VALIDATION / EVALUATION OF A MODEL

Validation or evaluation?

- Treat model as a scientific hypothesis
  - Hypothesis: does the model imitate the way the real world functions?
  - We want to validate or invalidate hypothesis - validation
- Treat model as engineering tool
  - The question is how good the tool is
  - We want to evaluate the quality of the model

The model as a scientific hypothesis

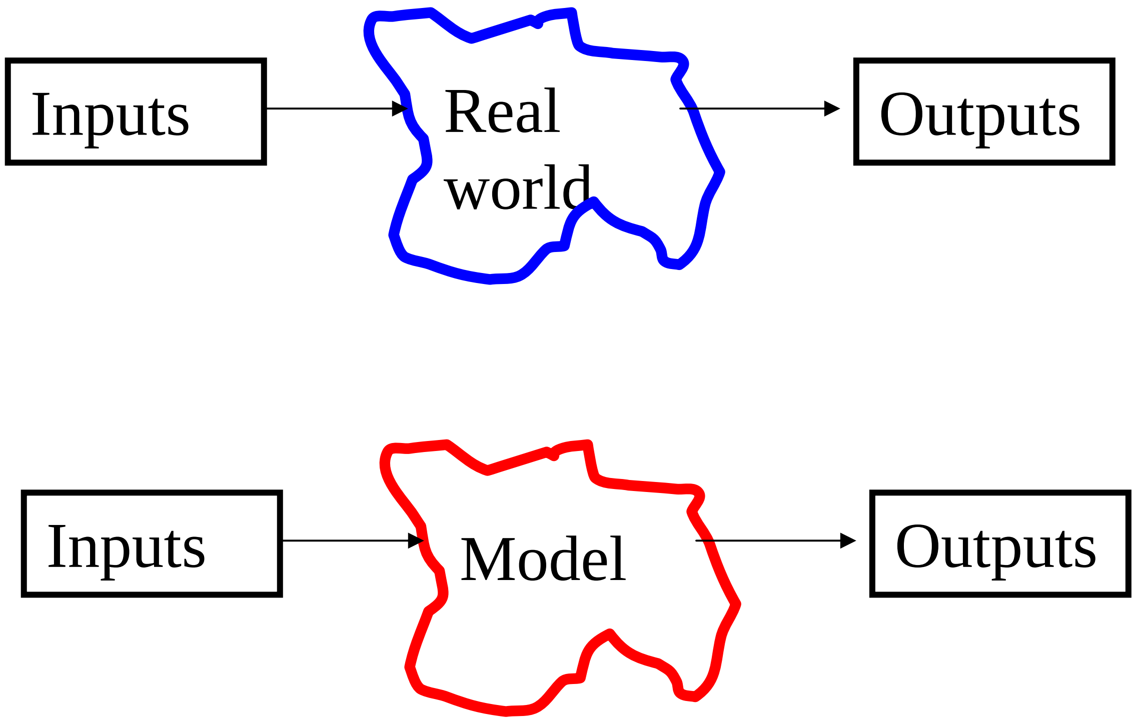
- Does the model behave in the same way as the real world for a set of conditions C.
  - “behaves like”: Each process gives results similar to measurements (within experimental error)

hypothesis

M behaves like R for C

- If the hypothesis is correct, then model predictions and observations will be the same

IF | M equivalent to R for C | AND | We are in C | THEN | M gives same results as R |

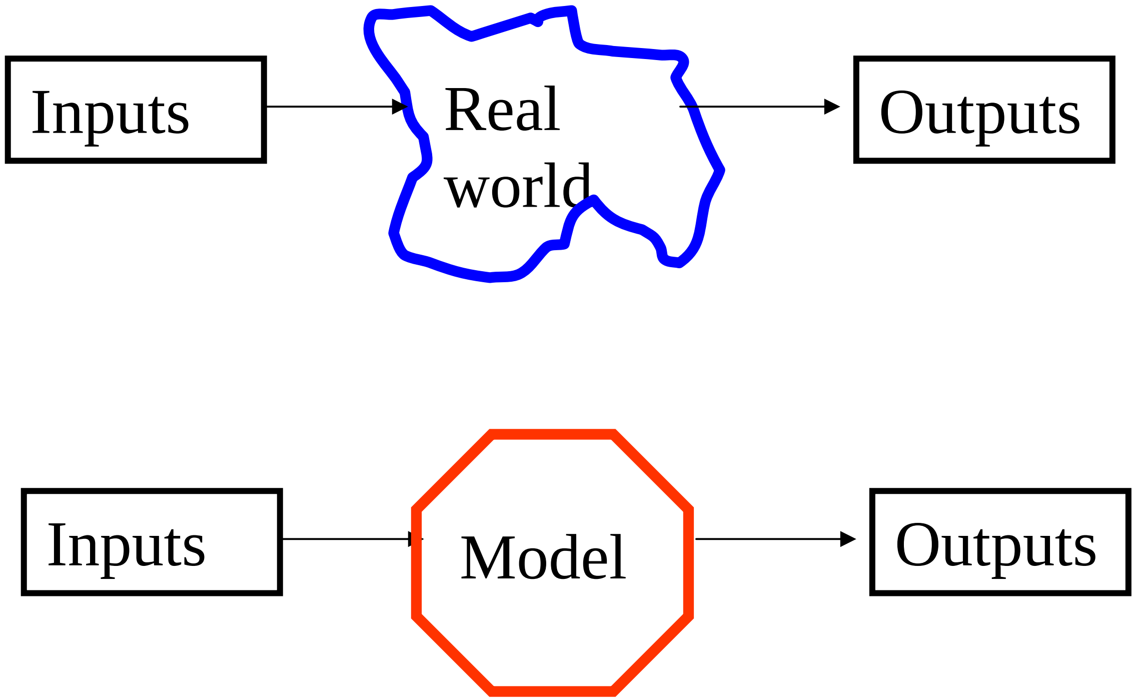


- What can we deduce from this syllogism?

IF M does NOT give same results as R AND We are in C THEN M NOT equivalent to R for C

~~IF M gives same results as R AND We are in C THEN M equivalent To R for C~~

- We can invalidate a model
- We cannot validate a model
  - The model may be right for the wrong reasons
    - e. g. even if aphid densities are correct, models of individual processes may e wrong



- Logically, we can’t validate a model
- In any case, we know that all models are false
  - A model is a simplification of reality
    - e.g. aphid-ladybeetle model is extreme simplification, ignores other populations, plant growth, etc. etc. etc.
  - It is not meant to be exactly the same as reality

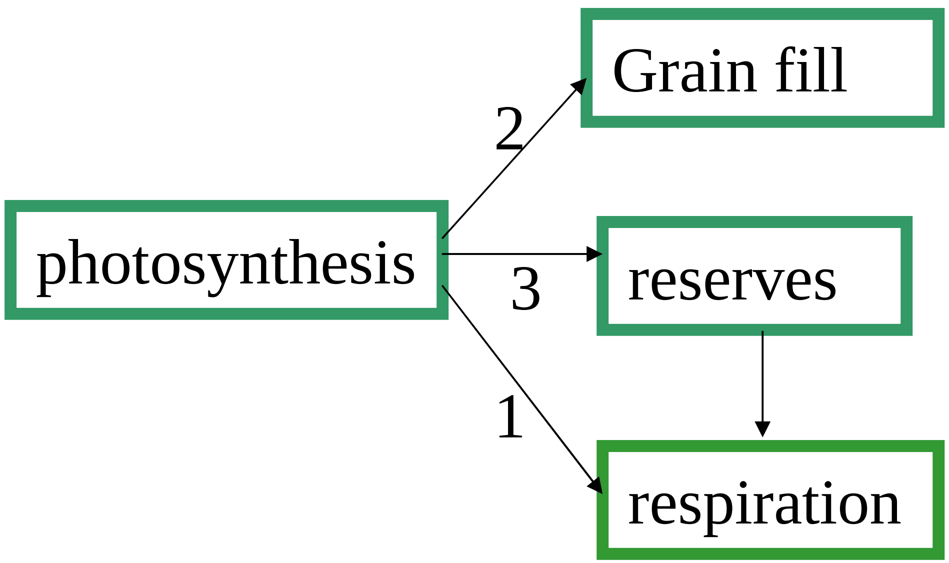
So a model as theory is useless?

- NO
  - Show that unlikely hypotheses are possible
  - Show that accepted hypotheses are wrong
  - Compare alternative hypotheses

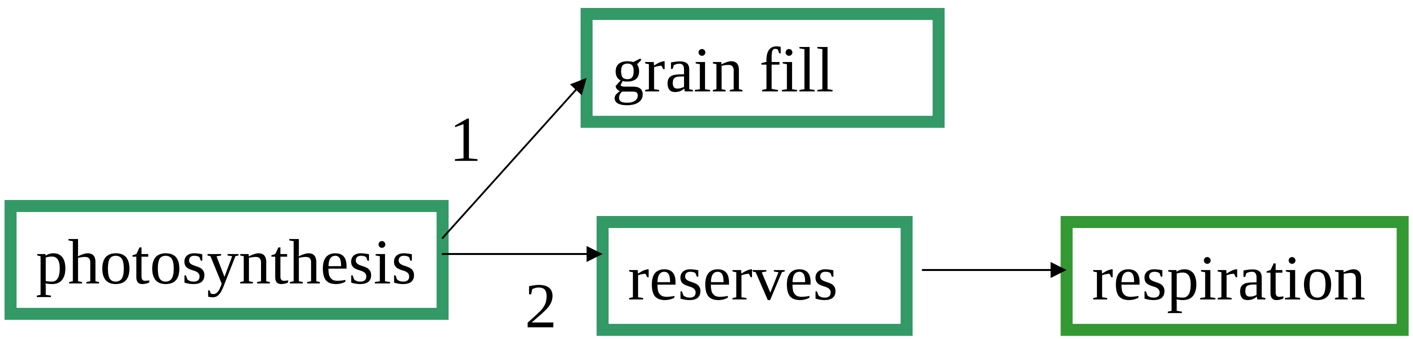
Example of comparison of hypotheses

- Respiration of wheat during grain filling. Does the C for respiration come directly from photosynthesis, or from reserves?

