Introduction to Machine Learning – Subset Selection

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Slides based off slides courtesy of Jordan Crouser (https://jcrouser.github.io/)

Plan for Today

- Validation / Error
- Linear Model selection and Regularization
  - Best Subset Selection
  - Stepwise Selection
  - Choosing the Optimal Model

Motivation

So far, we've thought about how to evaluate our models using error calculations.

Besides fit, what else might influence the effectiveness / accuracy of our models?

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Besides fit, what else might influence the effectiveness / accuracy of our models?

- https://www.ted.com/talks/joy_buolamwini_how_i_m_fighting_bias_in_algorithms?language=en
- http://gendershades.org/overview.html

Motivation

Moving back to linear models…

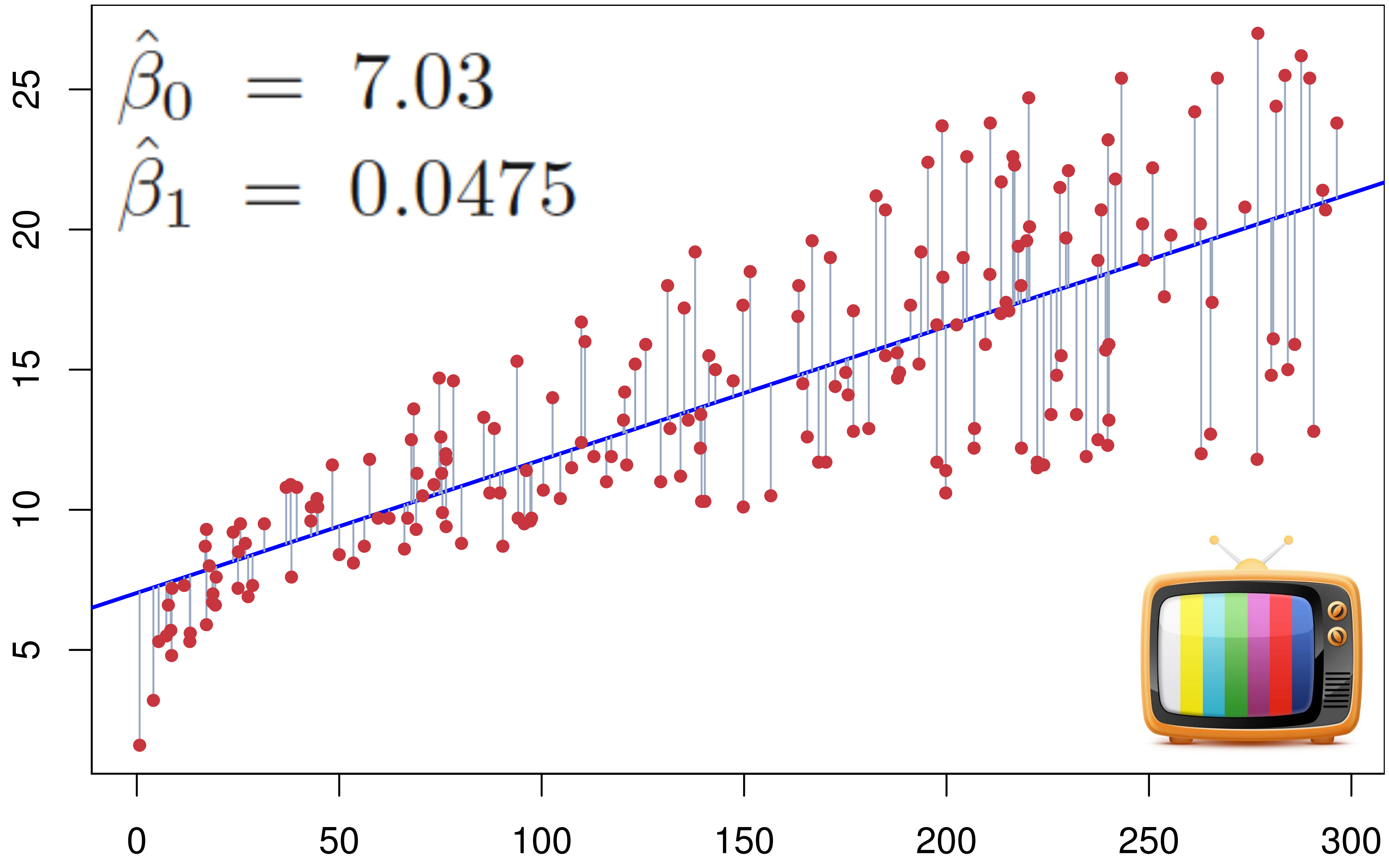
In regression, the standard model is:

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$$

How did we find the coefficients for this model?

