Lecture 7

Principles of Modeling for Cyber-Physical Systems

Instructor: Madhur Behl

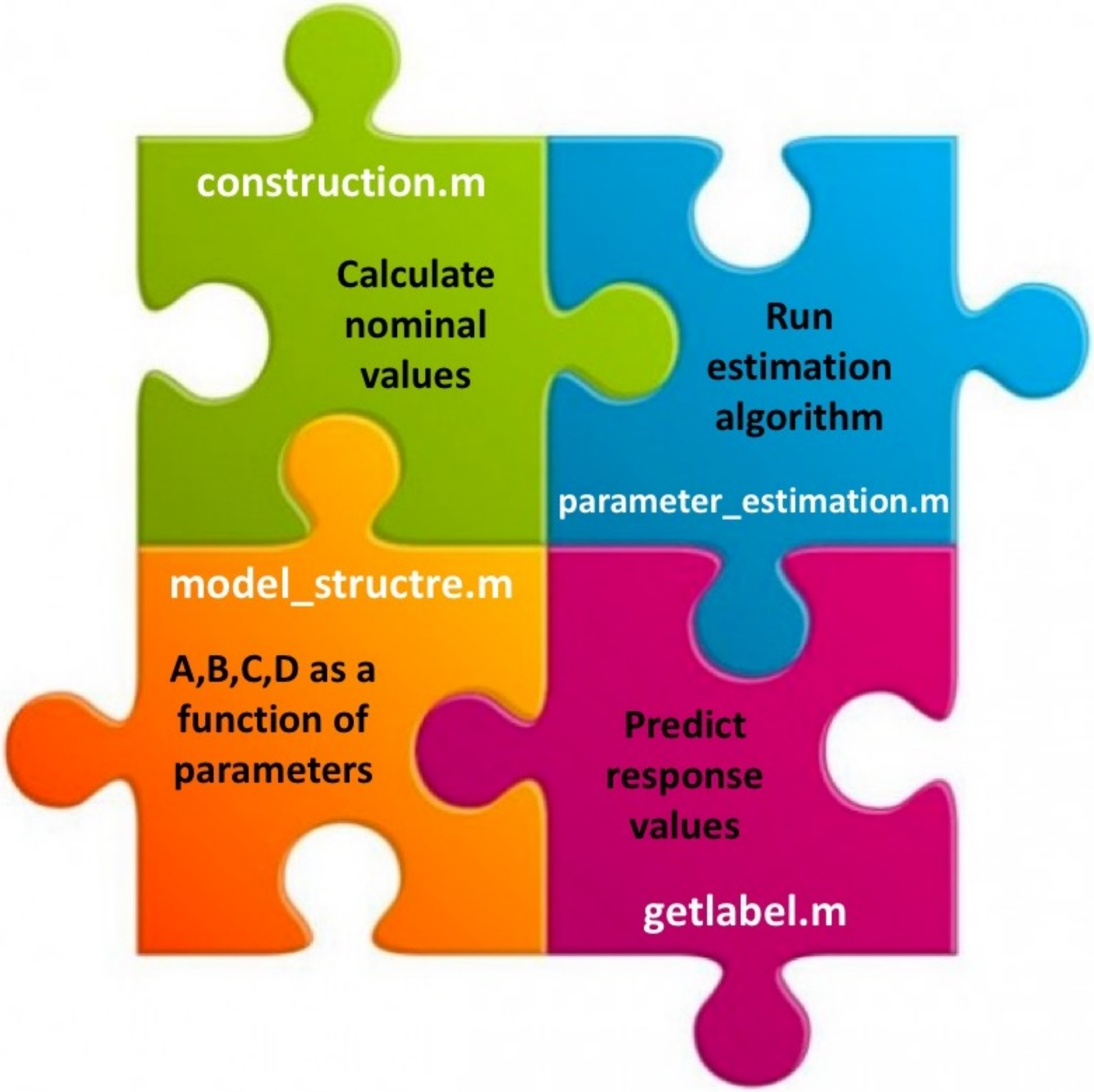
Topics we will cover

- Model evaluation
- Model sensitivity and uncertainty
- Model order reduction
- Model predictive control

But first..

- **Assignment 4 is out:**
  - getlabel.m – generate predicted model outputs for a given set of parameters
  - parameter_estimation.m – format i/o data and implement NLLS.
  - Model evaluation
  - Use the templates on Collab to save time.
  - Due in ~ >1 week. Thursday, October 11, by 11:59pm

Worksheet 4


construction.m
Calculate nominal values
Run estimation algorithm
parameter_estimation.m
model_structre.m
A,B,C,D as a function of parameters
Predict response values
getlabel.m

How do I know my model is any good ?

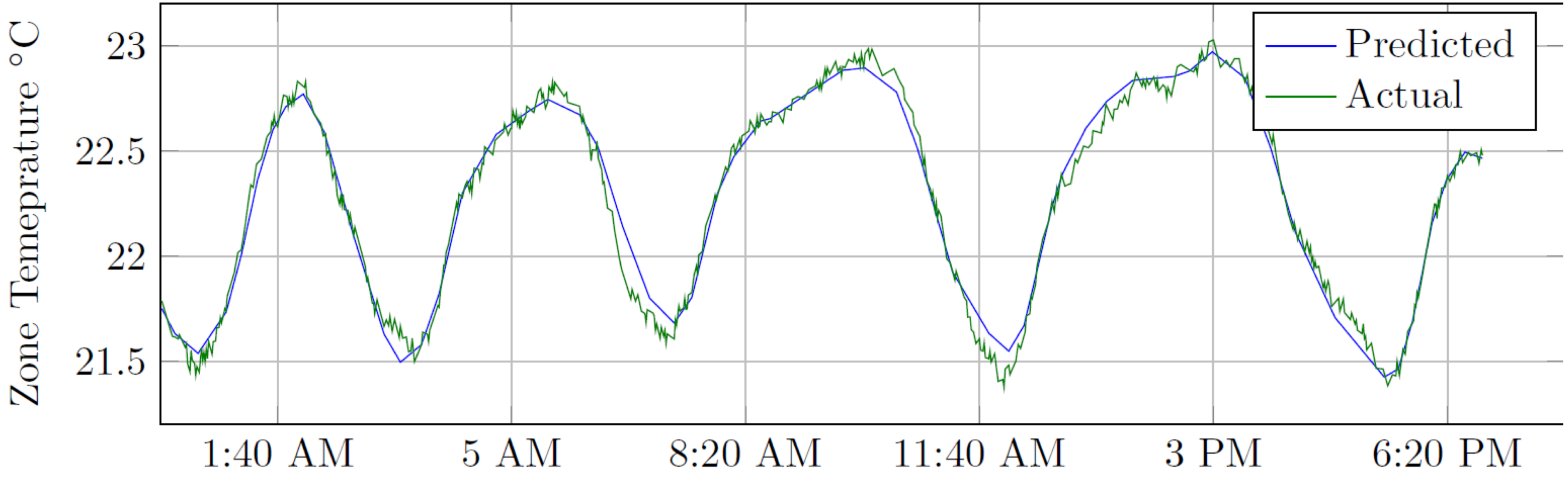
- **Purpose** – predict the zone temperature based on the disturbances and control inputs.