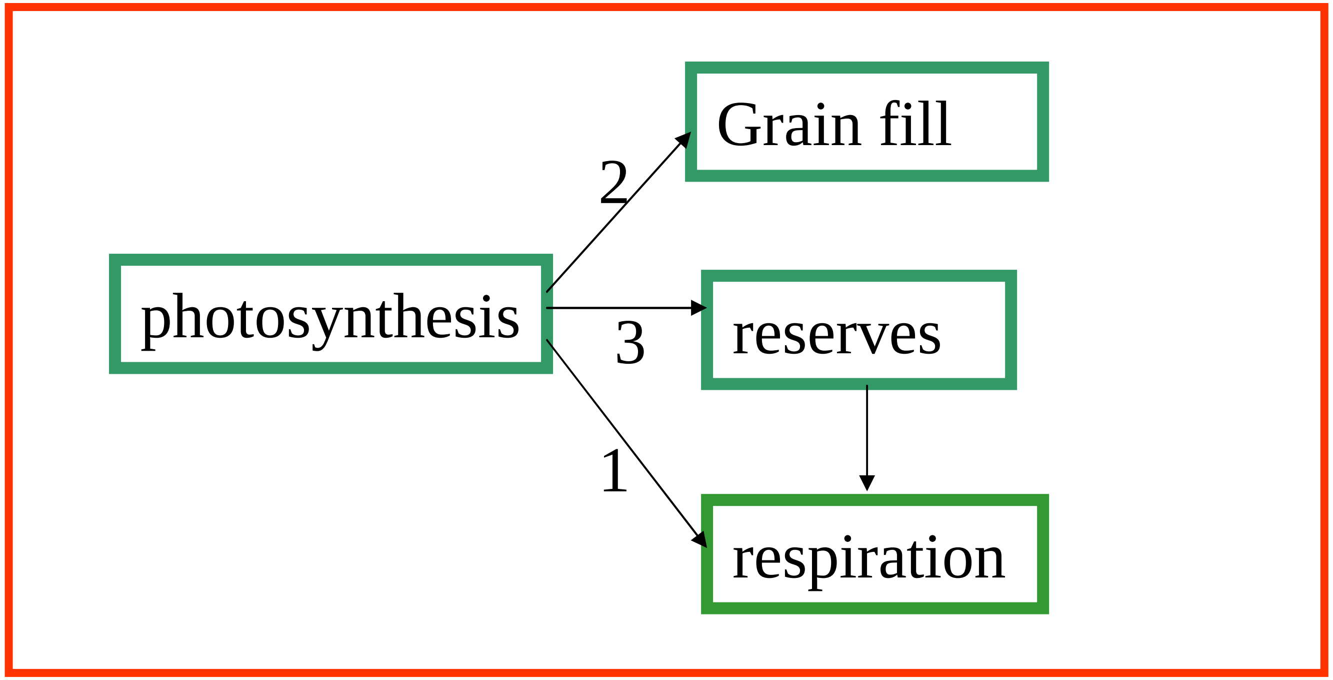
- Hypothesis 1 : C for respiration comes from photosynthesis if possible.

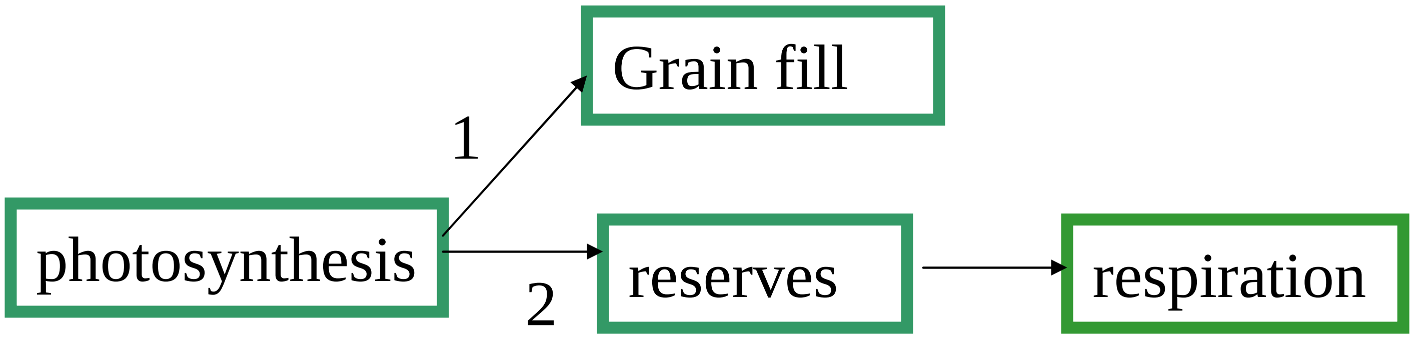


- Hypothesis 2: C for respiration comes from reserves



- Do experiments using pulses of ^{14}C marked air. Measure ^{14}C concentrations in grain and reserves.
- Develop 2 models, corresponding to above 2 hypotheses. Models predict ^{14}C concentrations in grain and reserves.
- Model based on hypothesis 1 is more consistent with data.


Grain fill
photosynthesis
reserves
respiration
2
3
1


Grain fill
photosynthesis
reserves
respiration
1
2

Conclusions?

- Hypothesis 1 is more apt to reproduce observed results.
- We don’t accept it as exactly true, but as better working hypothesis
  - So this is like engineering model?
  - Yes and no.
    - Yes because we look at how well model reproduces results.
    - No because we have drawn conclusions about mechanisms.

Engineering model

Evaluation

- We don't treat the model as a hypothesis but as a tool.
- We want it to reproduce important aspects of reality (e. g. predict yield, predict response to fetilizer)
- How well does model do that? That's what we evaluate.

The role of evaluation

- At the start of a modelling project
  - Define objectives and therefore evaluation criteria
- During the project
  - To choose between alternatives, evaluate each
  - Evaluation may give indication of how to improve model
- At the end of the project (or of a cycle)
  - Evaluation provides measure of quality of model

The practice of evaluation

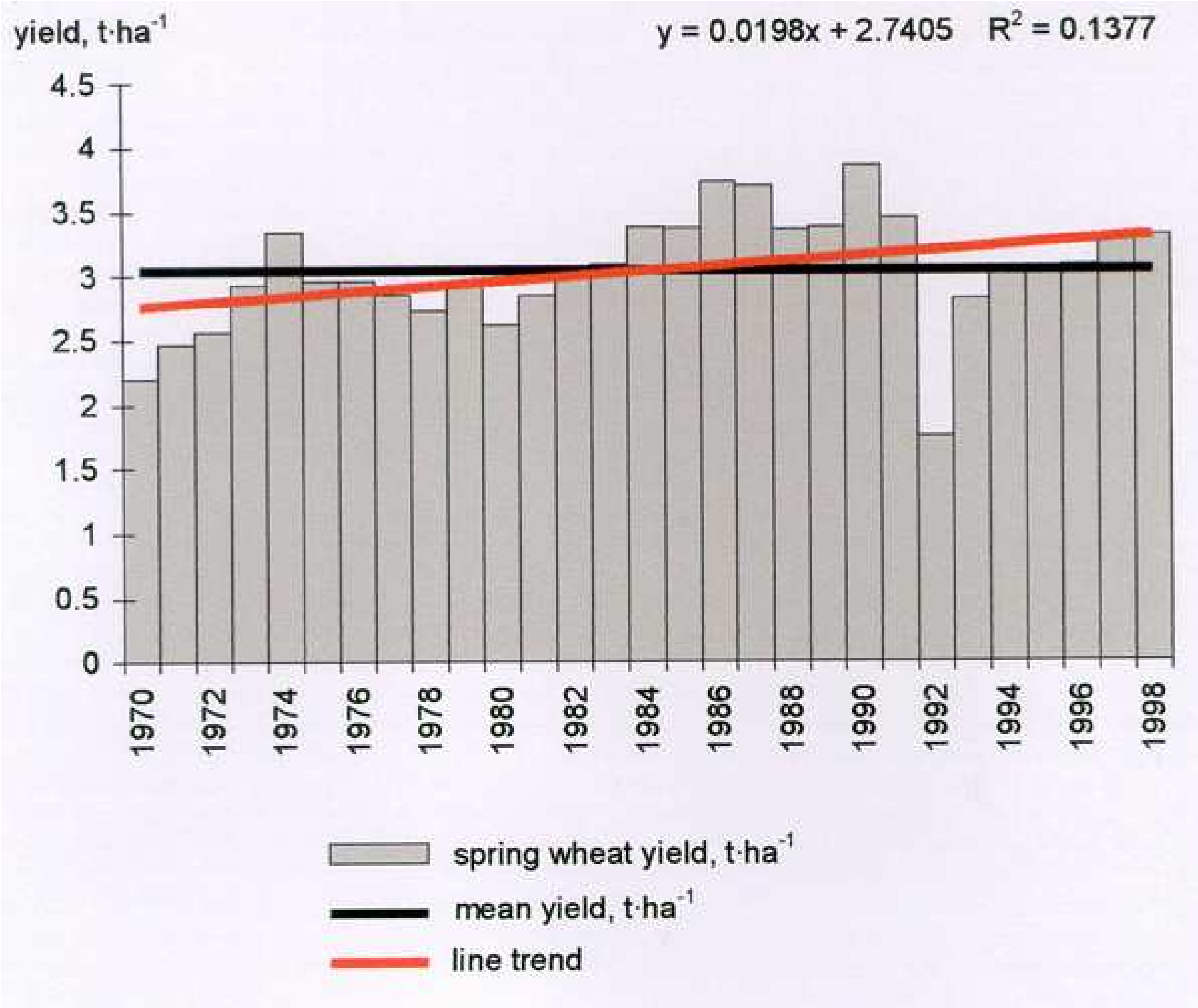
- Compare model to data, measure model quality
- Estimate how well model will predict for new cases

- Evaluation applies to all models. Both simple linear models and complex dynamic system models.
  - So we can use simple linear models to illustrate
  - We will point out specific aspects of dynamic system models

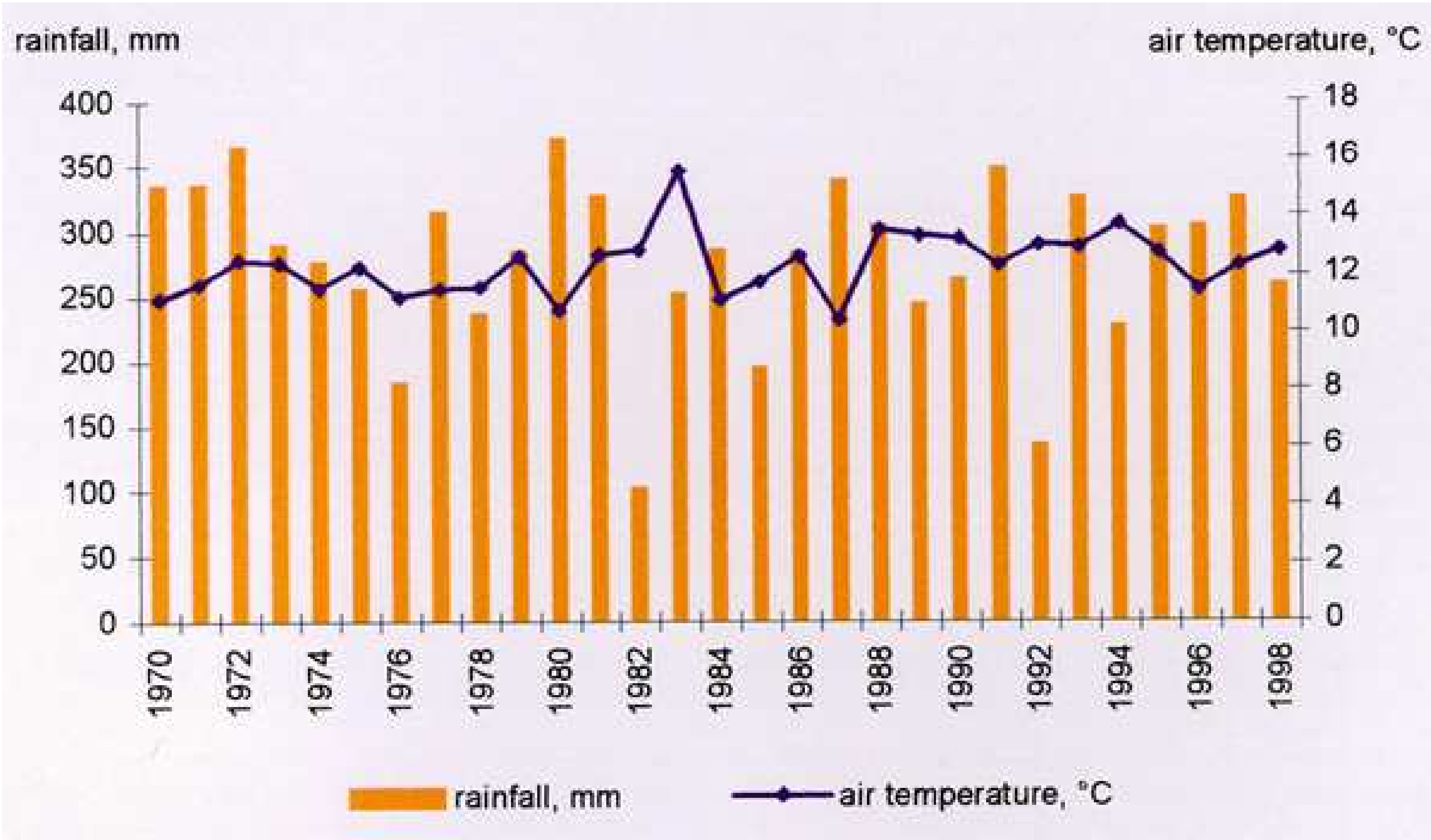
Examples of data and models

- Dynamic system models.
  - We have seen several examples
  - Dynamic system model for corn. Model is used to compare different irrigation strategies. We don't present model, just measured and calculated values.
- Static models
  - Predicting yield in a Polish region. To show that same problems arise for static and dynamic models.
  - An invented example, used to illustrate methods.