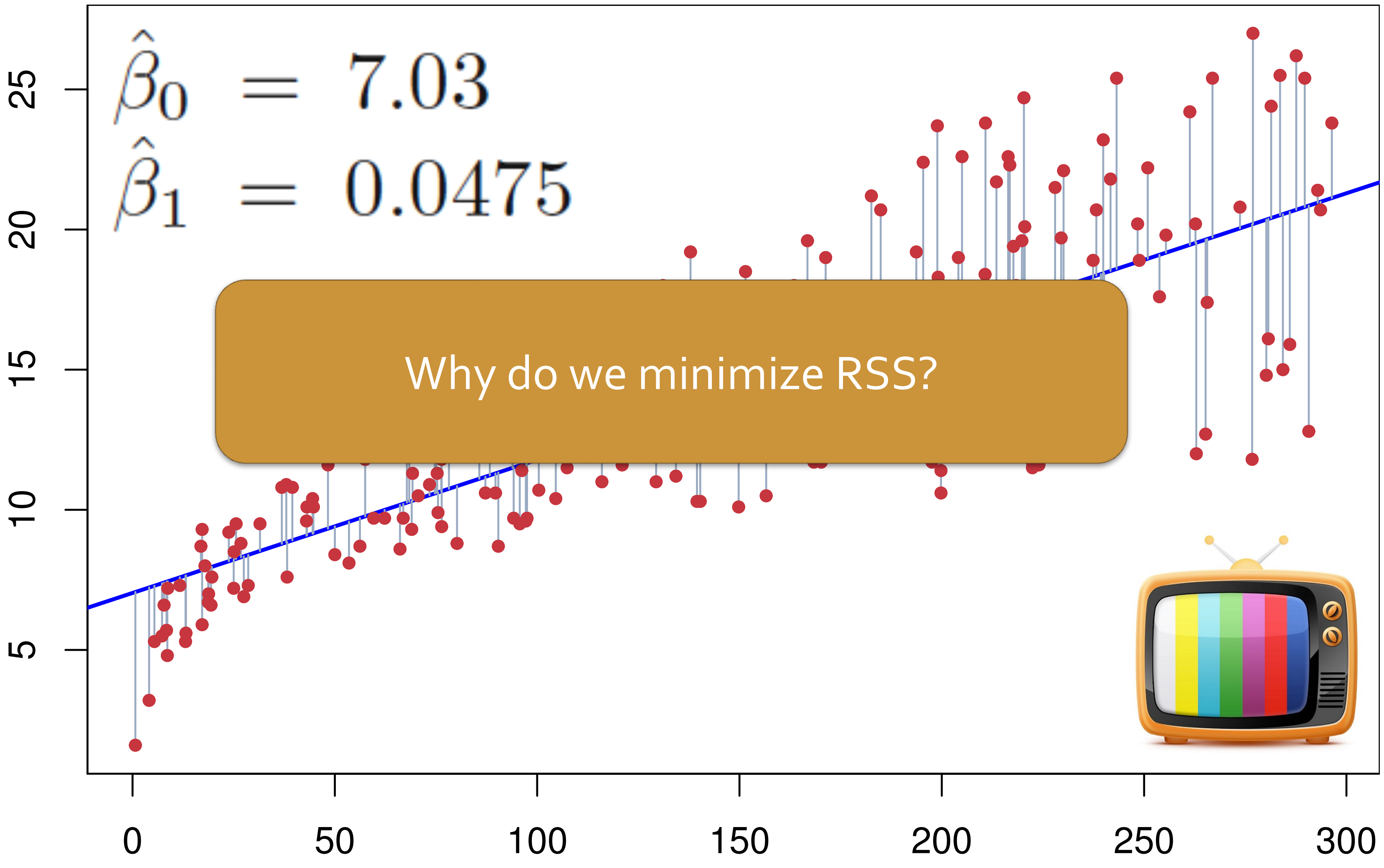
Motivation

Flashback: minimizing RSS



Motivation

Flashback: minimizing RSS



Why do we minimize RSS?