- **"Good"** = How accurate is the predicted zone temperature (response) ?

Predict response for optimal θ^*

$$\begin{pmatrix} y(0) \\ y(1) \\ \vdots \\ y(N-1) \end{pmatrix} = \boldsymbol{\mathcal{O}}_{\theta^*}\, x(0) + \boldsymbol{\mathcal{T}}_{\theta^*} \begin{pmatrix} u(0) \\ u(1) \\ \vdots \\ u(N-1) \end{pmatrix}$$

How do I know my model is any good ?



Quick review: Goodness of fit.

- Root mean squared error: RMSE
- Coefficient of determination: R^2
- Normalized root mean squared error: NRMSE
- Mean absolute error - MAE

What is Root Mean Squared Error (RMSE)?

$$SSE = \sum_{j=1}^{N} \left(y_{true,j} - \hat{y}_{predicted,j}\right)^2$$

Sum of squared error

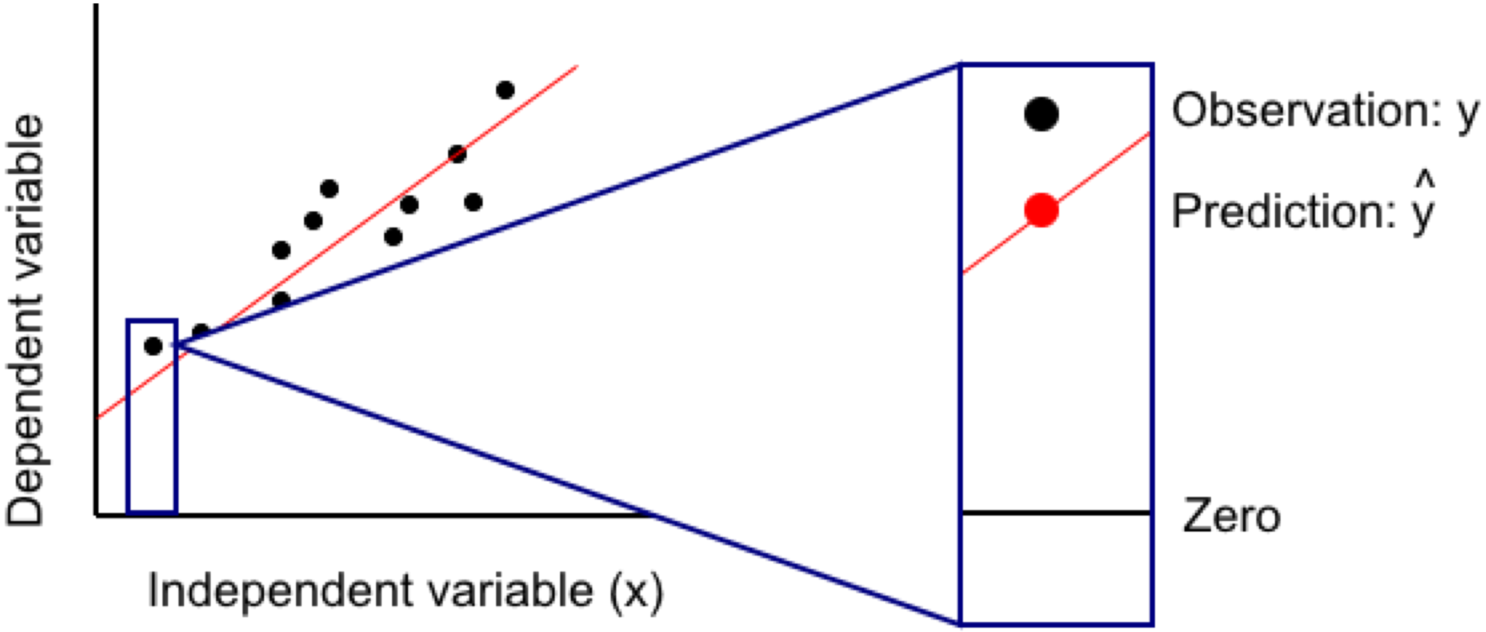
$$MSE = \frac{\sum_{j=1}^{N} \left(y_{true,j} - \hat{y}_{predicted,j}\right)^2}{N}$$

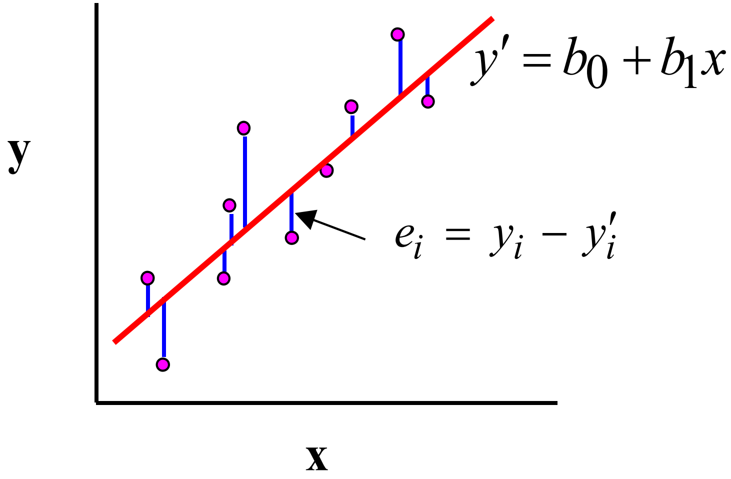
Mean squared error

$$RMSE = \sqrt{\frac{\sum_{j=1}^{N} \left(y_{true,j} - \hat{y}_{predicted}\right)^2}{N}}$$

