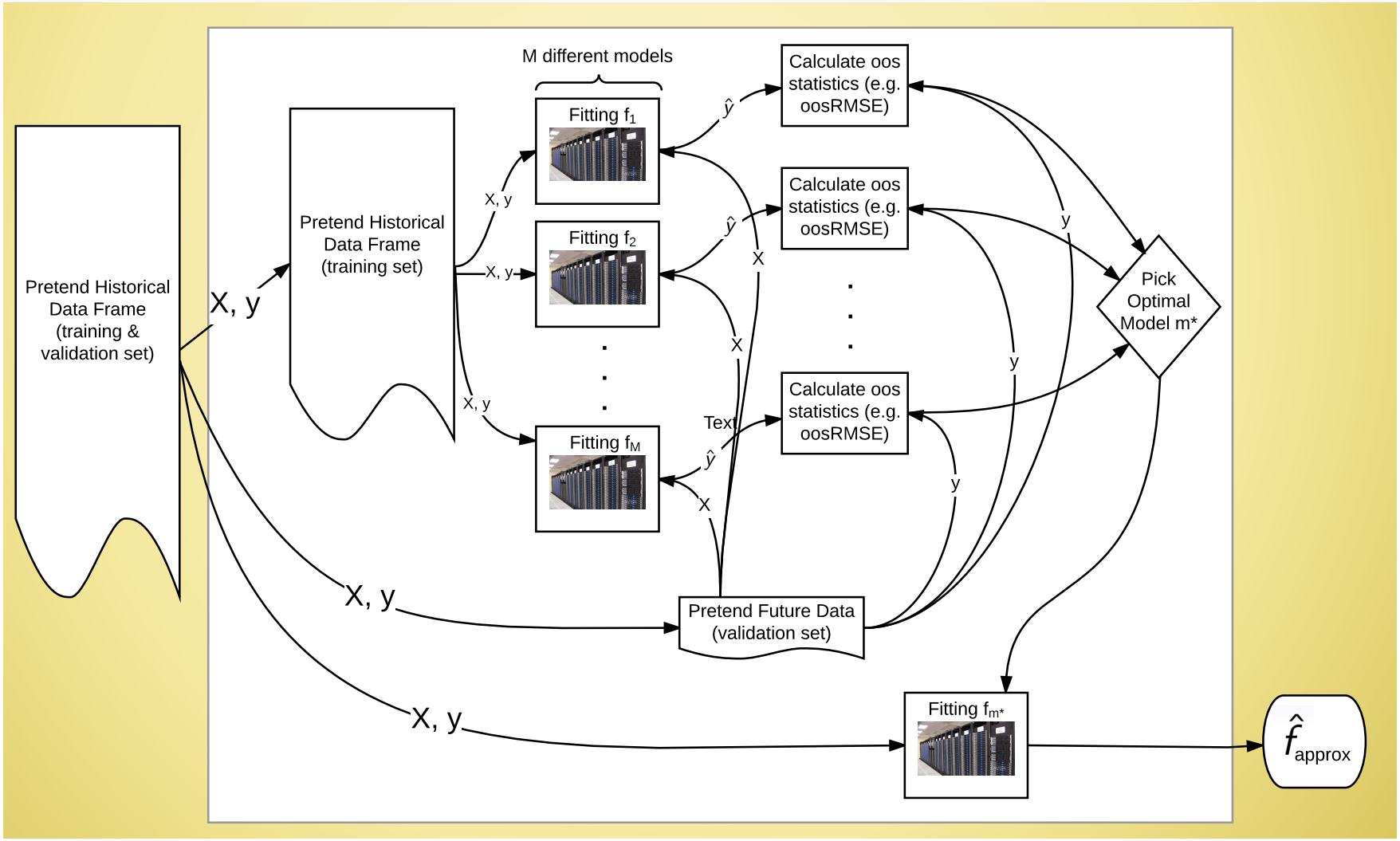