Spring wheat yield in the Zachodnie Pomorze Province 1970-1998.



Rainfall and mean air temperature from March 11 to August 20 in the Zachodnie Pomorze Province 1970-1998.



Relationship between spring wheat yield (t·ha-1) in the Zachodnie Pomorze Province and weather components 1970-1998

Regression equations R^2

Till April 30

$y = 1.40129 + 0.2396x_1 - 0.0448x_2 + 0.130222x_3 - 0.002306x_4$ 67.84

Till May 31

$y = 2.25358 + 0,2837x_1 - 0.01490x_2 + 0.15782x_3 - 0.01039x_5 - 0.020279x_6$ 79.31

Till June 30

$y = 3.77033 + 0.2557x_1 - 0.01218x_2 + 0.13753x_3 - 0.01265x_5 - 0.0235x_7 - 0,00273x_8$ 88.85

Till July 31

$y = 3.61260 + 0.02643x_1 - 0.01126x_2 + 0.13129x_3 - 0.01291x_5 - 0.02982x_7 + 0.03687x_9 - 0.00215x_{10} + 0.03107x_{11}$ 90.5

Artificial data and model

- Invent formula for generating data. This is « real world ». Generate sample of 8 data values. Those are « measurements ».

$$Y = \theta_1 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_4 x_4 + \theta_5 x_5 + \varepsilon$$

- Model has same form (linear model with 5 explanatory variables)
- Use data to estimate model parameters
- Estimate 0,2,3,4, or 6 parameters. Others have default values that are different than true values.

$$\hat{Y} = \hat{\theta}_1 + \hat{\theta}_1 x_1 + \hat{\theta}_2 x_2 + \hat{\theta}_3 x_3 + \hat{\theta}_4 x_4 + \hat{\theta}_5 x_5$$

Data for artificial example

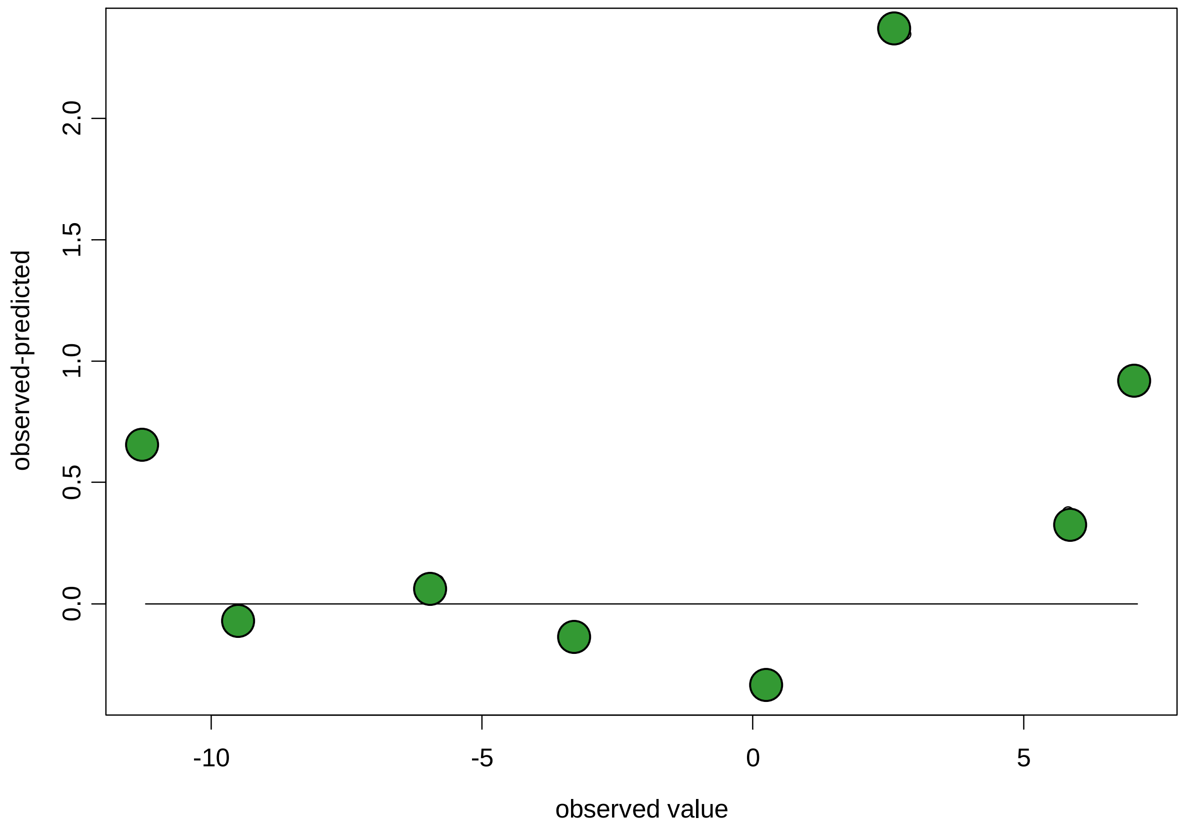
$$f(X\;;\hat{\theta}) = \hat{\theta}^{(0)} + \hat{\theta}^{(1)} * x^{(1)} + \hat{\theta}^{(2)} * x^{(2)} + \hat{\theta}^{(3)} * x^{(3)} + \hat{\theta}^{(4)} * x^{(4)} + \hat{\theta}^{(5)} * x^{(5)}$$

$x^{(1)}$	$x^{(2)}$	$x^{(3)}$	$x^{(4)}$	$x^{(5)}$	Y	$\hat{Y}$
-1.6339	0.7977	0.4416	-0.4463	-0.4728	-9.3896	-9.3144
-0.9485	1.0700	0.5047	0.5308	-0.3257	-3.2312	-3.0994
-0.2512	0.1952	0.5099	0.8226	0.4495	0.3732	0.7236
0.3789	1.0193	-0.2185	0.8163	-1.9263	7.1024	6.1808
0.1464	1.1373	1.0657	1.6325	-0.5528	5.8245	5.4485
-1.1984	-1.7925	0.3530	-0.2601	0.2617	-11.2130	-11.8425
-0.9720	-0.1533	0.1113	1.1251	0.1019	-5.8110	-5.9035
0.3931	-1.2031	2.0132	-0.7947	-1.4396	2.8158	0.4690

Graphs

Artificial model
Residuals (observed – calculated)