Root mean squared error

A simple example

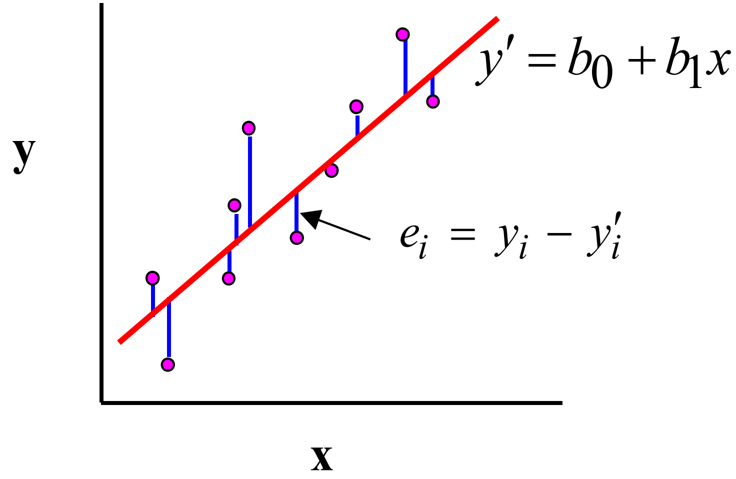




A simple example

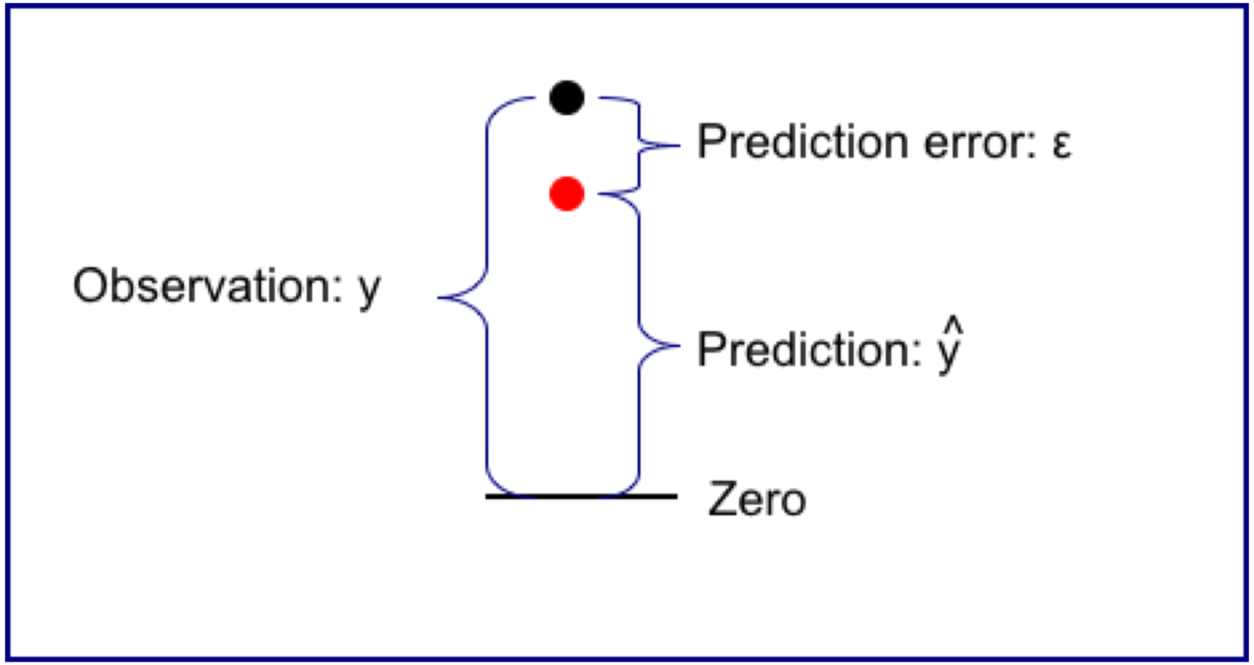
$$y_i = b_0 + b_1 x_i + e_i$$

- y_i: observed response
- b_0: estimate of β_0
- b_1: estimate of β_1
- e_i: residual



Sum of squared error (SSE): $S(b_0, b_1) = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - y_i')^2$