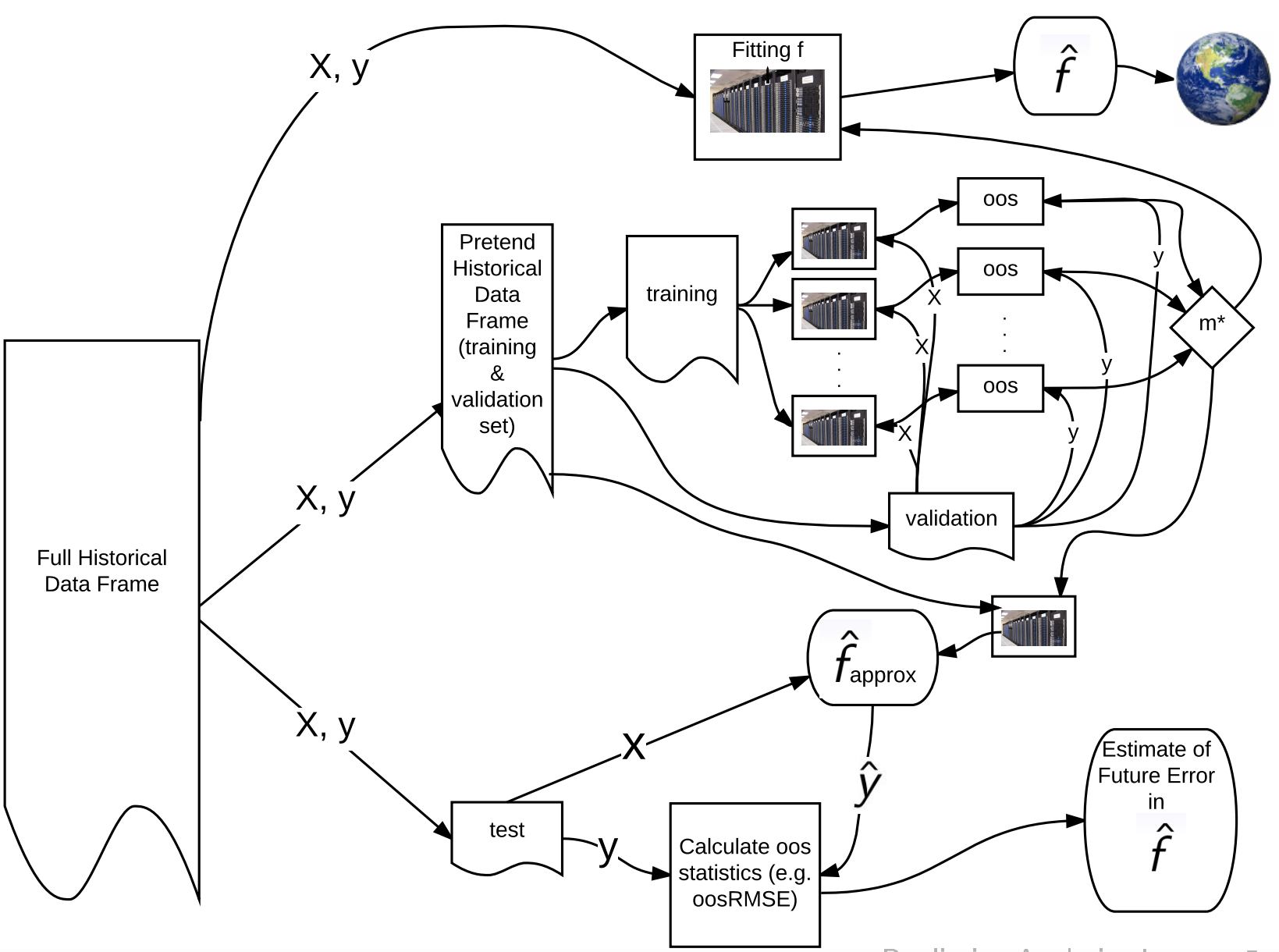