residual

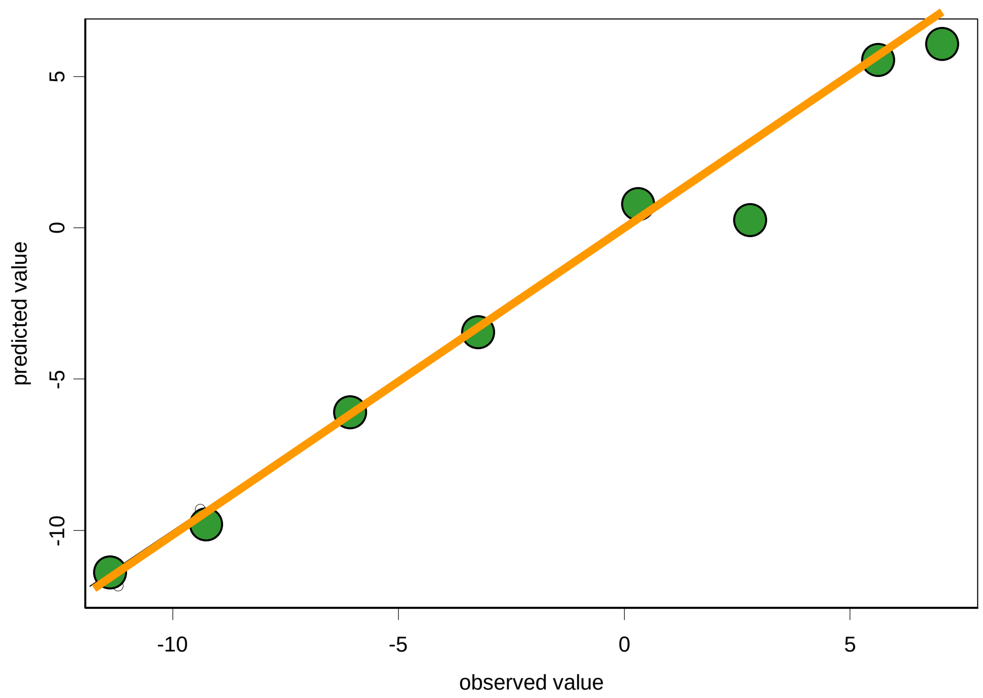


Observed values

Artificial example

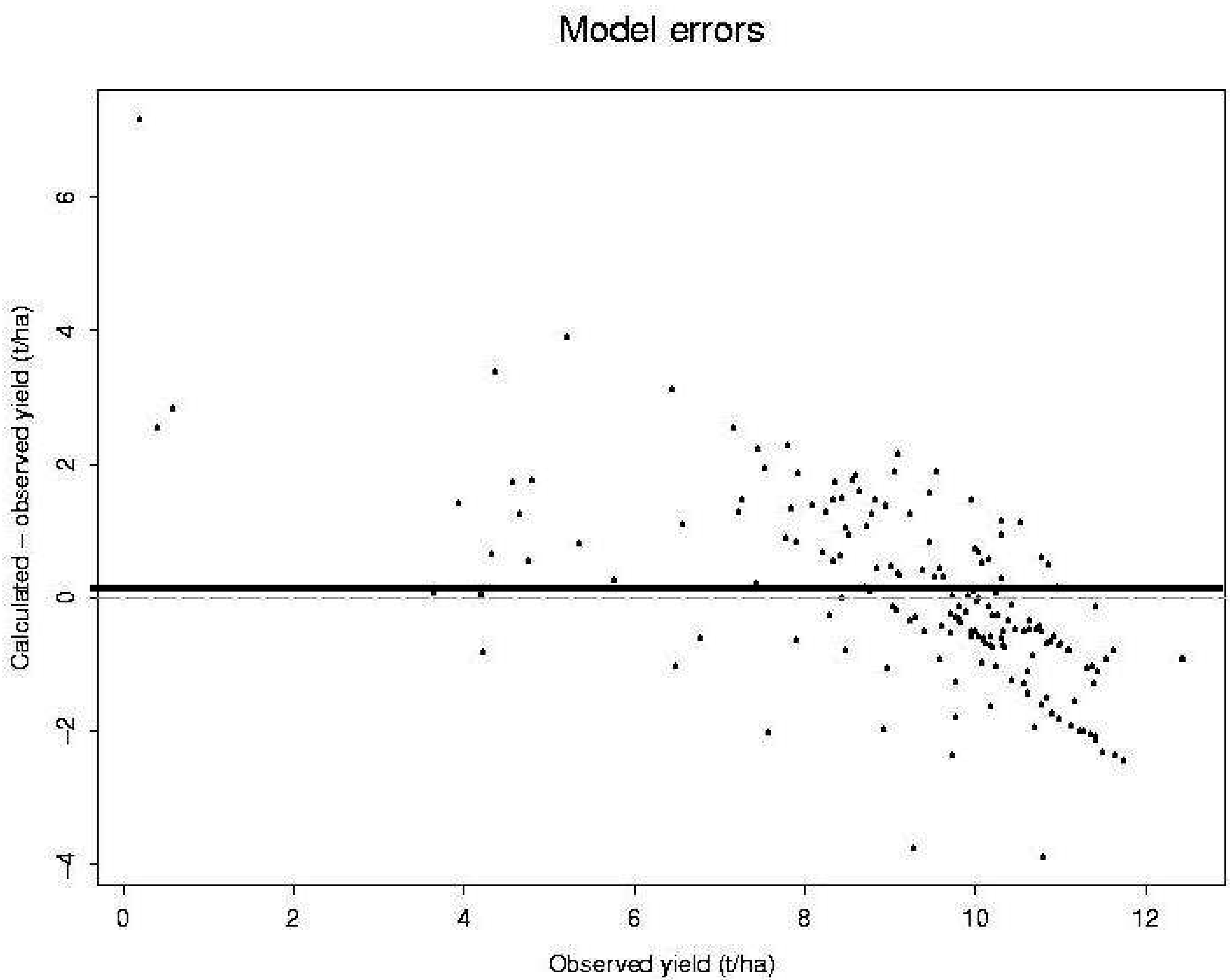
Calculated vs observed values

Calculated values

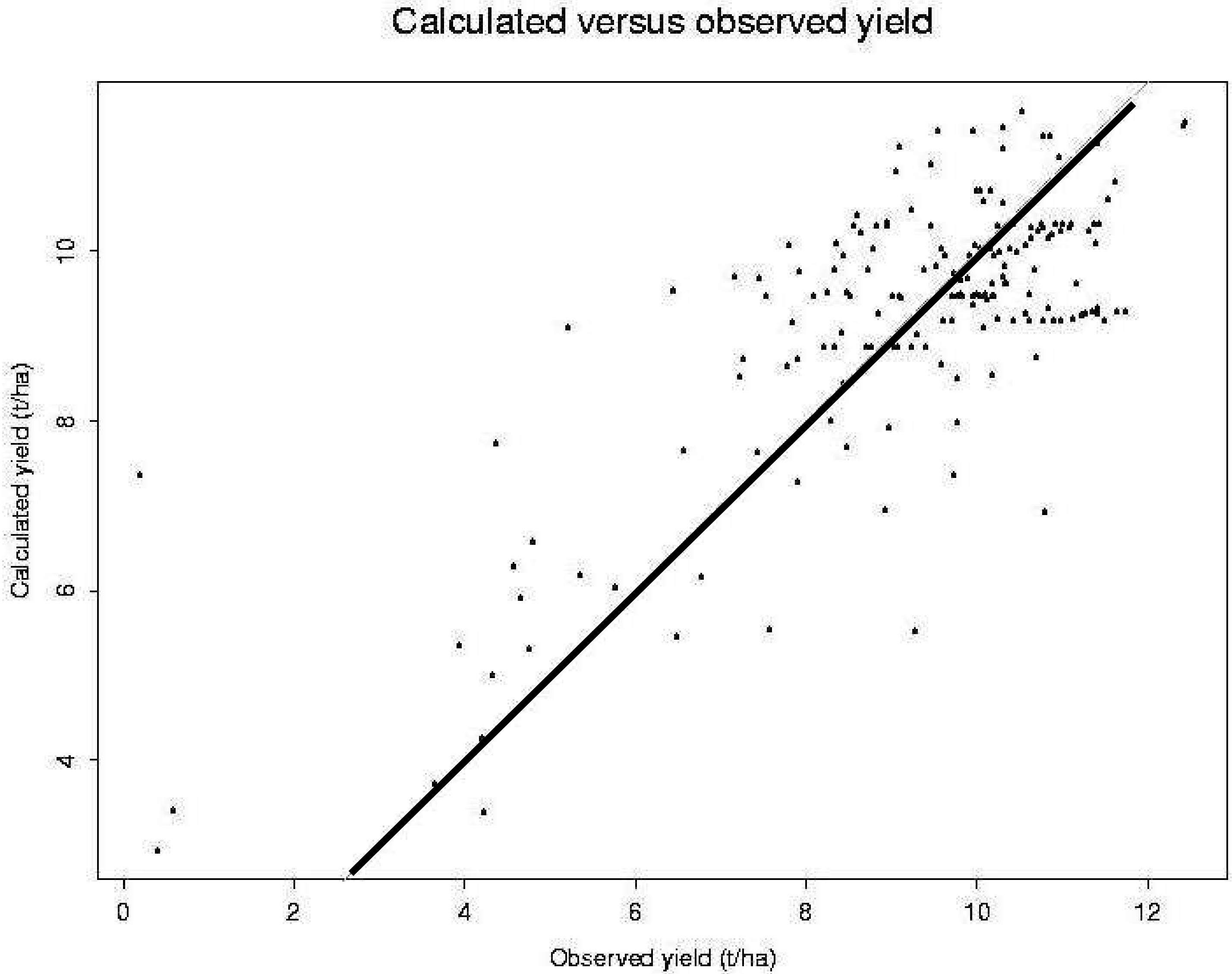


Observed values

Corn model. Residuals



Corn model. Observed vs calculated



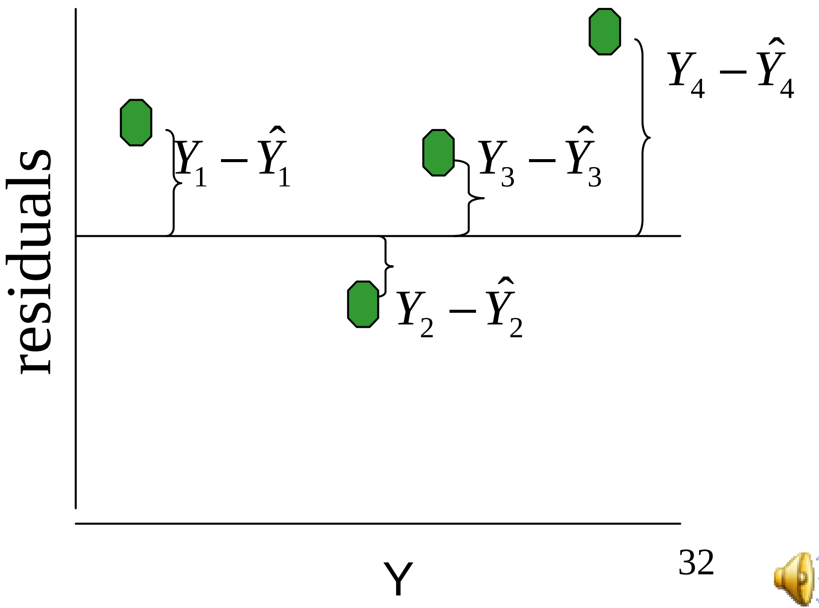
Measures of error

- Summarize information about differences between measured and calculated values

MSE

- Mean Squared Error (the most common measure)

$$MSE = (1/N)\sum_{i=1}^{N}(Y_i - \hat{Y}_i)^2$$



RMSE and MAE

name	equation	value for example
mean squared error	$MSE = \frac{\sum (Y_i - \hat{Y}_i)^2}{N}$	0.88 (t/ha)²
root mean squared error	$RMSE = \sqrt{MSE}$	0.94 (t/ha)
mean absolute error	$MAE = \frac{\sum \left\| Y_i - \hat{Y}_i \right\|}{N}$	0.62 (t/ha)

R squared

$$R^2 = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \overline{y})^2}$$

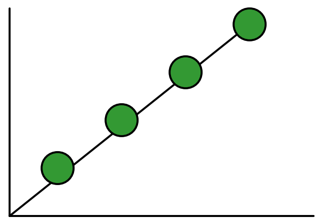
- R^2 if model is perfect?
  - $R^2=1$
  - Can R^2 be > 1?
  - No.
- R^2 if model is just average of observed values?
  - $R^2=0$
  - Can R^2 be less than 0?
  - Yes, for complex models
- This criterion also called efficiency
- For yield example, $R^2=0.98$

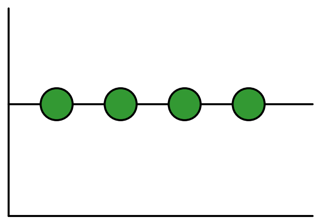
R^2 and graphs

Calculated vs. observed

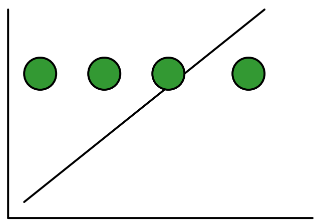
Residuals

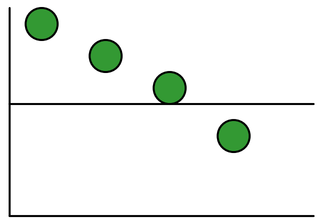
$R^2=1$ $Y_i=\hat{Y}_i$





$R^2=0$ $Y_i=\hat{Y}_i$





Components of model error

- To better understand origin of error
- May give ideas of how to improve model

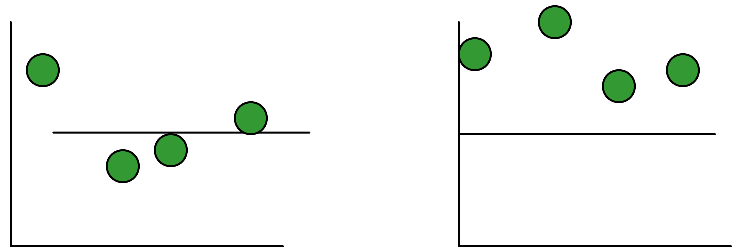
Components of MSE

MSE=bias^2 + variability difference + remainder

Bias term

residuals

Small bias　　Large bias



$$\text{bias}^2 = \frac{\sum (Y_i - \hat{Y}_i)^2}{N}$$

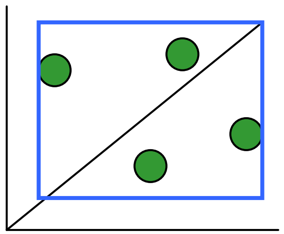
- If bias is large
  - Left out or underestimated a factor that systematically increases or decreases response
  - For example, underestimated harvest index (relation of yield to total biomass)
  - In example, $\text{bias}^2=0.23$ (MSE=0.88)