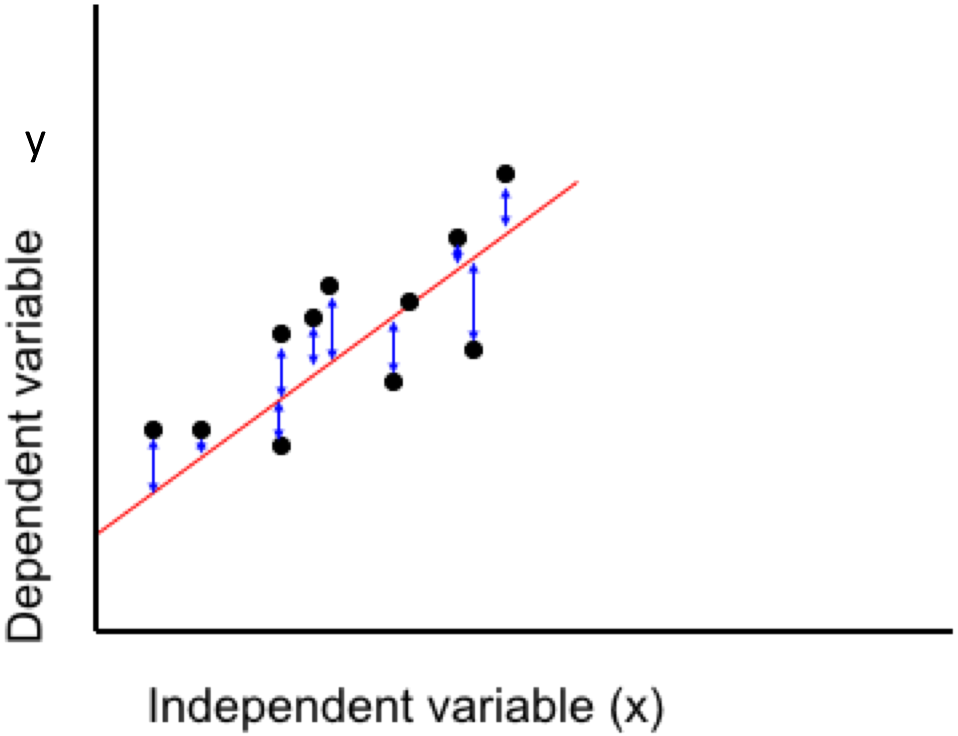
A simple example



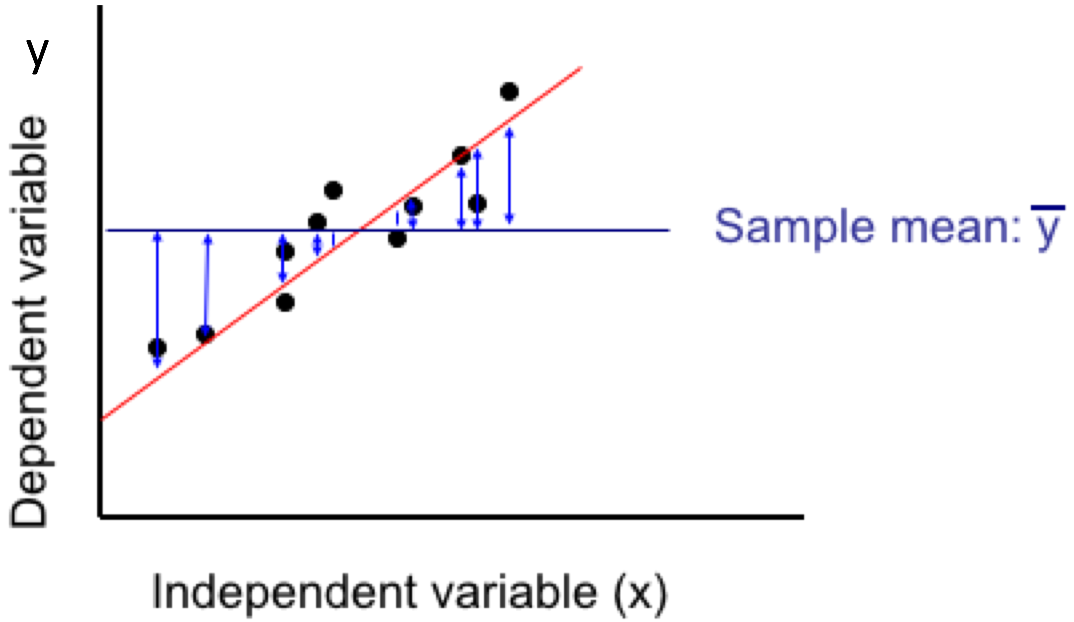
$$y = \hat{y} + \varepsilon$$

Actual = Explained + Error

How much variation in *y* can the model explain ?



Total variation in *y*



$$SE_{\bar{y}} = \sum_{j=1}^{N} \left(y_{true,j} - \bar{y}_{sample}\right)^2$$

How much variation in y is described by the model ?

$$SE_{\bar{y}} = \sum_{j=1}^{N} \left(y_{true,j} - \bar{y}_{sample}\right)^2$$

$$SSE = \sum_{j=1}^{N} \left(y_{true,j} - \hat{y}_{predicted,j}\right)^2$$

$$\frac{SEE}{SE_{\bar{y}}}$$

Ratio of variation of error not explained by model to total variation in y

R^2: Coefficient of determination

$$SE_{\bar{y}} = \sum_{j=1}^{N} \left(y_{true,j} - \bar{y}_{sample}\right)^2$$

$$SSE = \sum_{j=1}^{N} \left(y_{true,j} - \hat{y}_{predicted,j}\right)^2$$

$$R^2 = 1 - \frac{SEE}{SE_{\bar{y}}}$$

Coefficient of determination

SSE is low
"Good" fit
R^2 close to 1

Normalized Root Mean Squared Error (NRMSE)

$$NRMSE = \frac{RMSE}{y_{true_{max}} - y_{true_{min}}} \; or \; \frac{RMSE}{\bar{y}_{true}}$$

$$RMSE = \sqrt{\frac{\sum_{j=1}^{N} \left(y_{true,j} - \hat{y}_{predicted}\right)^2}{N}}$$

Root mean squared error

Madhur Behl madhur.behl@virginia.edu

MAE: Mean absolute error

$$MAE = \frac{1}{N}\sum_{j=1}^{N}\left|y_{true,j} - \hat{y}_{predicted,j}\right|$$

MAE measures the average magnitude of the errors in a set of predictions, without considering their direction

MAE v RMSE: Similarities

- Both MAE and RMSE express average model prediction error in units of the variable of interest.
- Both metrics can range from 0 to ∞ and are indifferent to the direction of errors.
- They are negatively-oriented scores, which means lower values are better.

MAE v RMSE:

RMSE is more useful when large errors are particularly undesirable.

RMSE does not necessarily increase with the variance of the errors.

MAE v RMSE: Example 1

CASE 1: Evenly distributed errors

ID	Error	|Error|	Error^2
1	2	2	4
2	2	2	4
3	2	2	4
4	2	2	4
5	2	2	4
6	2	2	4
7	2	2	4
8	2	2	4
9	2	2	4
10	2	2	4

MAE	RMSE
2.000	2.000

MAE v RMSE: Example 1

CASE 1: Evenly distributed errors

ID	Error	|Error|	Error^2
1	2	2	4
2	2	2	4
3	2	2	4
4	2	2	4
5	2	2	4
6	2	2	4
7	2	2	4
8	2	2	4
9	2	2	4
10	2	2	4

MAE	RMSE
2.000	2.000

CASE 2: Small variance in errors

ID	Error	|Error|	Error^2
1	1	1	1
2	1	1	1
3	1	1	1
4	1	1	1
5	1	1	1
6	3	3	9
7	3	3	9
8	3	3	9
9	3	3	9
10	3	3	9