This procedure was completely valid as long as we did not touch the test set, right? As long as we operate only within the training set... we're OK!

Training ⇒ Training & Validation



3-way Splitting: The Full Picture



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Just like in the previous 2-way training-test split, you can overfit the training, get killed on the test set and be stuck. How could you similaryl overfit here? Be careful of optimizing to the validation set. Models $1, 2, \ldots, M$ should still be reasonable thought-through models.

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Back to Wine...

We can do a single 3-partition split in JMP using the validation column... then data filter... then fit the 6 models again... then use model comparison to select best model ... then undo the filter ... then use model comparison again to find our test set error (the guess of the generalization error)... then build the full model for public consumption.

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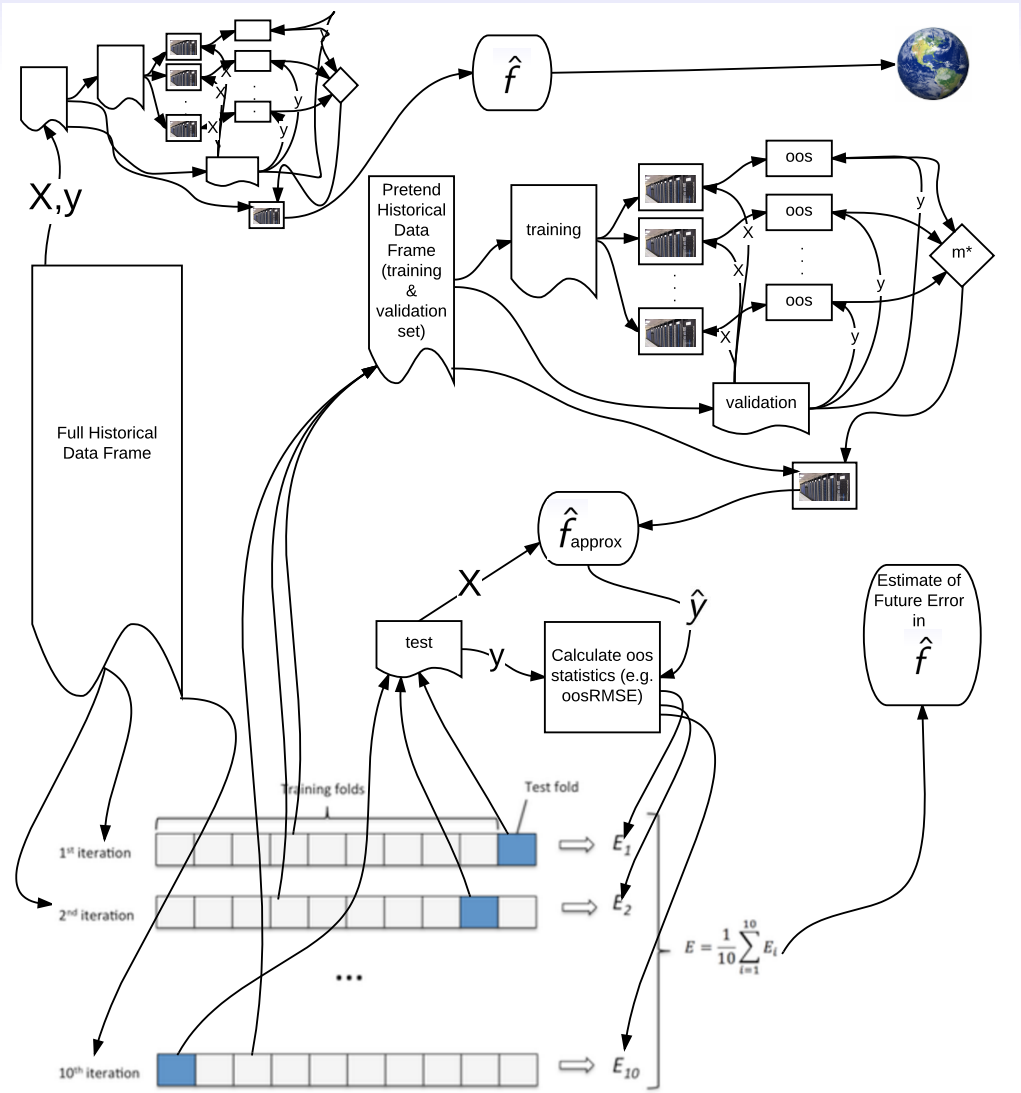