Motivation

Least Squares

Assumption 1: we're fitting a linear model

Assumption 2: the true relationship between the predictors and the response is linear

What can we say about the **bias** of our least-squares estimates?

Motivation

Least Squares

Assumption 1: we're fitting a linear model

Assumption 2: the true relationship between the predictors and the response is linear

Consider:

- Case 1: the number of observations in the training data is much larger than the number of predictors (n >>p)
  - Variance should be low; our model will perform well on test observations

Motivation

Least Squares

Assumption 1: we’re fitting a linear model

Assumption 2: the true relationship between the predictors and the response is linear

Consider:

- Case 2: the number of observations is not much larger than the number of predictors ($n \approx p$)
  - Variance will get (pretty) high; performance of the model will suffer

Motivation

Least Squares

Assumption 1: we're fitting a linear model

Assumption 2: the true relationship between the predictors and the response is linear

Consider:

- Case 3: the number of observations smaller than the number of predictors ($n < p$)
  - Variance will be infinite; we will no longer get a unique least squares estimate

Motivation

So what can we do in cases where $n < p$ or $n \approx p$?

Ideas?

Subset selection

So what can we do in cases where $n < p$ or $n \approx p$?

Subset selection

- If we have too many predictors, we can get rid of some to improve model performance

- But how will we choose?

Ideas?

Subset selection

So what can we do in cases where $n < p$ or $n \approx p$?

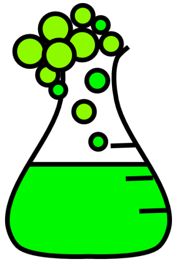
Subset selection

- If we have too many predictors, we can get rid of some to improve model performance

- But how will we choose?
  - For each possible subset of predictors
    - Fit least squares
  - Choose the "best" model from the collection