MAE	RMSE
2.000	2.236

MAE v RMSE: Example 1

CASE 1: Evenly distributed errors

ID	Error	|Error|	Error^2
1	2	2	4
2	2	2	4
3	2	2	4
4	2	2	4
5	2	2	4
6	2	2	4
7	2	2	4
8	2	2	4
9	2	2	4
10	2	2	4

MAE	RMSE
2.000	2.000

CASE 2: Small variance in errors

ID	Error	|Error|	Error^2
1	1	1	1
2	1	1	1
3	1	1	1
4	1	1	1
5	1	1	1
6	3	3	9
7	3	3	9
8	3	3	9
9	3	3	9
10	3	3	9

MAE	RMSE
2.000	2.236

CASE 3: Large error outlier

ID	Error	|Error|	Error^2
1	0	0	0
2	0	0	0
3	0	0	0
4	0	0	0
5	0	0	0
6	0	0	0
7	0	0	0
8	0	0	0
9	0	0	0
10	20	20	400

MAE	RMSE
2.000	6.325

MAE v RMSE: Example 2

CASE 4: Errors = 0 or 5

ID	Error	|Error|	Error^2
1	5	5	25
2	0	0	0
3	5	5	25
4	0	0	0
5	5	5	25
6	0	0	0
7	5	5	25
8	0	0	0
9	5	5	25
10	0	0	0

MAE	RMSE
2.500	3.536

CASE 5: Errors = 3 or 4

ID	Error	|Error|	Error^2
1	3	3	9
2	4	4	16
3	3	3	9
4	4	4	16
5	3	3	9
6	4	4	16
7	3	3	9
8	4	4	16
9	3	3	9
10	4	4	16

MAE	RMSE
3.500	3.536

Madhur Behl madhur.behl@virginia.edu

MAE v RMSE

[MAE] ≤ [RMSE] ≤ [MAE * sqrt(n)]

MATLAB implementation

goodnessOfFit

Goodness of fit between test and reference data

Syntax

```
fit = goodnessOfFit(x,xref,cost_func)
```

Predicted response

Measured response

`cost_func` — Cost function to determine goodness of fit.

`cost_func` is specified as one of the following values:

- `'MSE'` — Mean square error:

  $$fit = \frac{\|x - xref\|^2}{Ns}$$

  where, N_s is the number of samples, and ‖ indicates the

- `'NRMSE'` — Normalized root mean square error:

  $$fit(i) = 1 - \frac{\|xref(:, i) - x(:, i)\|}{\|xref(:, i) - mean(xref(:, i))\|}$$

  where, ‖ indicates the 2-norm of a vector. `fit` is a row v

  NRMSE costs vary between `-Inf` (bad fit) to 1 (perfect
  `xref`.

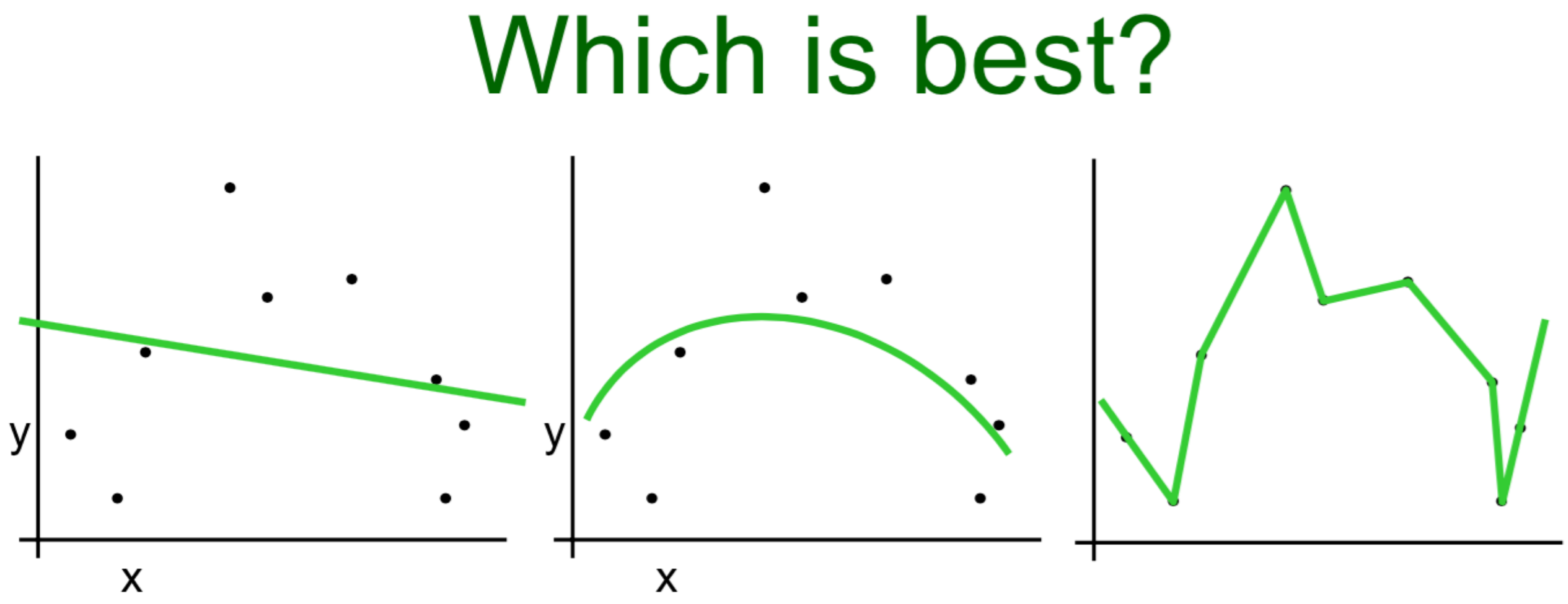
- `'NMSE'` — Normalized mean square error:

  $$fit(i) = 1 - \frac{\|xref(:, i) - x(:, i)\|^2}{\|xref(:, i) - mean(xref(:, i))\|^2}$$