Variability difference

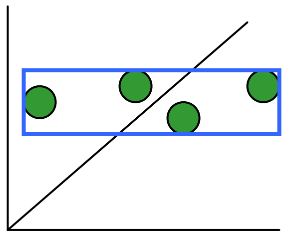
$$\text{variability difference} = (\sigma_Y - \sigma_{\hat{Y}})^2$$

Calculated vs observed values

small



large



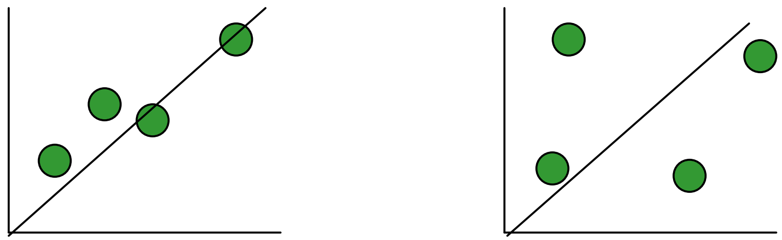
- If SDSD is large
  - Left out or underestimated a factor that sometimes increases or decresaes response
  - For example, effect of water stress
  - In example variability difference = 0.06 (MSE=0.88)

Remainder

$$\text{remainder} = 2\sigma_Y \sigma_{\hat{Y}} (1 - \text{correlation coefficient})$$

Calculated vs observed values

small large



- If LCS is large
  - Sorry, error is in details of model
  - In example, remainder=0.59 (MSE=0.88)

Criteria for model comparison

- Can we use criteria we have seen?
  - Graphs, MSE, R^2

MSE and R^2

- What will be effect of adding extra variables to model, and estimating their parameters, on MSE and R^2?
  - MSE will decrease, R^2 will increase
  - Because adding extra terms allows better fit
  - MSE=0.16 (was 0.21)
  - R^2=0.56 (was 0.45)

- Should we add extra variables in this case?
- Should we always add extra variables?
  - Is a more complex model always better than a simpler model?
  - Should we always put all our knowledge of the system into a model?

- The answer is no. Next we explain why.
  - Note that this implies that MSE and R^2 are not good for comparing models of different complexity.

Summary to here

- Common methods of evaluation
  - Graphs
  - MSE, R^2
- Decomposition of MSE can give indication of source of errors
- MSE and R^2 are not suited for comparing models of different complexity

EVALUATING PREDICTIONS

- Often, the goal is to predict for different situations
  - Could be future (prediction) or could be past (unobserved situations)
  - So we need to compare prediction errors of models. That is topic of this section.
  - (In other cases, we are interested in using a model to make decisions. In that case, we need to compare the quality of decisions based on different models. That is another lecture).
- In this case we are not really interested in MSE or R^2 per se.
  - We have data, don't need model for those situations
  - We would be interested in MSE if it gave information about predictions. Does it?

- First, define prediction quality

Prediction for what situations?

- Define target population = situations where we want to use model.
  - For model of animal metabolism rate, random selection of animals (of given race, age).
  - Corn yield in southwestern France. Random fields in region, random climate for region, certain management practices

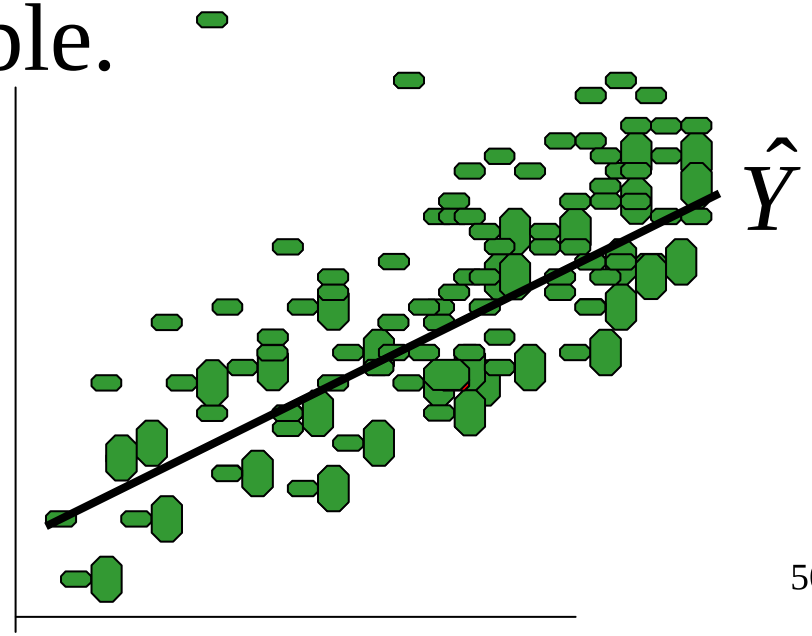
Prediction of what variables?

- Prediction quality depends on what we predict. Define target variables.
  - e. g. Aphid-ladybeetle model may have different error for prey population in margins, aphid population in wheat, ladybeetle population, total predation, etc.

A criterion of prediction error

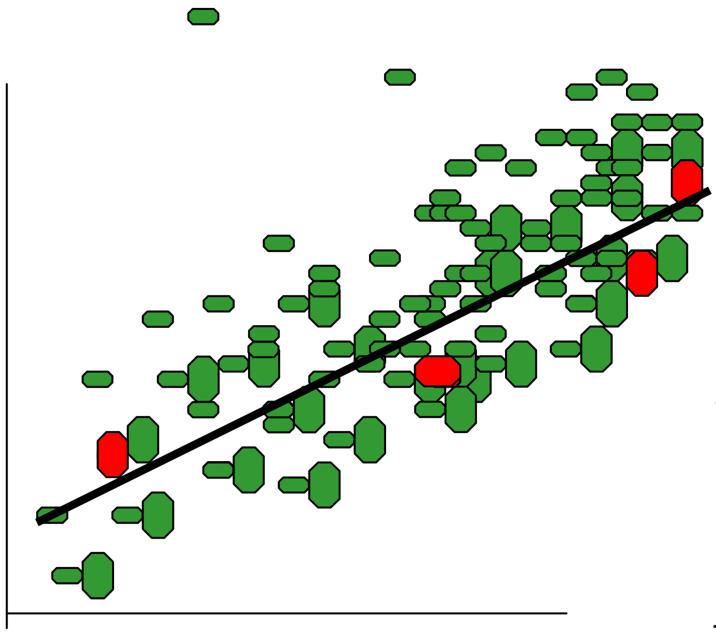
- A common measure of prediction error is MSEP=mean squared error of prediction.
- Expectation over target population. Y is target variable.

$$MSEP = E\left[\left(Y - \hat{Y}\right)\right]^2$$



The difference MSE, MSEP

- MSE is adjustment error (based on measurements)
- MSEP is prediction error (for full target population)



- target population
- measurements

$$MSEP = E\left[\left(Y - \hat{Y}\right)\right]^2$$

$$MSE = (1/N)\sum_{i=1}^{N}(Y_i - \hat{Y}_i)^2$$

- The difference between MSE and MSEP is very important.
  - Conceptually.
  - Practically. MSE and MSEP can be very different.

Estimate value of MSEP

- MSEP measures average squared error over target population. At best, we only have measurements for a sample.
- How can we measure MSEP?
  - We can't
- How can we estimate MSEP?
  - Based on measurements (no other choice)

- MSEP looks like MSE (a sum of squared errors).
- Is MSE a good estimator of MSEP?
  - We have a sample of measurements. On the average over possible samples, is MSE=MSEP?

$$MSEP = E\left[\left(Y - \hat{Y}\right)\right]^2$$

$$MSE = (1/N)\sum_{i=1}^{N}(Y_i - \hat{Y}_i)^2$$

MSE estimates MSEP if…

- Our measurements are representative of the target population
- The measurements weren’t used to develop the model
  - Often, measurements used to estimate parameter values
  - But could also be used to choose form of function etc.

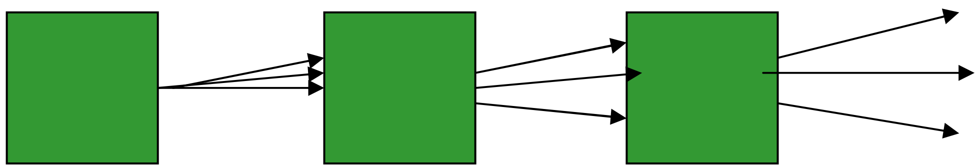
Representative sample

- If data are not representative of target population, of course MSE is not a good measure of MSEP

- Insure by random sampling
  - For complex systems, random sampling may not be possible.
    - e.g. agronomy experiments at field stations, not farmer fields.
  - With many explanatory variables, even random sample may not be representative
    - e.g. climate. With only a few years sampled, hard to say if this is representative sample.

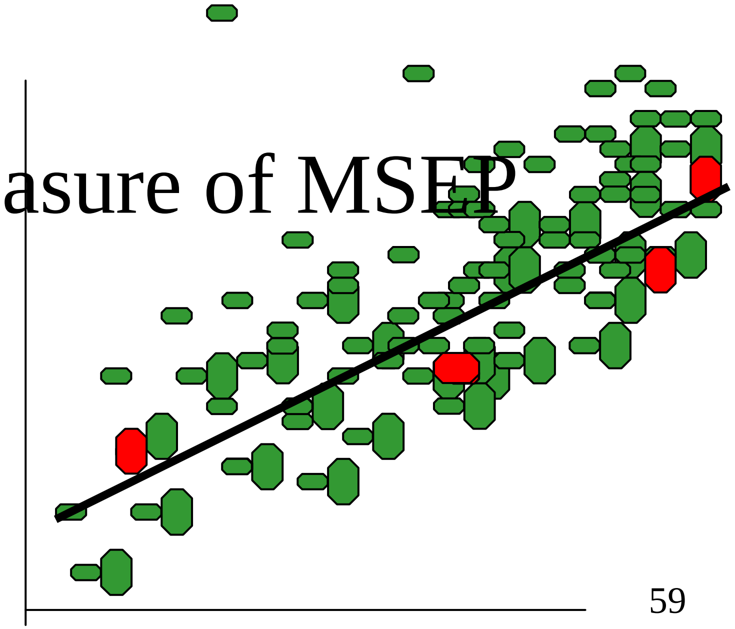
If sample from target population unavailable

- Can estimate error in each part off model, and use model to get overall error
  - In particular, parameter error
  - If we know possible distribution of parameter values, run model to get distribution of responses
    - See uncertainty analysis, Bayesian estimation



If measurements used to develop model?