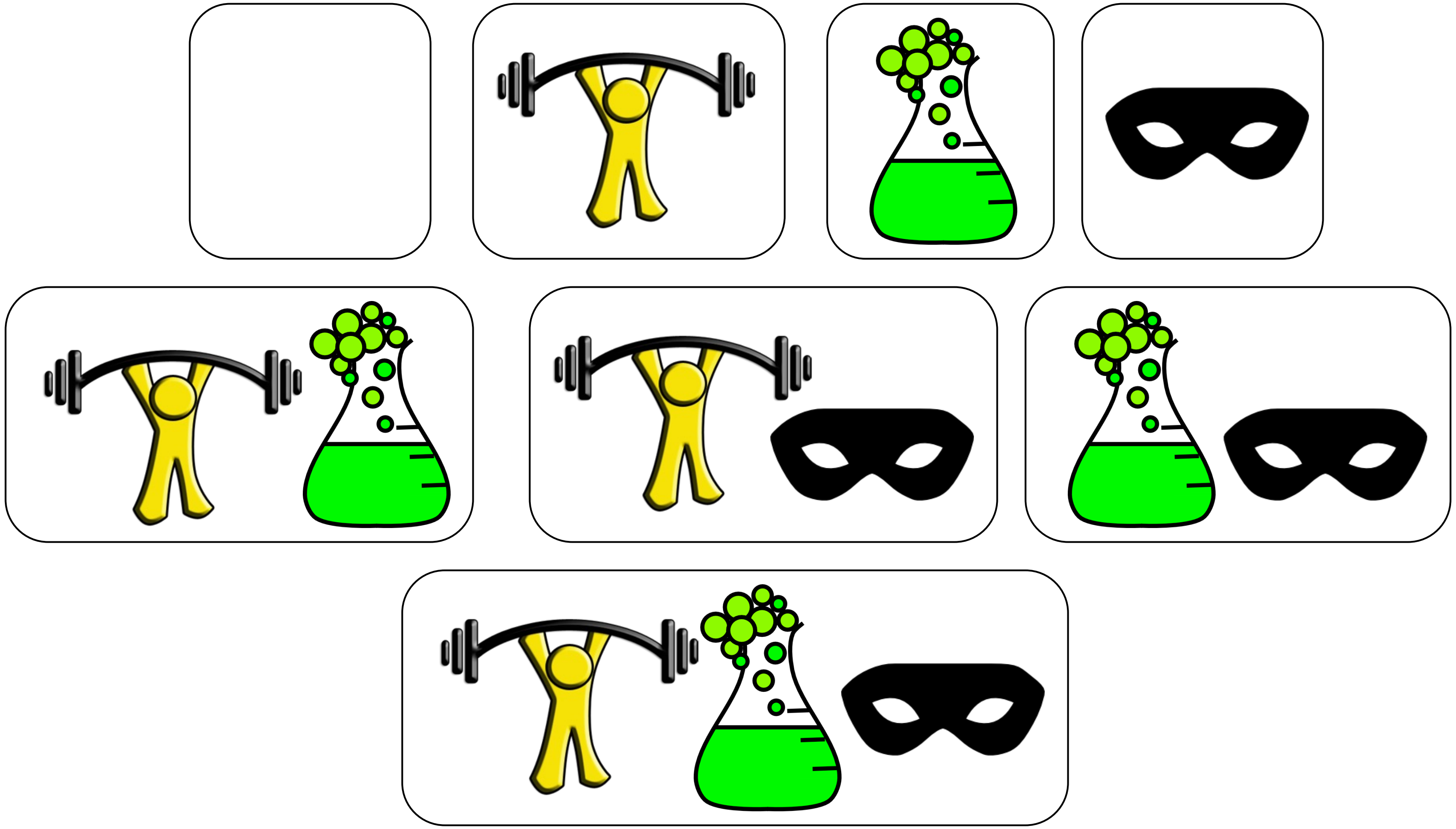
Subset selection

Superhero Example

$height = \beta_1 \big($  $\big) + \beta_2 \big($  $\big) + \beta_3 \big($  $\big)$