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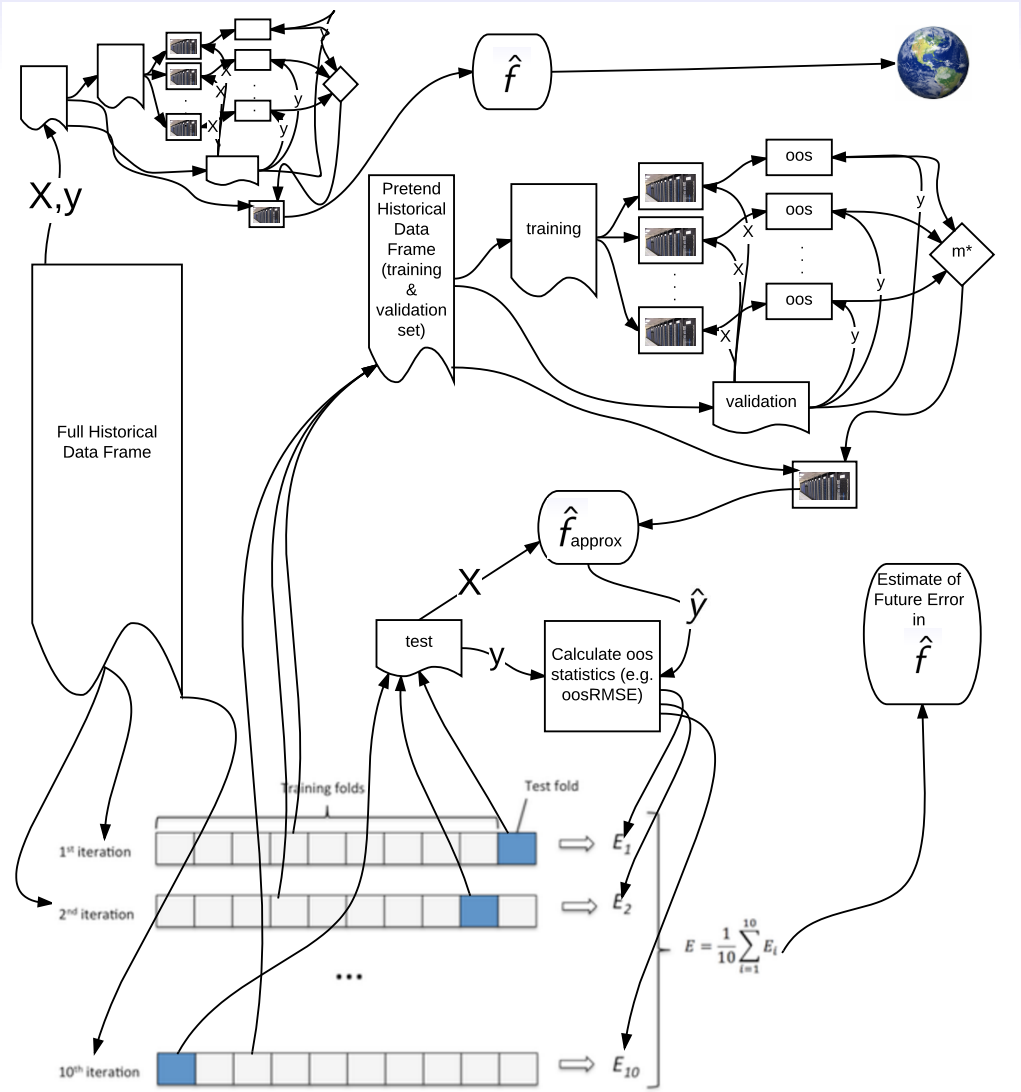