- Typically, use measurements to estimate model parameters.
- Then model fits measurements better than new data
- So MSE isn't a good measure of MSEP



Example. MSEP $\neq$MSE

Adjusted parameters	$MSE(\hat{\theta})$	$MSEP(\hat{\theta})$
$\theta^{(0)},\theta^{(1)}$	4.6077	4.30
$\theta^{(0)},\theta^{(1)},\theta^{(2)}$	0.0143	0.07
$\theta^{(0)},\theta^{(1)},\theta^{(2)},\theta^{(3)}$	0.0119	0.06
$\theta^{(0)},\theta^{(1)},\theta^{(2)},\theta^{(3)},\theta^{(4)}$	0.0040	0.10
$\theta^{(0)},\theta^{(1)},\theta^{(2)},\theta^{(3)},\theta^{(4)},\theta^{(5)}$	0.0003	0.42

Conclusions about MSE and MSEP

MSEP$\neq$MSE

For large p/n, MSEP>>MSE

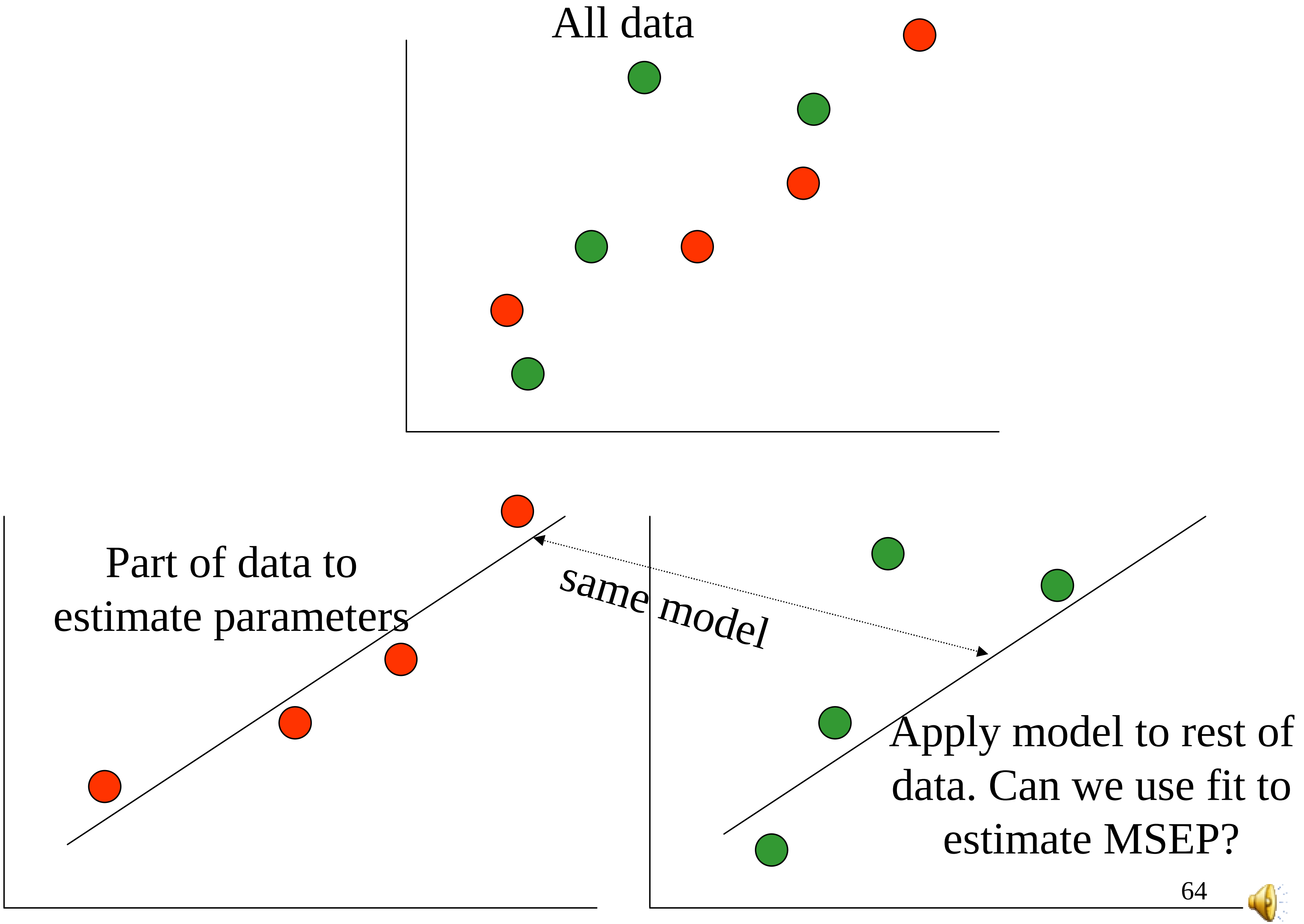
MSE always decreases as model complexity increases

MSEP has a minimum for some number of parameters

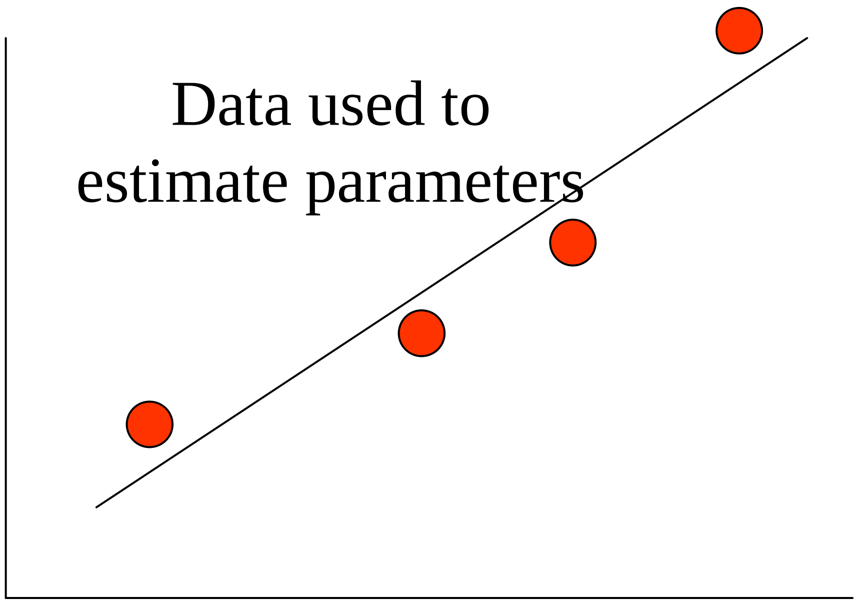
How can we estimate MSEP if data is used in model development?

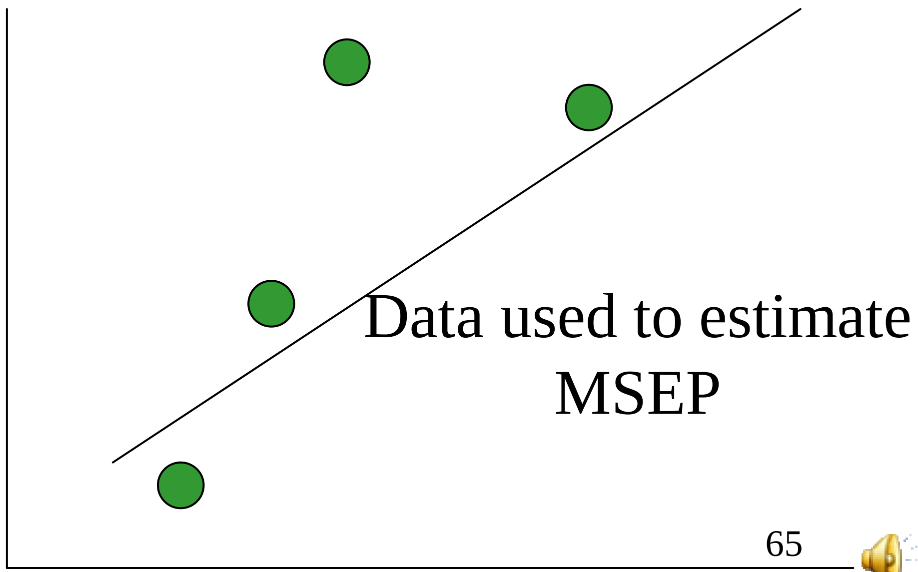
- This is important practical question
- We need estimate of error

Data splitting

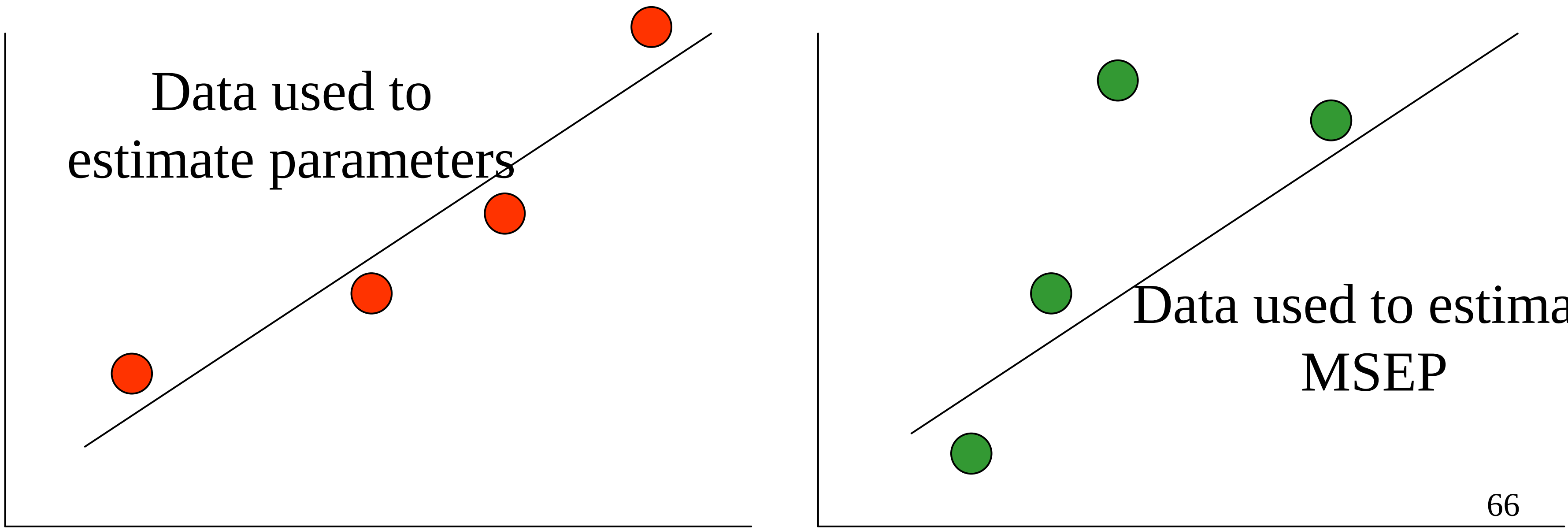

All data
Part of data to
estimate parameters
same model
Apply model to rest of
data. Can we use fit to
estimate MSEP?