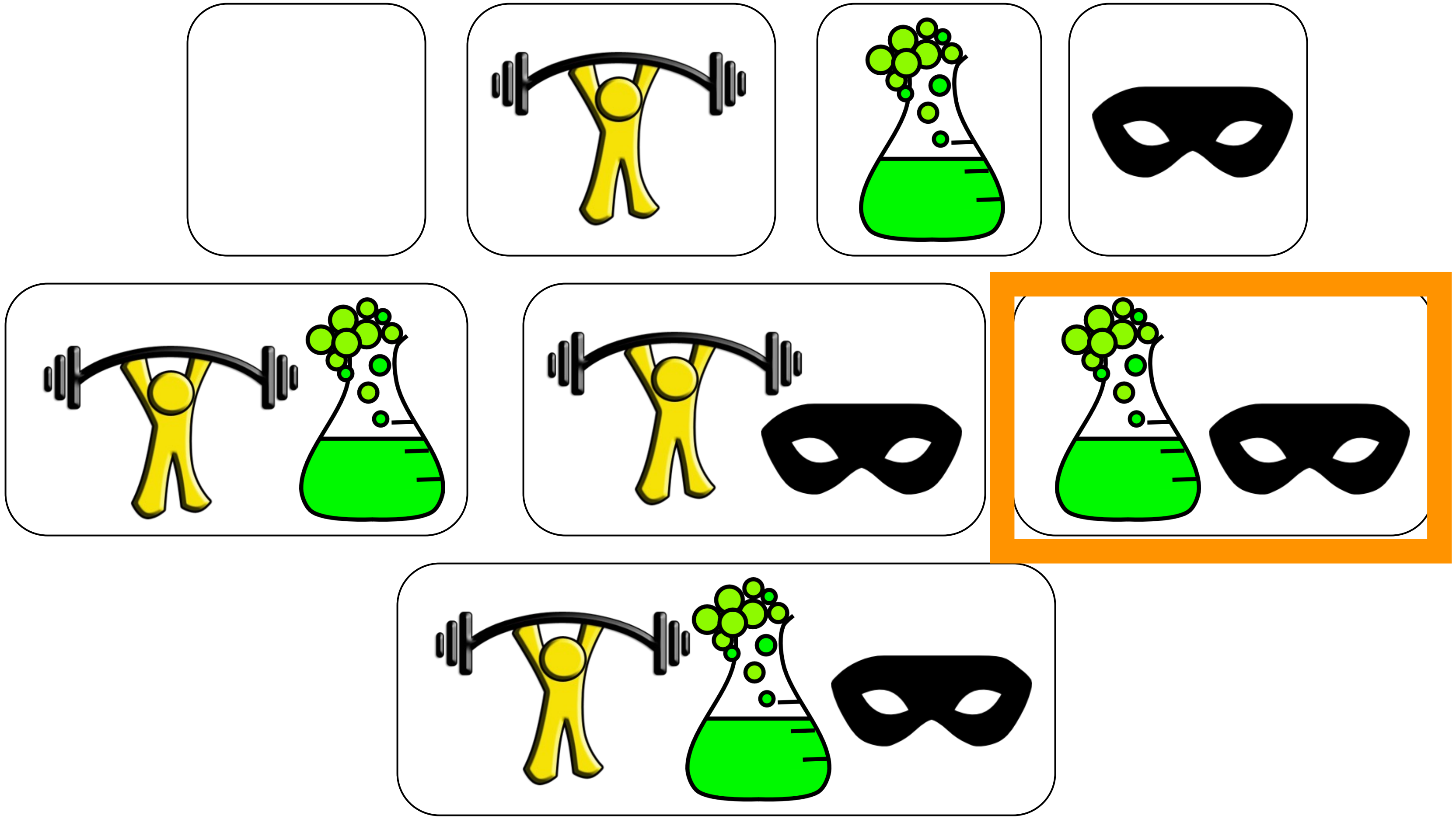
Superhero Example

Subset selection



Superhero Example

Subset selection



Subset selection

Algorithm

Start with the null model, M_0 (no predictors)

For $k = 1, 2, \ldots, p$

Fit all $\binom{p}{k}$ models that contain exactly k predictors

Keep only the one that has the smallest RSS. Call it M_k

Select the "best" model from $M_0, M_1, \ldots M_p$

Subset selection

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Can we do this for models that are not least-squares regression models?

Subset selection

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What drawbacks do you see to this approach?

Subset selection

Model overload

- Number of possible models on a set of p predictors is

$$\sum_{k=1}^{p} \binom{p}{k} = 2^p$$

How many possible models do we get for 10 predictors? For 20?