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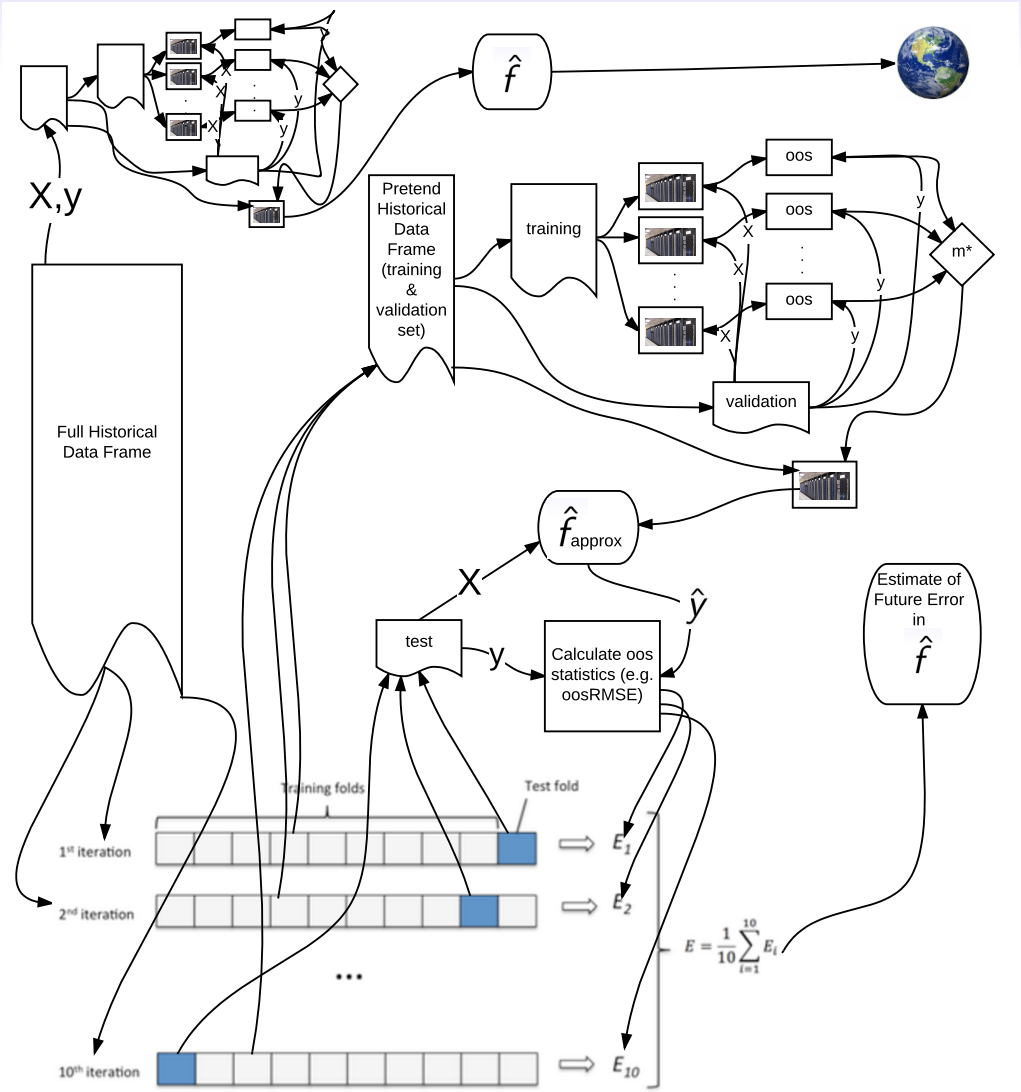

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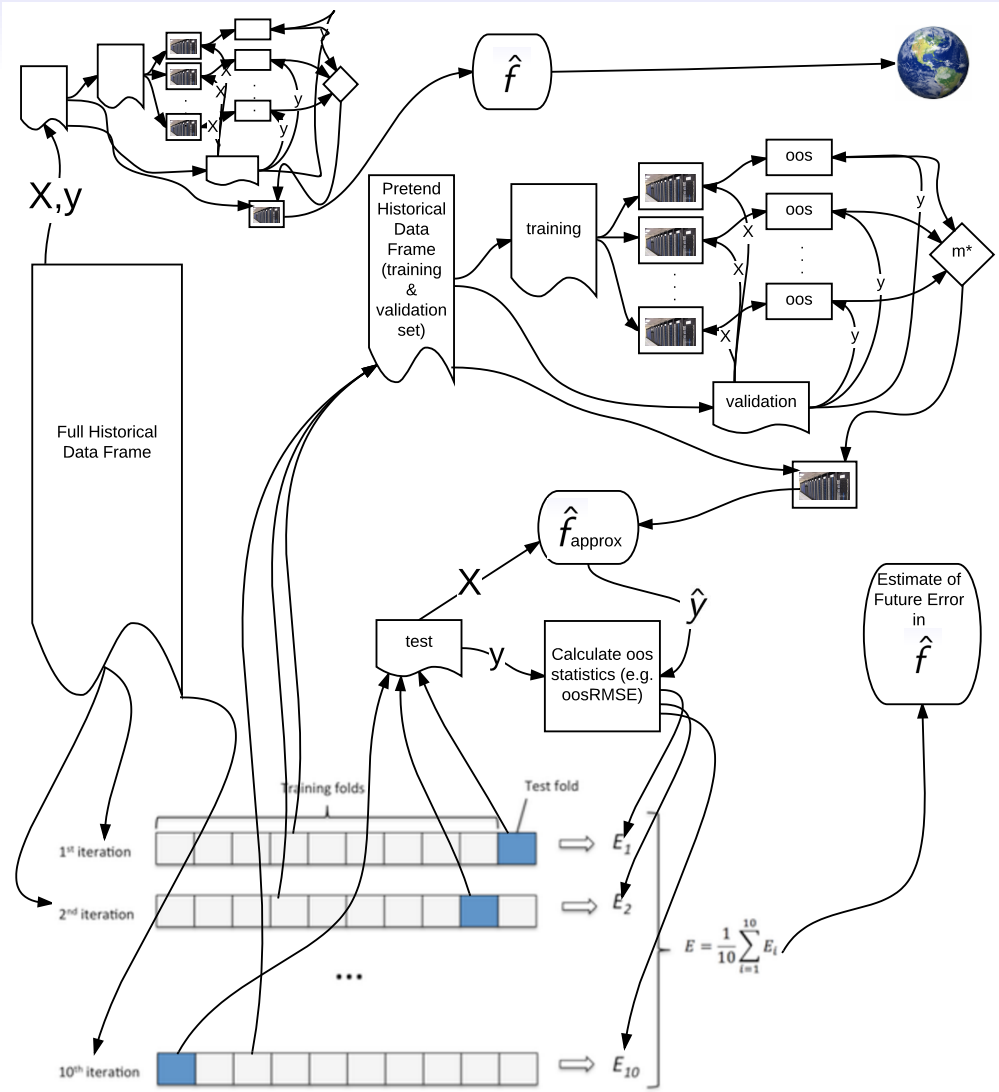