- Yes, use MSE for second part of data to estimate MSEP (if data are from target distribution)
- Second part of data wasn't used to estimate parameters





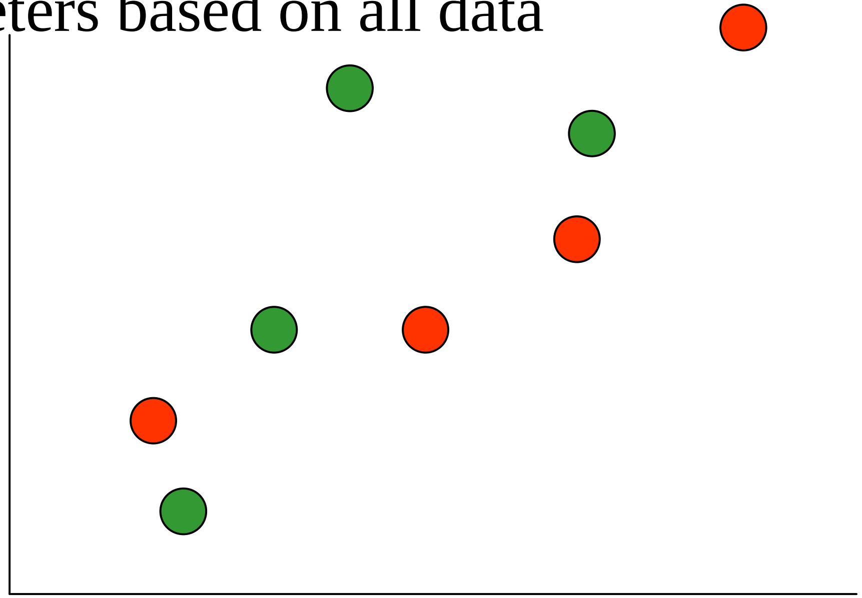
- What are disadvantages of data splitting?
  - Arbitrary division of data into two parts
  - Use only part of data to estimate parameters
  - Use only part of data to estimate MSEP



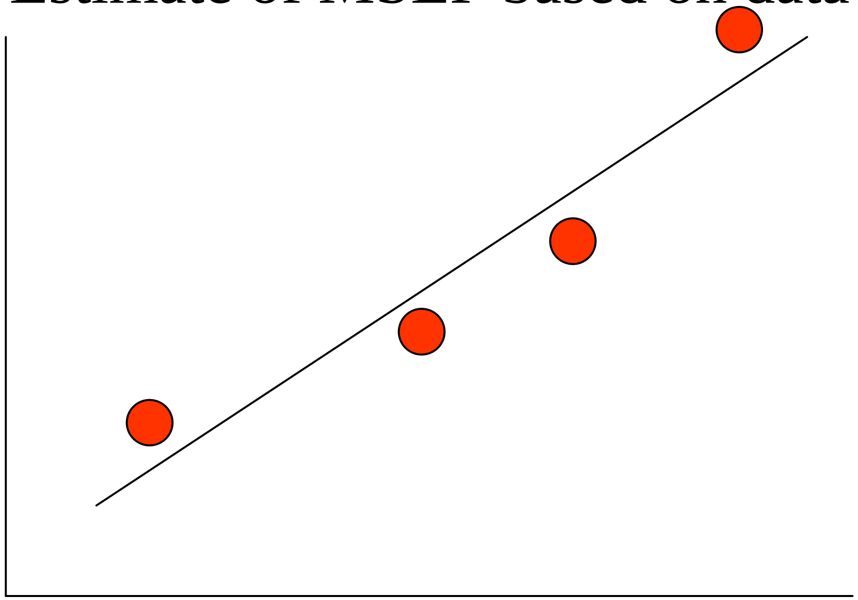
Other strategy

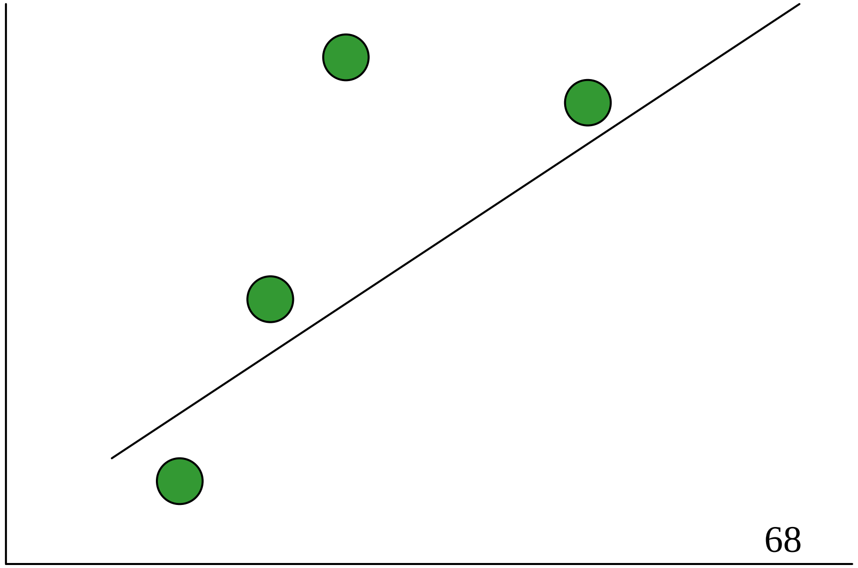
- Use all data to estimate parameters, then data splitting to estimate MSEP

Proposed parameters based on all data



Estimate of MSEP based on data splitting

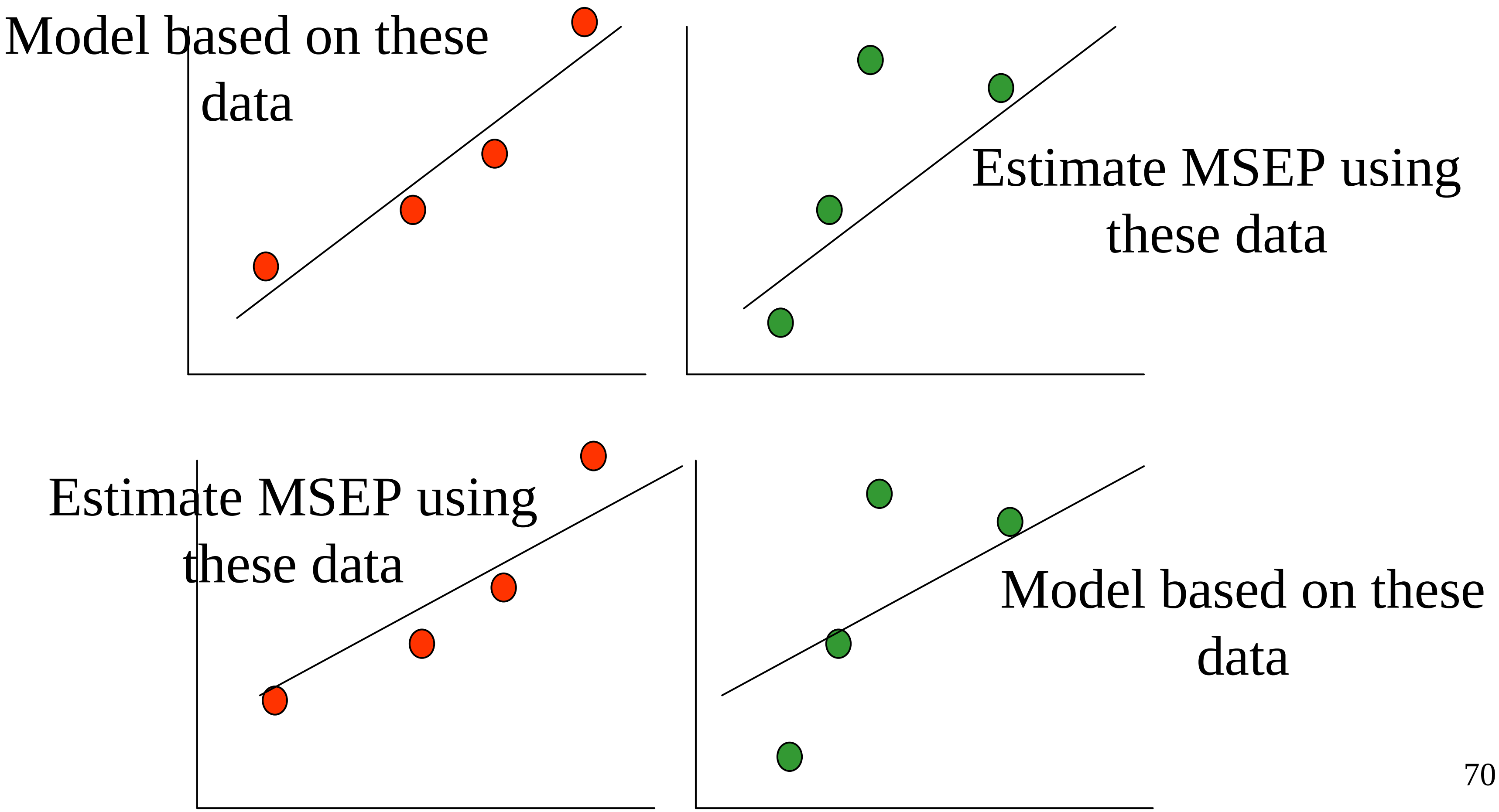




- What do you think of that?
- We want two things: parameter estimates for model and estimate of MSEP.
- This way, get best parameter estimates (use all data)
- And MSEP is correctly estimated.
  - The only problem is that MSEP refers to model based on half the data.
  - This probably overestimates MSEP for model based on all data.

Other strategy

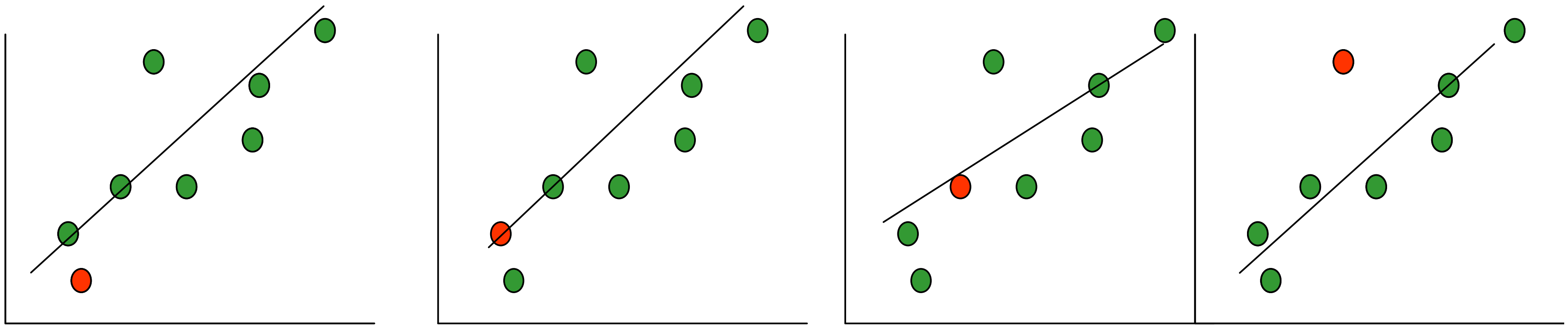
- As above, but do data splitting twice. Then use average MSEP.



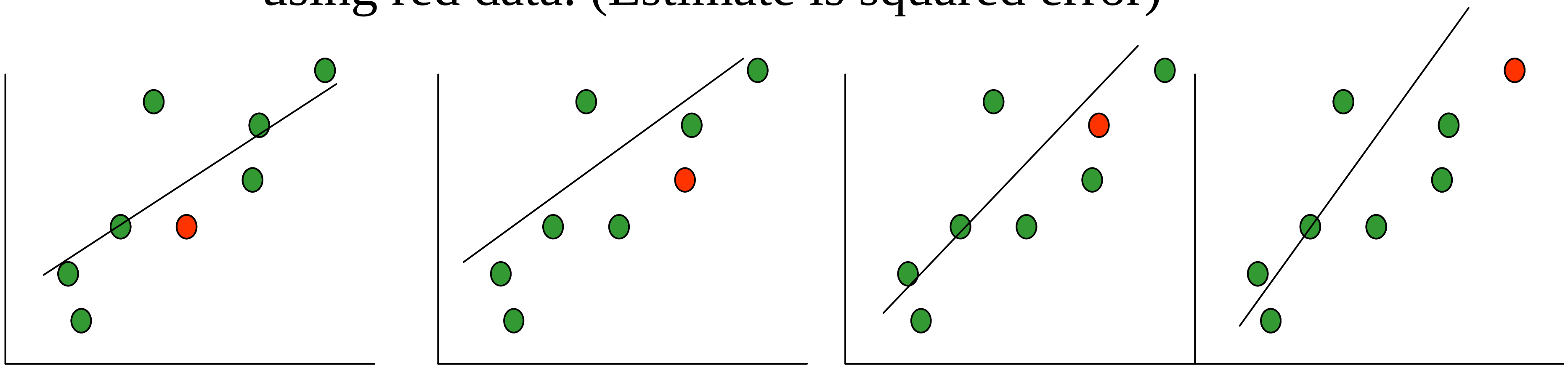
- What do you think of that?
- Less arbitrary
  - But split into two groups is still arbitrary
- Use all data to estimate MSEP
- But model for calculating MSEP isn't model that is proposed.
- Could we do better?