Subset selection

Model overload

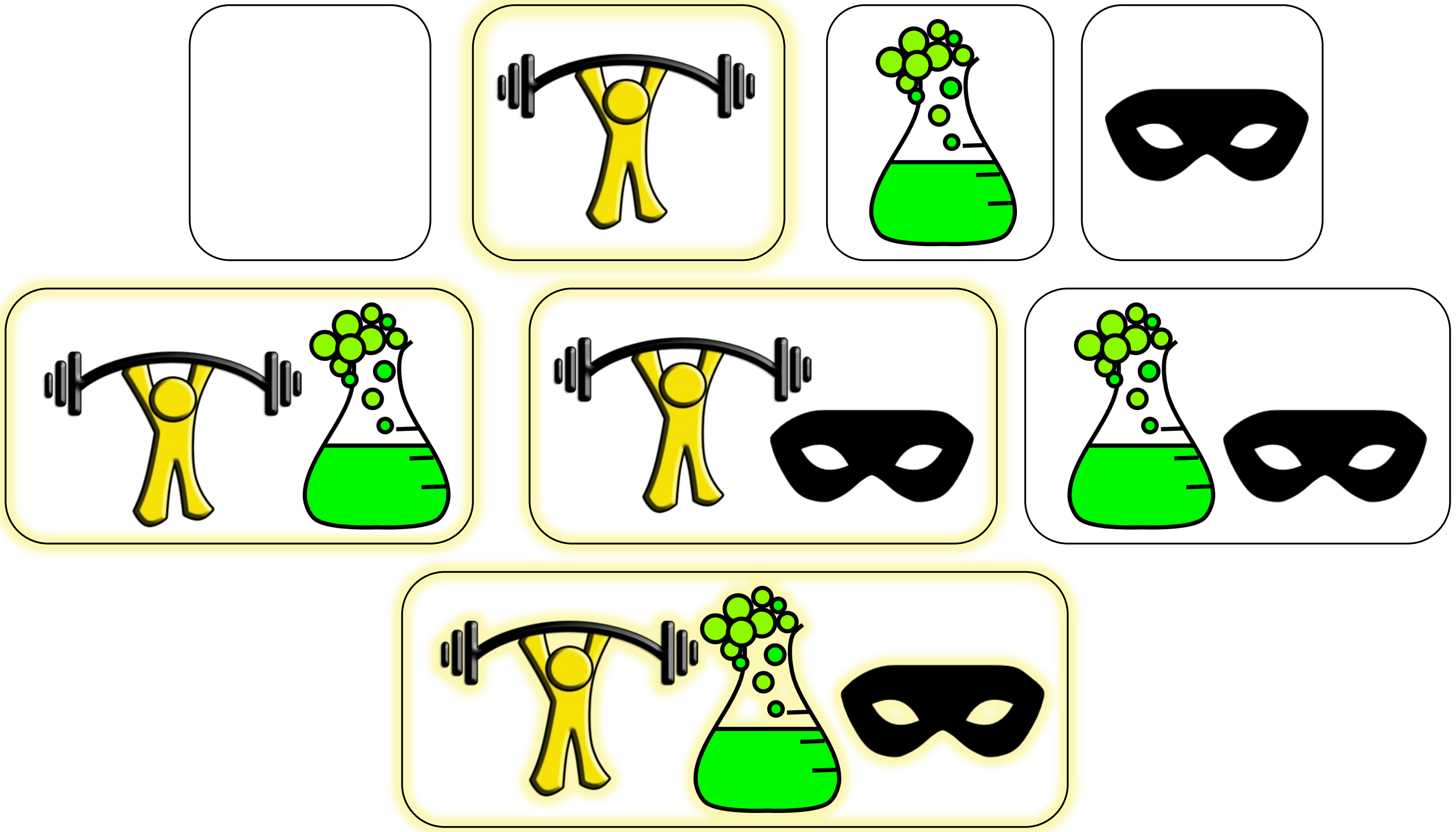
- Number of possible models on a set of p predictors is

$$\sum_{k=1}^{p} \binom{p}{k} = 2^p$$

As we fit more and more models, what happens to our estimated coefficients?

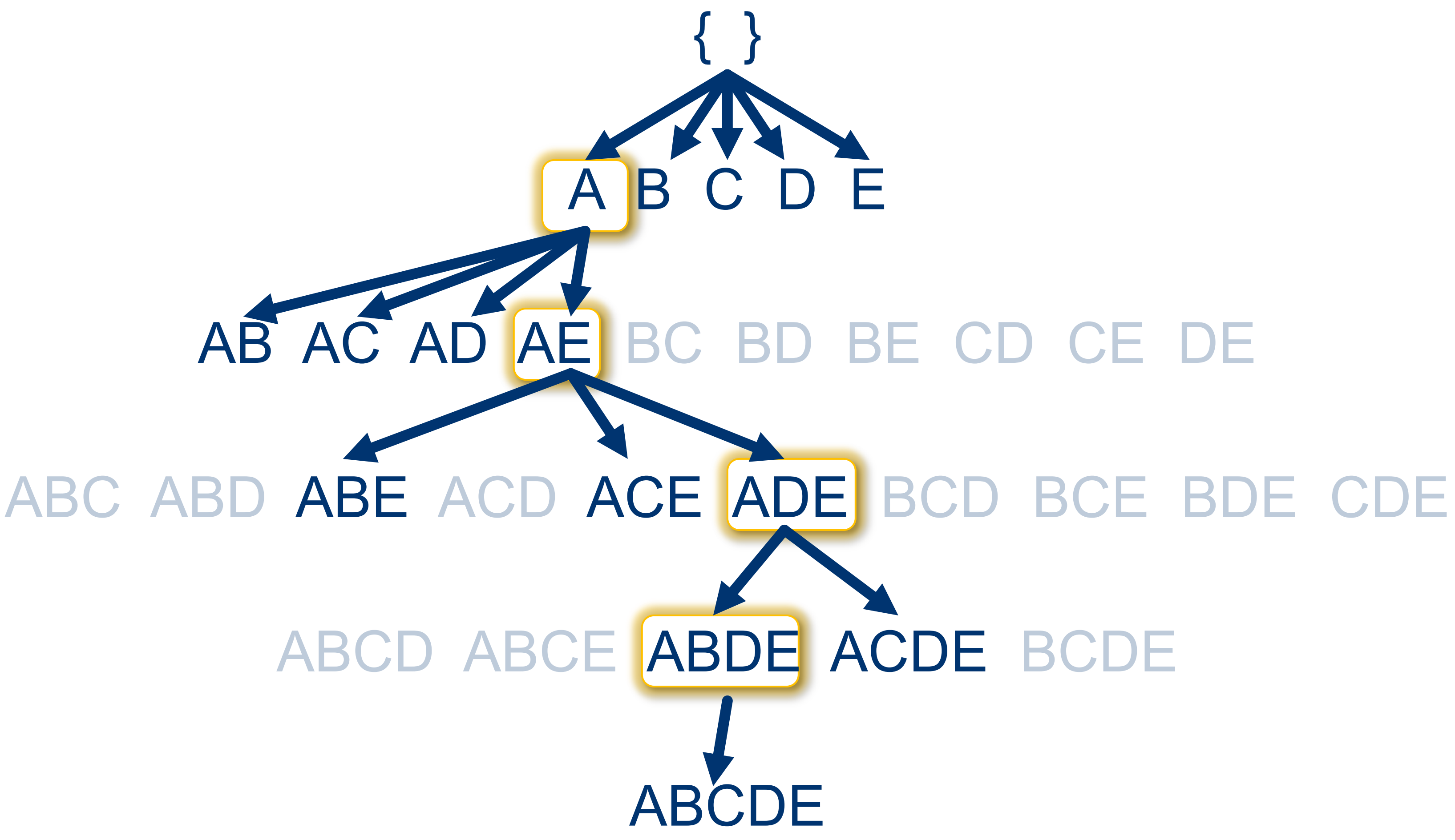
What if we could eliminate some of our model options?