  where, ‖ indicates the 2-norm of a vector. `fit` is a row v

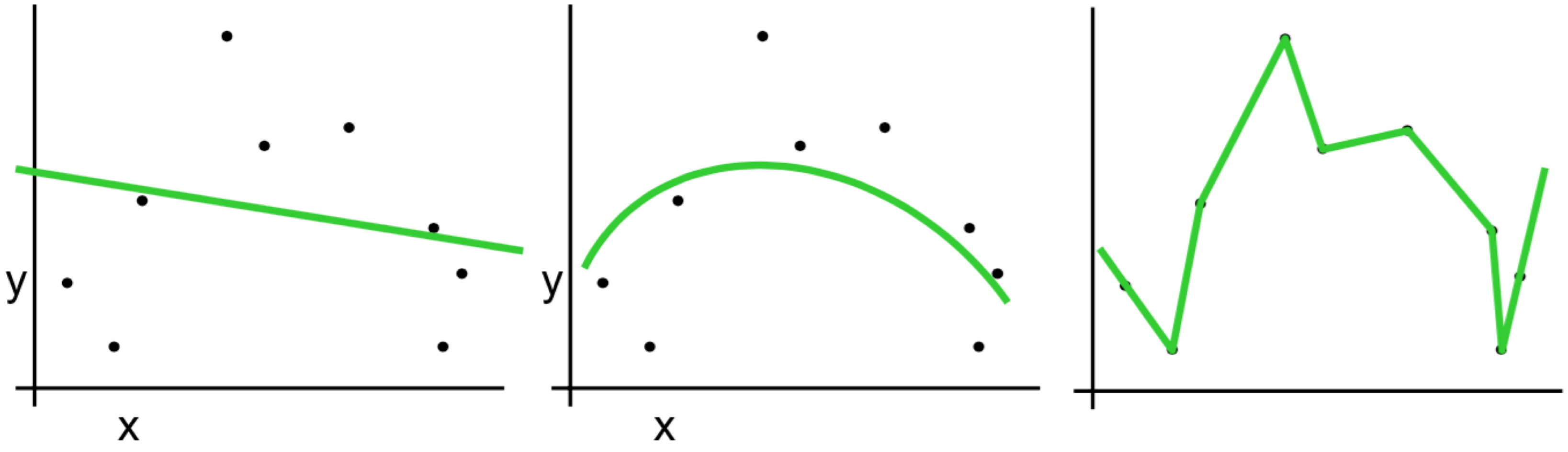
  NMSE costs vary between `-Inf` (bad fit) to 1 (perfect fi

Regress to impress !



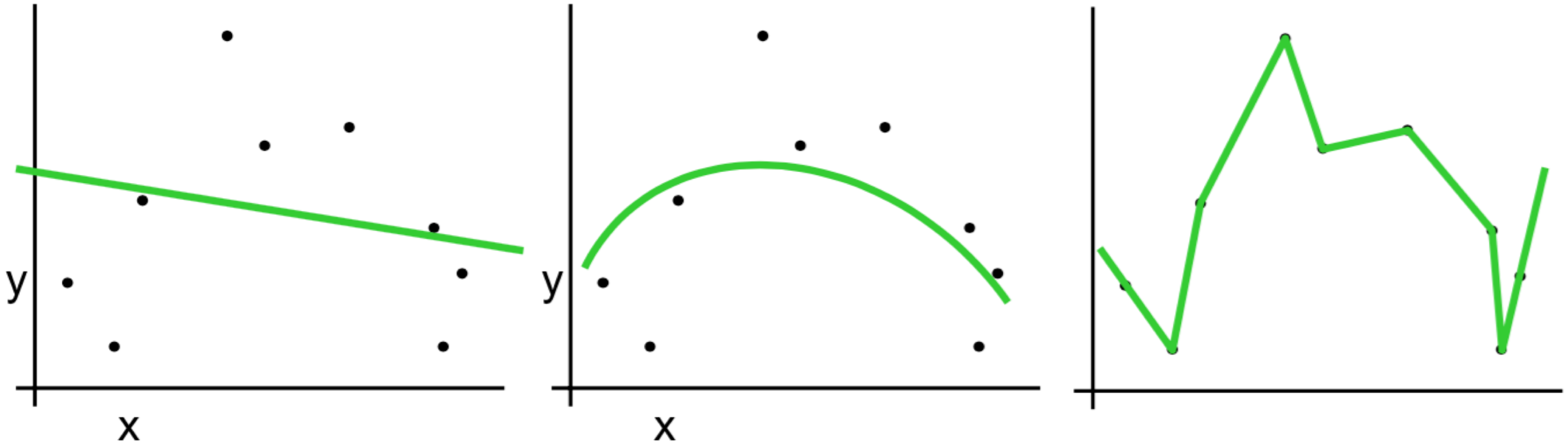
Regress to impress !

Which is best?



Why not choose the method with the best fit to the data?