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Without CV, it was just model m^*. But here m^* varies with the 10 folds! You are testing the entire procedure i.e. given models $1, 2, \ldots, M$, pick the best one and ship it. How well you do in the future is estimated by the CV test set.

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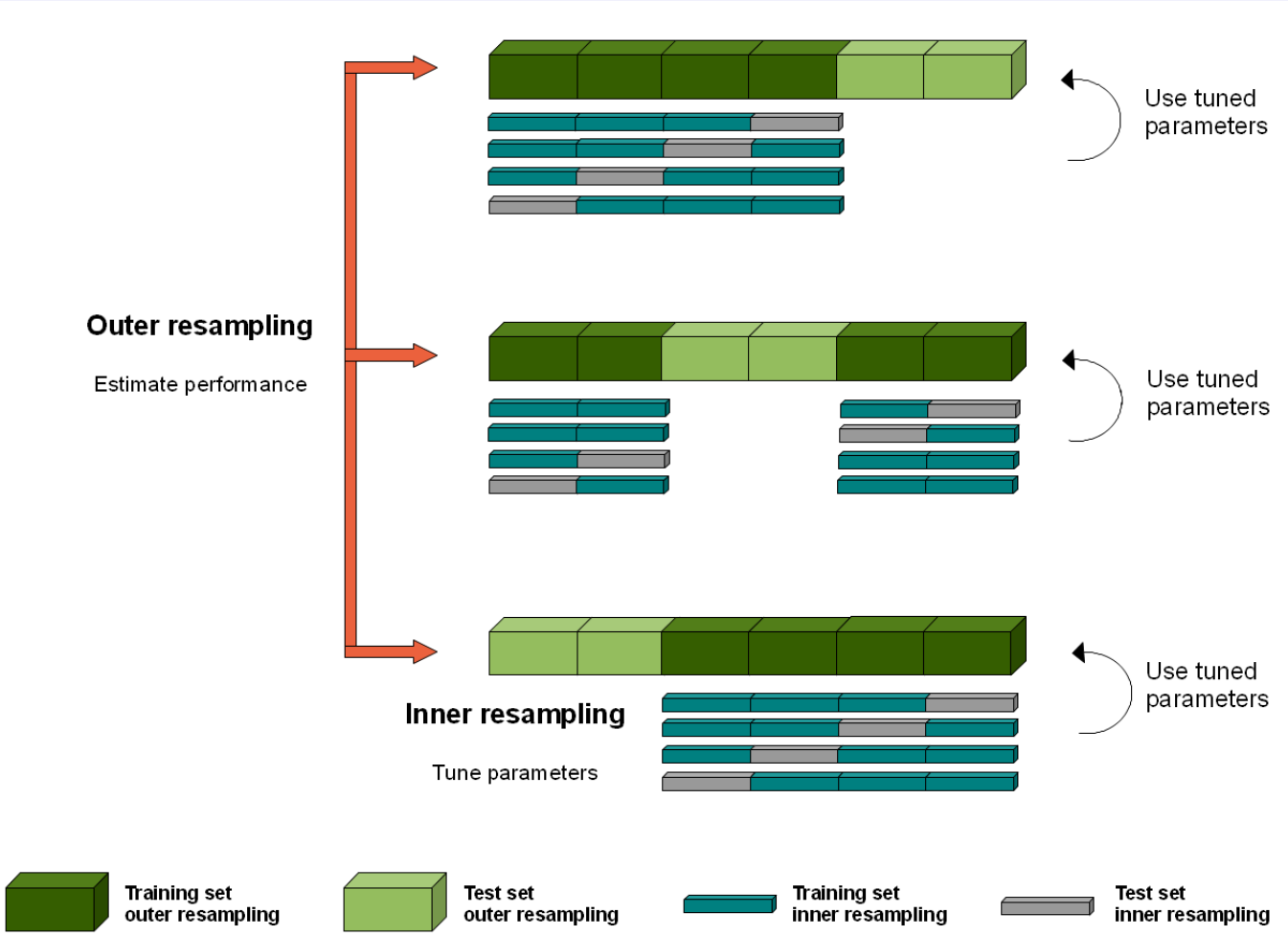
Neither R nor JMP (to my knowledge) can do this out-of-the-box. In R, even with MLR, you have to program it (MLR uses it for tuning an algorithm). Maybe I will write to them?