Subset selection



Subset selection

Ex. when $p = 5$



Forward selection

Algorithm

Start with the null model, M_0 (no predictors)

For $k = 1, 2, \ldots, p$

Fit all $(p-k)$ models that augment M_{k-1} with exactly one predictor

Keep only the one that has the smallest RSS. Call it M_k

Select the "best" model from $M_0, M_1, \ldots M_p$

Stepwise selection

Far fewer models than best subset

- Number of possible models on a set of p predictors is

$$\sum_{k=0}^{p-1}(p-k) = 1 + \frac{p(p+1)}{2}$$

How many possible models do we get for 10 predictors? For 20?

Forward selection

Algorithm

Start with the null model, M_0 (no predictors)

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Keep only the one that has the smallest RSS. Call it M_k

Select the "best" model from $M_0, M_1, \dots M_p$

What potential downsides do you see?

Backward selection

Algorithm

Start with the full model, M_p (all predictors)

For $k = p, p-1, \dots, 1$

Fit all k models that reduce M_{k+1} by exactly one predictor

Keep only the one that has the smallest RSS. Call it M_k

Select the "best" model from $M_0, M_1, \dots M_p$

Backward selection

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Choosing the Optimal Model

Recall: measures of **training** error (RSS and R^2) are not good predictors of **test** error.

In addition, they are not good ways of comparing models with different numbers of predictors.

Why?

Choosing the Optimal Model

Recall: measures of **training** error (RSS and R^2) are not good predictors of **test** error

We have two options for estimating test error:

- Directly estimate using a validation set or CV
- **Indirectly estimate by making an adjustment to the training error to account for bias**

Adjusted R^2

Intuition: once all of the useful variables have been included in the model, adding additional junk variables will lead to only a small decrease in RSS

$$R^2 = 1 - \frac{RSS}{TSS}, (TSS = \sum(y_i - \bar{y})^2)$$

$$R^2_{Adj} = 1 - \frac{\frac{RSS}{n-d-1}}{\frac{TSS}{n-1}}, d = num\_predictors$$

To maximize R^2_{Adj} (get the best fit), we need to minimize $\frac{RSS}{n-d-1}$

As d increases, what will happen to this term?