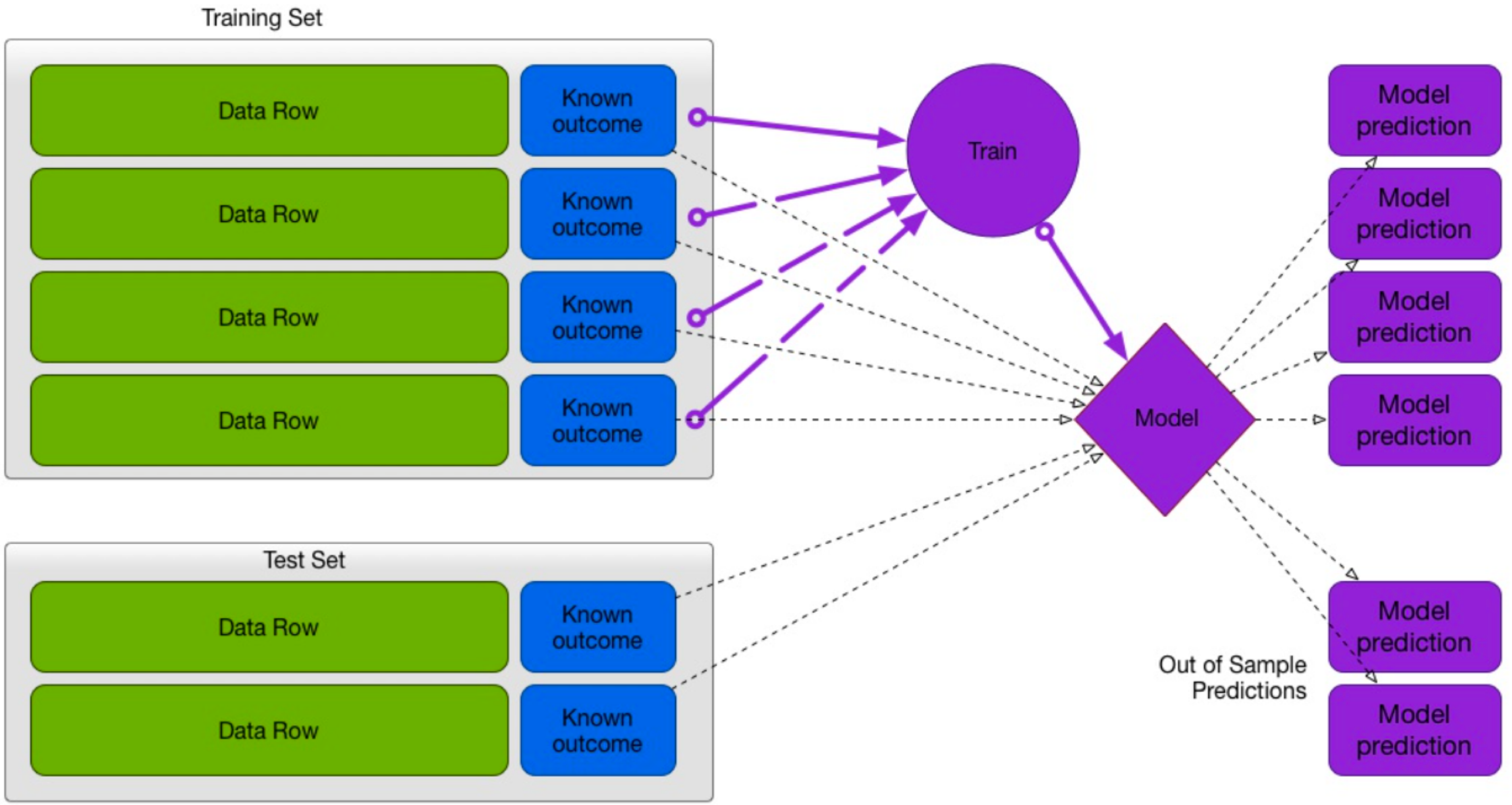
What do we really want?



Why not choose the method with the best fit to the data?

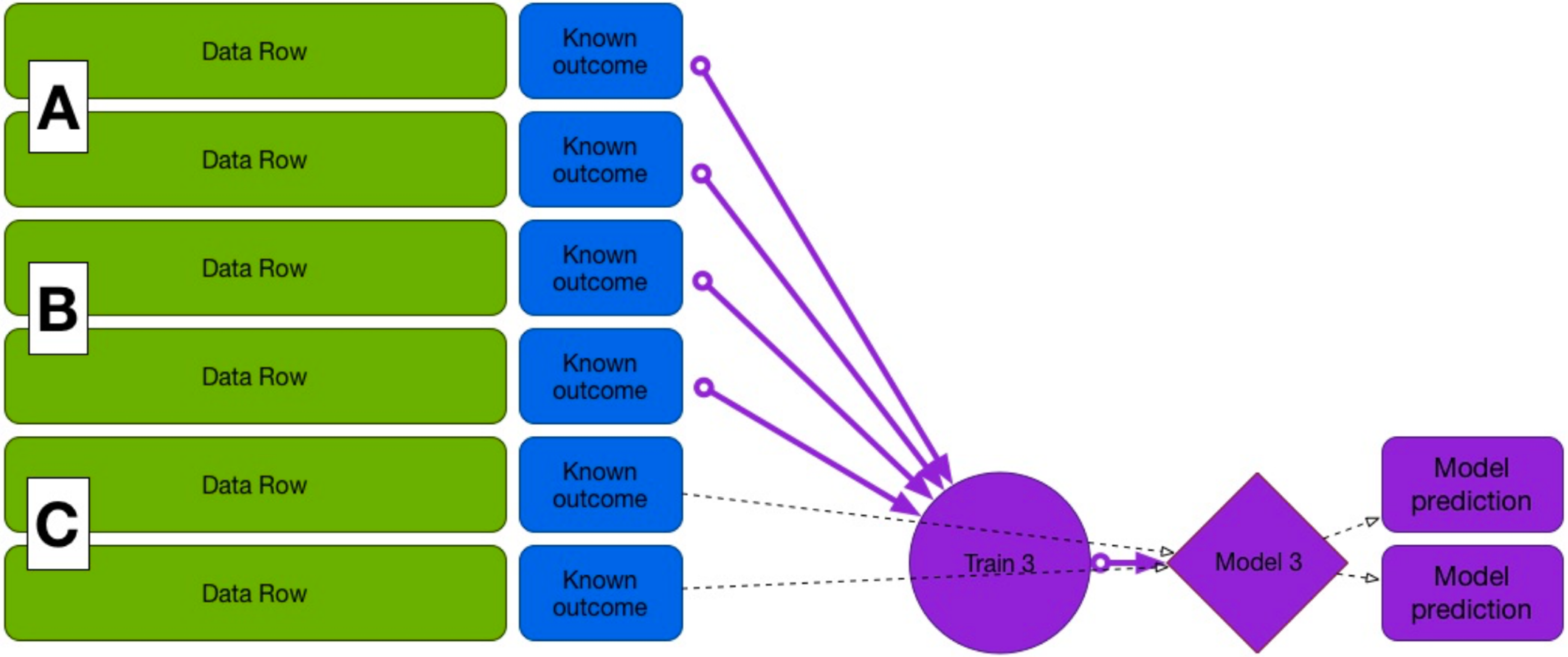
"How well are you going to predict future data drawn from the same distribution?"