Nested Resampling for Tuning



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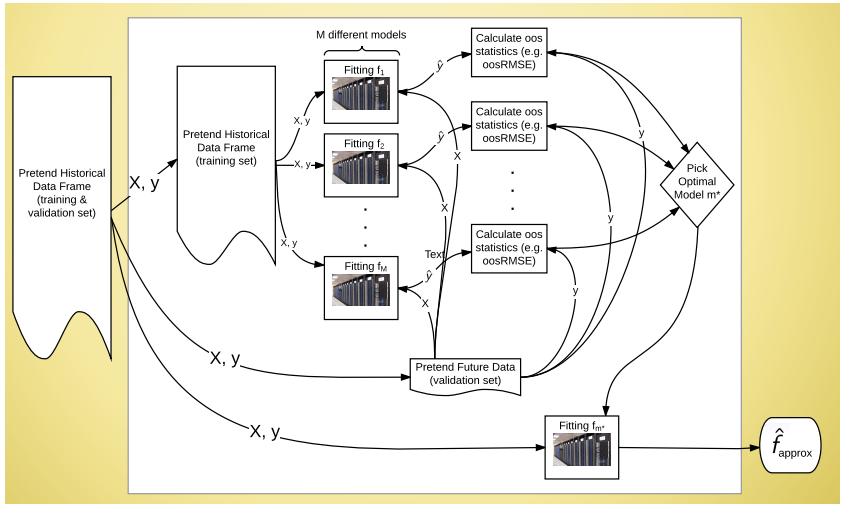

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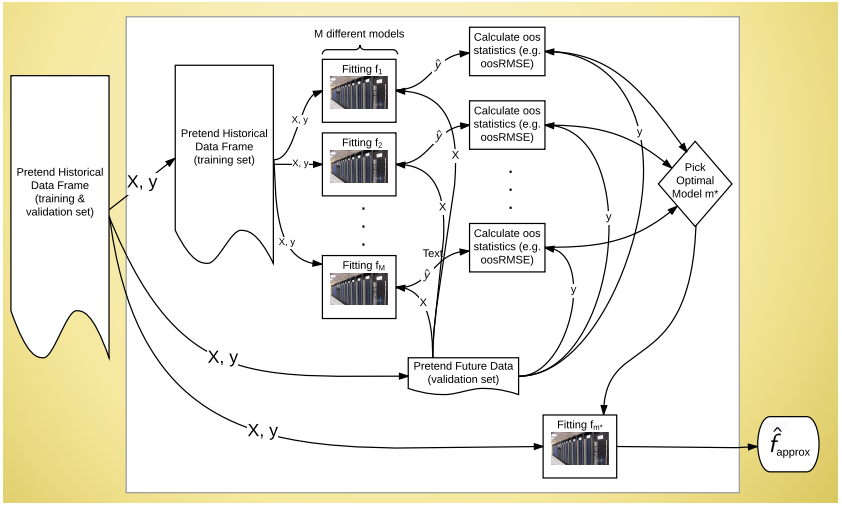