AIC, BIC, and C_p

Other ways to penalize RSS when more predictors are added:

$$C_p = \frac{1}{n}(RSS + 2d\hat{\sigma}^2), \hat{\sigma}^2 = estimate\ of\ variance\ of\ \epsilon_i$$

As d increases, what will happen to C_p?

AIC, BIC, and C_p

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$$AIC = \frac{1}{n}(RSS + 2d\hat{\sigma}^2)$$

$$BIC = \frac{1}{n}(RSS + \log(n)\, d\hat{\sigma}^2)$$

As d increases, what will happen to BIC? How will this differ if d is very large vs small?

AIC, BIC, and C_p

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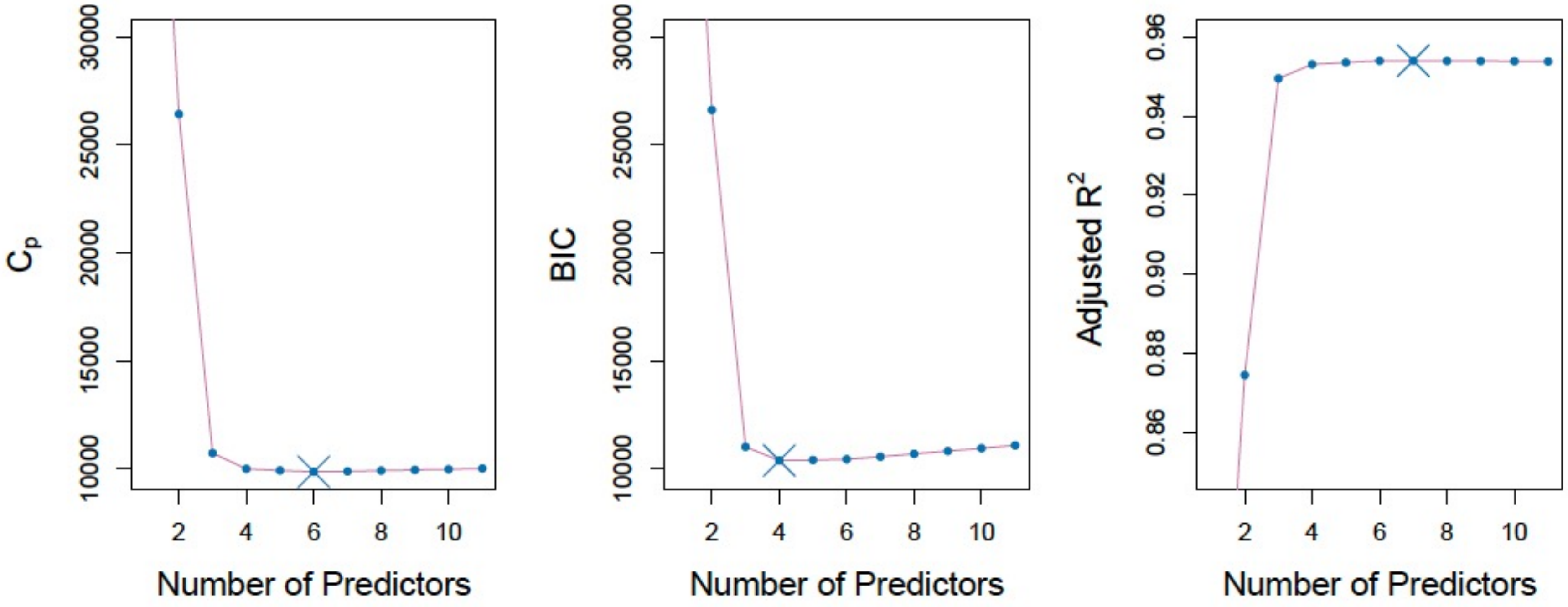
$$AIC = \frac{1}{n}(RSS + 2d\hat{\sigma}^2)$$

$$BIC = \frac{1}{n}(RSS + \log(n)\, d\hat{\sigma}^2)$$

All of these measures are supported by statistical theory. AIC and BIC are also defined for more general models beyond least squares.

AIC, BIC, and C_p

Credit dataset



Choosing the optimal model

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When do we use one vs the other?

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- With the computers we have today, CV is no longer as expensive and is the preferred method

Choosing the optimal model

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What if all models have about the same error (within one SE of each other)?

- Go with the simplest!