Test/train split



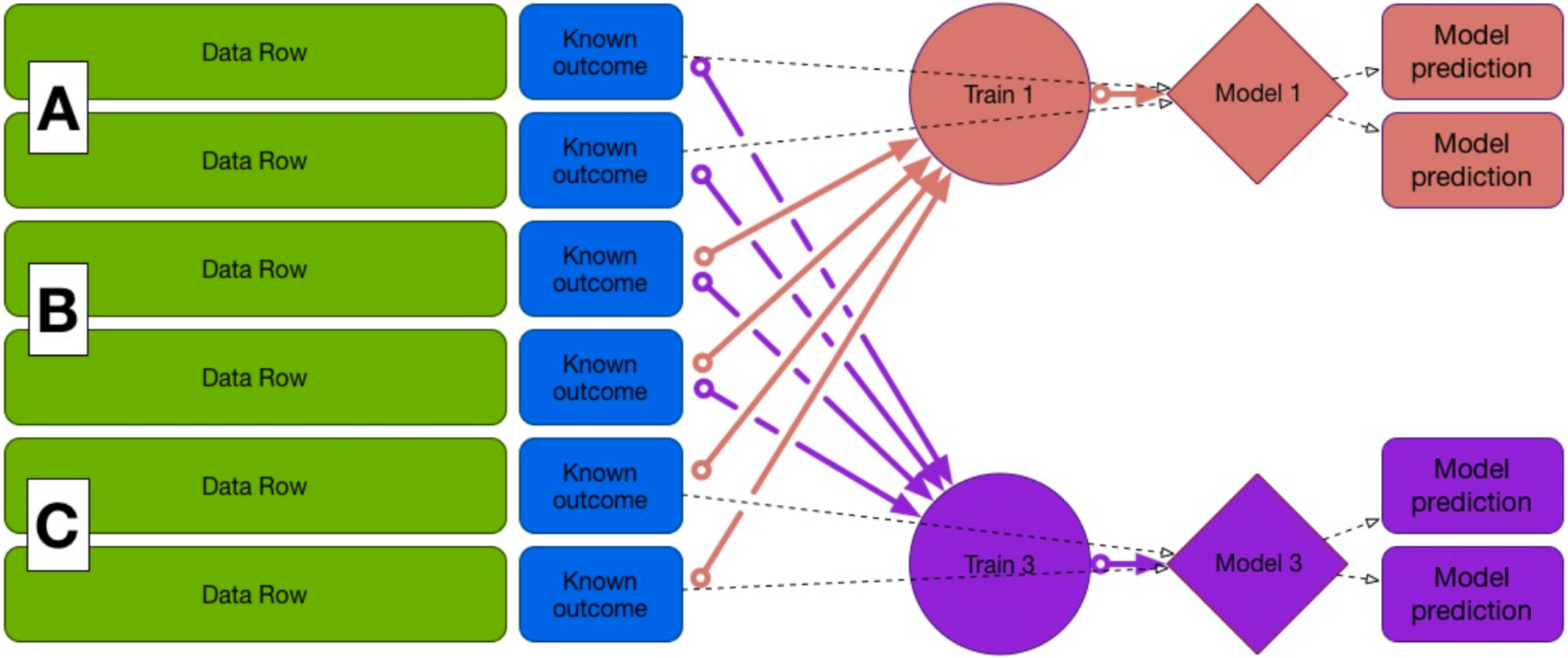
Madhur Behl madhur.behl@virginia.edu

Cross validation

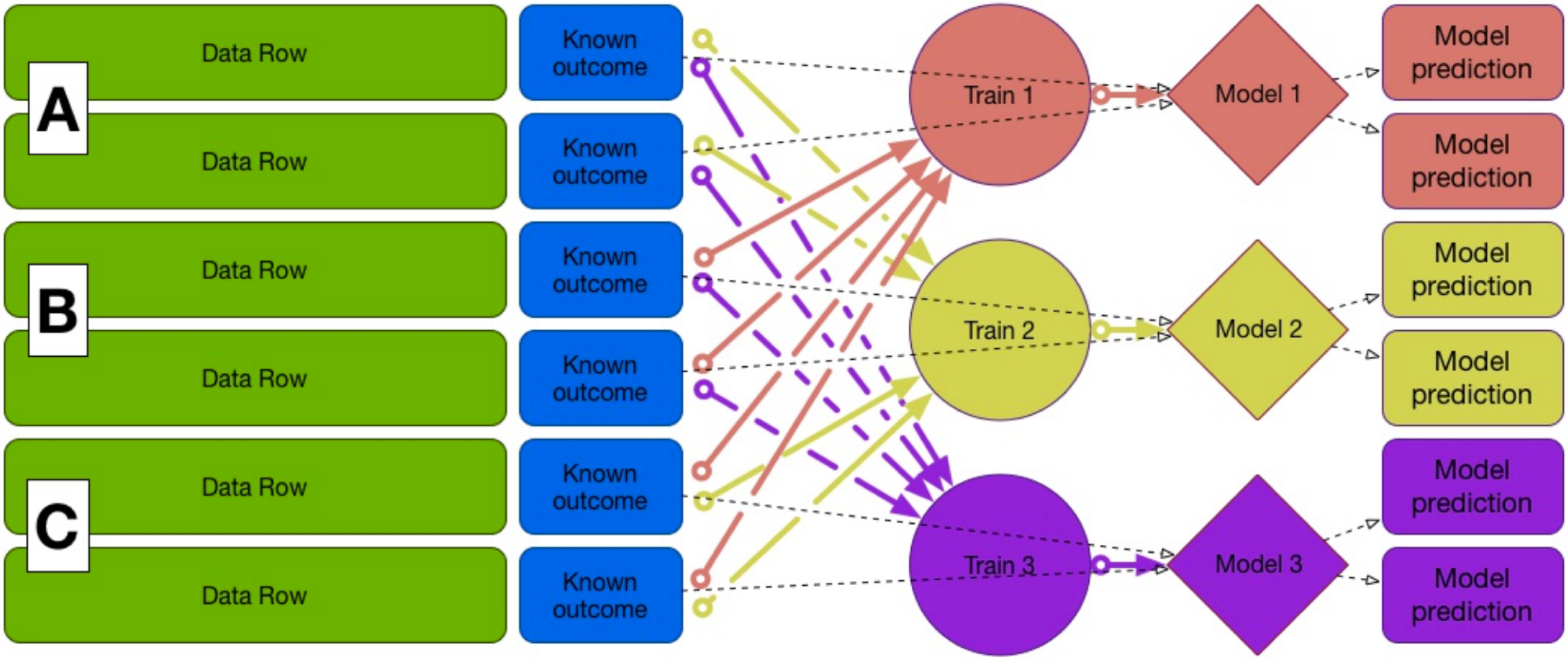


Madhur Behl madhur.behl@virginia.edu

Cross validation



Cross validation



Worksheet 4 discussion