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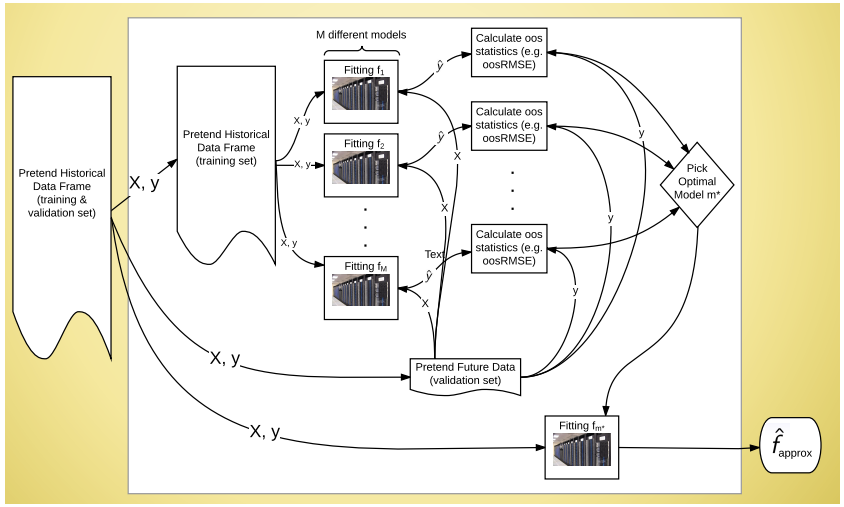

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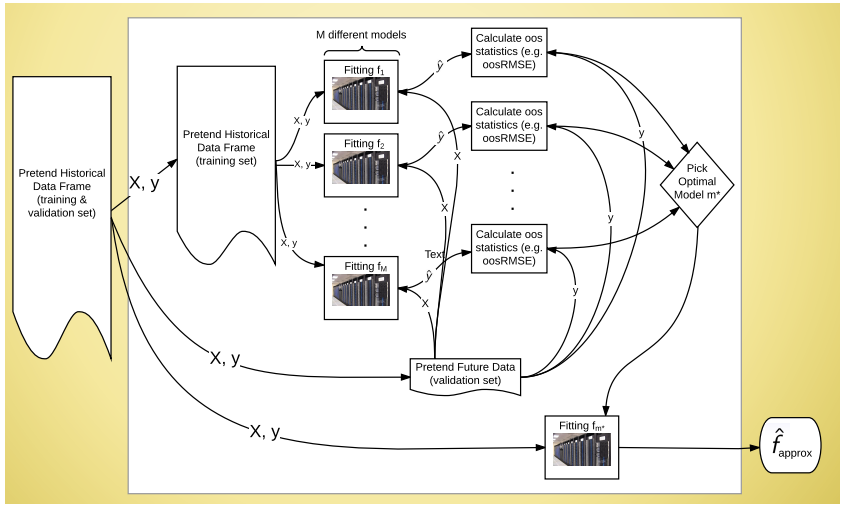

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The first component (the log-likelihood) represents in-sample fit. $\ell()$ is like R^2 though... as the fit gets closer to the points, the likelihood goes to 1 (and the log likelihood goes to 0). The $2p$ term is a reality check. If you have more features, you are going to overfit. So each additional feature must be justified in terms of the increase in log-likelihood.

Estimating Overfitting (again)

If you choose the feature to give you the best in-sample R^2, you will eventually take all the features (until $n = p + 1$) and you will get $R^2 = 100\%$. We need a metric to tell us when we may be overfitting and halt at that moment. Here are a few:

1. oos RMSE (keep a holdout set and quit when this starts increasing)
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$$AICc = AIC + \frac{2p(p+1)}{n-p-1}$$

Needless to say, this is all approximate since we are assuming OLS and a whole bunch of other things (beyond scope of course).

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This is not the only way to fit a flexible model and hedge against overfitting. We will do more such models. But first, we will talk about "missing data" as it's more relevant to the project which is due soon.