Cross validation

- Similar to above ideas.



Develop model using only green data. Estimate MSEP using red data. (Estimate is squared error)



For N data values, repeat N times. Final estimate of MSEP is average of N MSEP estimates.

Calculation with cross validation

$\boxed{Y1}$ Y2 Y3 ……. YN $\qquad$ $Y_1 - f_{-1}(U_1)$

Y1 $\boxed{Y2}$ Y3 ……. YN $\qquad$ $Y_2 - f_{-2}(U_2)$

Y1 Y2 Y3 ……. $\boxed{YN}$ $\qquad$ $Y_N - f_{-N}(U_N)$

$$\hat{M}SEP = 1/n \sum \left[Y_i - f_{-i}(U_i) \right]^2$$

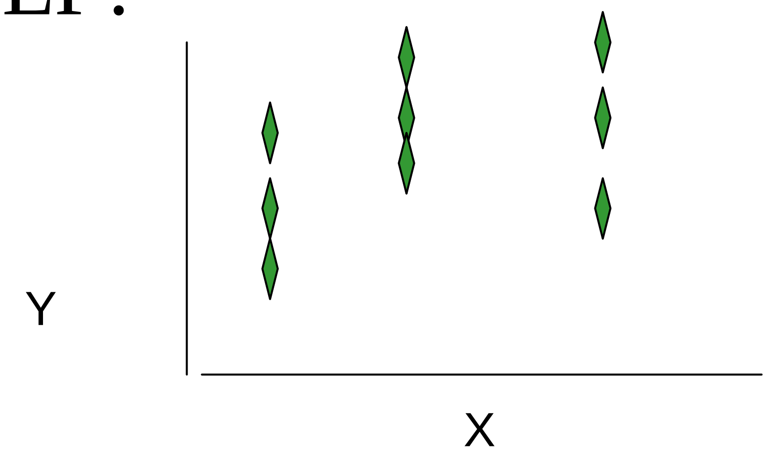
- What do you think of that?
- Proposed model based on all data.
- Evaluation based on model that uses all data but 1. So should be close to proposed model.

Decompose MSEP

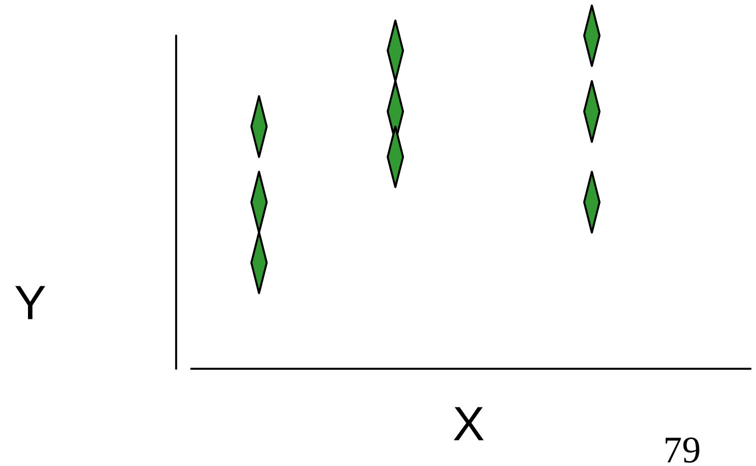
- MSEP can be written as the sum of two terms
- To help understand what determines predictive quality

First term

- Model has some explanatory variables
- They do not explain all the variability in Y
  - e.g. Temp, geometry, initial values don't explain all aphid-ladybeetle dynamics
- What is relation between unexplained variability and MSEP?

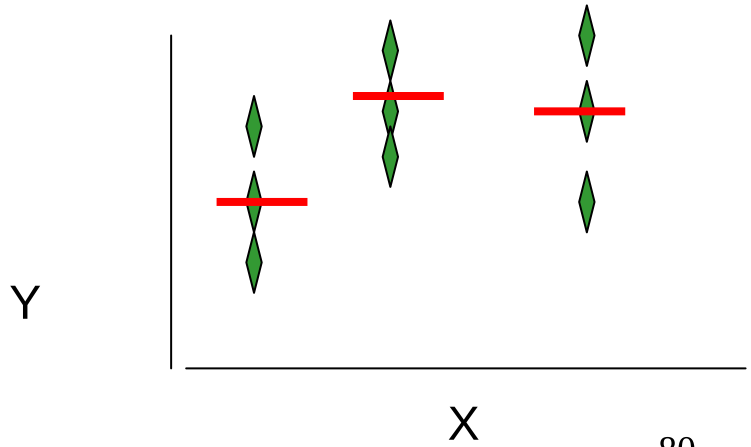


- For each value of explanatory variables X, model has unique prediction. Can’t be exact for all
- What is best possible model?



- Best possible model (smallest MSEP) equals average at each X.
- Remaining error is average variance for fixed X.

$$E_X\{\, \mathrm{var}(Y|X)^2\}$$

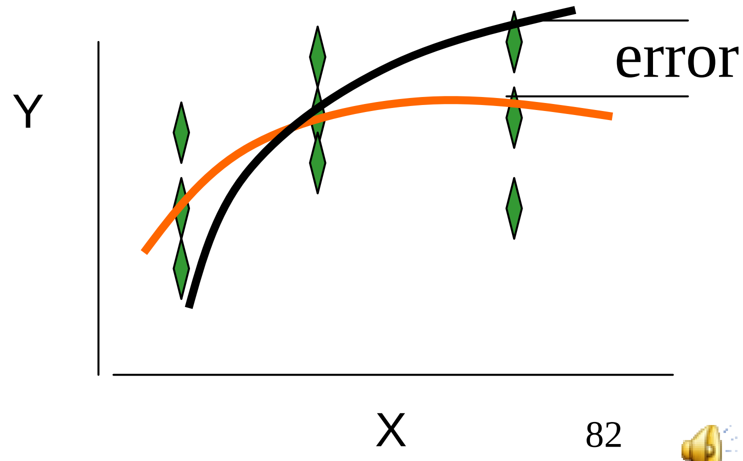


- Average variance for fixed X is lower limit for MSEP. Just depends on choice of explanatory variables.
- What is effect of adding more explanatory variables (more detailed model)?
  - Adding explanatory variables always reduces average variance for fixed X.
  - But some explanatory variables are important, others less important or irrelevent.
- What is second term in MSEP?

Second contribution to MSEP

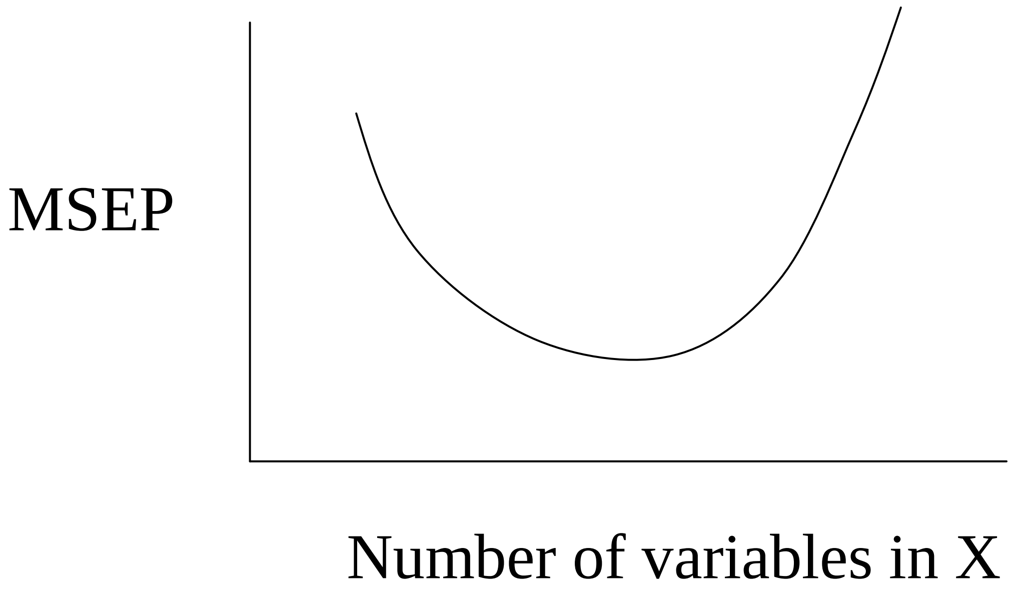
- Actual model will not be best model
  - Equations not exactly "correct".
  - Parameters not exactly "correct".
- Second term, model error for fixed X, measures difference between actual model and best model .

$$E_X\{\,[E_Y(Y|X) - \hat{Y}(X)]^2\}$$



- What is effect of extra detail (more variables in X or more equations) on second term?
  - This leads to more parameters. Each must be estimated. In general, more overall error.

- Overall effect of adding more variables in X?
  - Reduces average variance for fixed X.
  - But in general increases model error for fixed X



- What is good strategy?
  - Add important variables, that reduces average variance for fixed X a lot.
  - Don’t add unimportant variables.
  - Appropriate model complexity will depend on amount of data for estimating parameters.
  - This is particularly important for dynamic system models, where very complex models are possible

Example

Model	Variables in model Parameters in the model	*First term*	*2nd term*	$MSEP(\hat{\theta})$
$f_1(X;\ \theta)$	$x^{(1)}$ $\theta^{(0)}, \theta^{(1)}$	4.04	0.36	4.40
$f_3(X;\ \theta)$	$x^{(1)}\ x^{(21)}\ x^{(3)}$ $\theta^{(0)}, \theta^{(1)}, \theta^{(2)}, \theta^{(3)}$	0.04	0.01	0.05
$f_5(X;\ \theta)$	$x^{(1)}\ x^{(2)}\ x^{(3)}\ x^{(4)}\ x^{(5)}$ $\theta^{(0)}, \theta^{(1)}, \theta^{(2)}, \theta^{(3)}, \theta^{(4)}, \theta^{(5)}$	0.04	0.35	0.39

Summary

- Common criterion of prediction error is MSEP
  - Specify target population, target variables
- MSE is not in general a good estimator of MSEP
  - In particular if measured sample is not representative of target population, or if sample is used for parameter estimation
  - The difference between MSE and MSE depends on p/n
- MSEP is the result of two contributions
  - Variation due to fact that explanatory variables don’t explain all variability
  - Differences between model and best model
- MSEP has a minimum for some intermediate level of complexity

Evaluating decisions based on a model

- Not exactly the same as a good model for prediction.
- See David Makowski lecture.

THE END

References for examples

- Gent, M. P. N., 1994, Photosynthate Reserves during Grain Filling in Winter Wheat, Agron J 86:159-167
- Michalska, B. and Witos, A. 2000. Weather-based spring wheat yielding forecasting. EJPAU online. http://www.ejpau.media.pl/volume3/issue2/agronomy/art-04.html