KNN Regression and Generalization

Applied Machine Learning
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Dall-E

Previous Lecture Recap

- **Data** is a set of numbers that contains information. Images, audio, signals, tabular data and everything else must be represented as a vector of numbers to be used in ML.
- **Information** is the power to predict something – a lot of the challenge in ML is in transforming the data to make the desired information more obvious
- In machine learning, we have
  - **Sample**: a data point, such as a feature vector and label corresponding to the input and desired output of the model
  - **Dataset**: a collection of samples
  - **Training set**: a dataset used to train the model
  - **Validation set**: a dataset used to select which model to use or compare variants and manually set parameters
  - **Test set**: a dataset used to evaluate the final model
- In a **classification** problem, the goal is to map from features to a categorical label (or “class”)
- Nearest neighbor (or **K-NN**) algorithm can perform classification by retrieving the K nearest neighbors to the query features and assigning their most common label
- We can measure **error** and **confusion matrices** to show the fraction of mistakes and what kinds of mistakes are made

Machine learning model maps from features to prediction

$$f(x) \rightarrow y$$

Features

Prediction

Examples

- Classification: predict label
  - Is this a dog or a cat?
  - Is this email spam or not?

- Regression: predict value
  - What will the stock price be tomorrow?
  - What will be the high temperature tomorrow?

- Structured prediction: predict a set of related values
  - What is the pose of this person?

Key principle of machine learning

Given feature/target pairs $(X_1, y_1), \ldots, (X_n, y_n)$:

if X_i is similar to X_j, then y_i is probably similar to y_j

Fundamentally, learning depends on:

1. Representation of samples
2. Similarity function

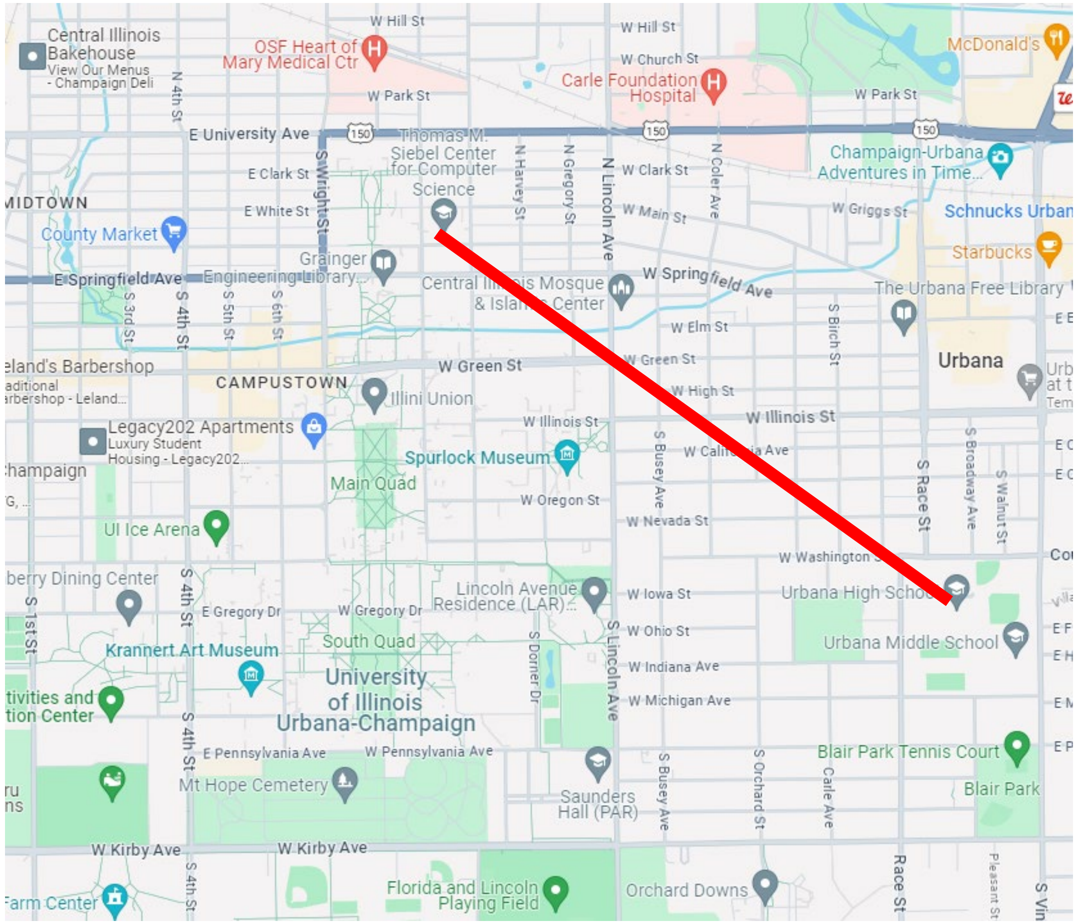
Today's lecture

- Similarity measures
- Regression
- Generalization

Common Distance/Similarity Measures

- L2: Euclidean

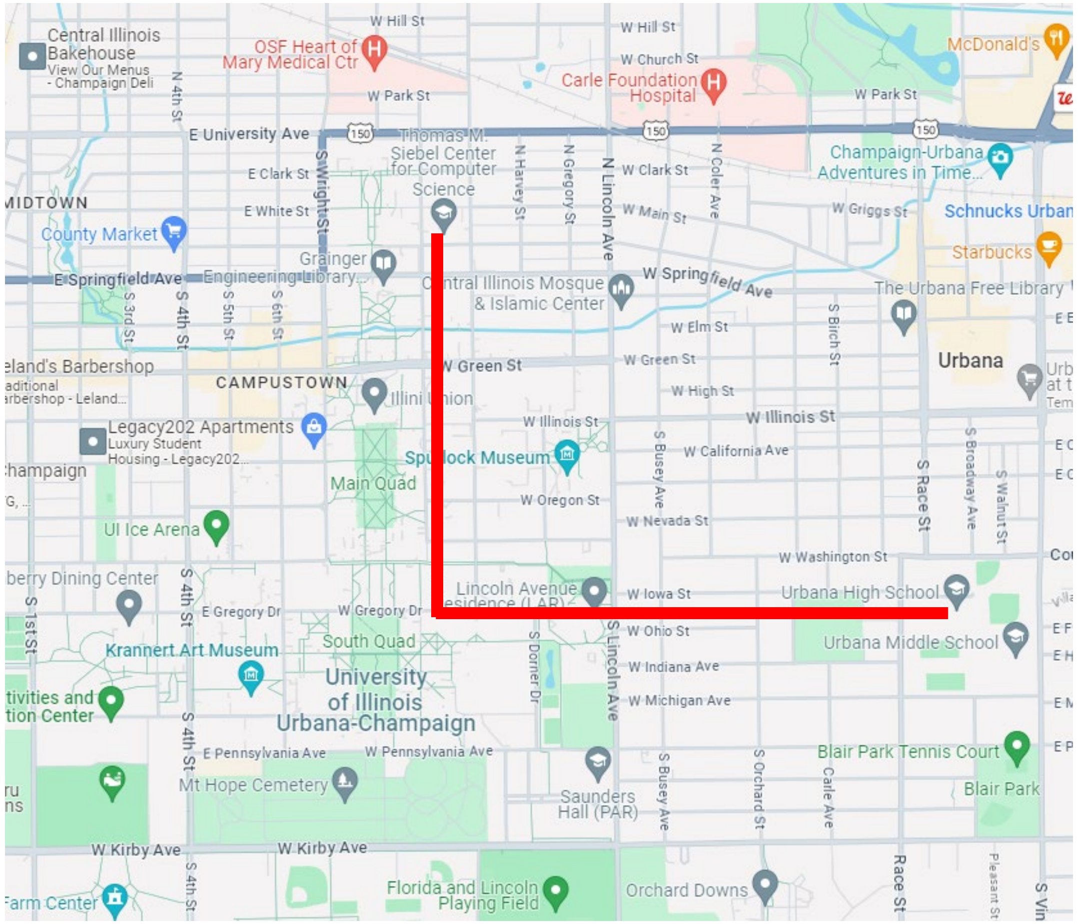
$$d_2(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\|_2$$
$$= \sqrt{\sum_i (x_i - y_i)^2}$$



Common Distance/Similarity Measures

- L1: City-Block

$$d_1(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\|_1$$
$$= \sum_i |x_i - y_i|$$



Common Distance/Similarity Measures

- Dot product, Cosine

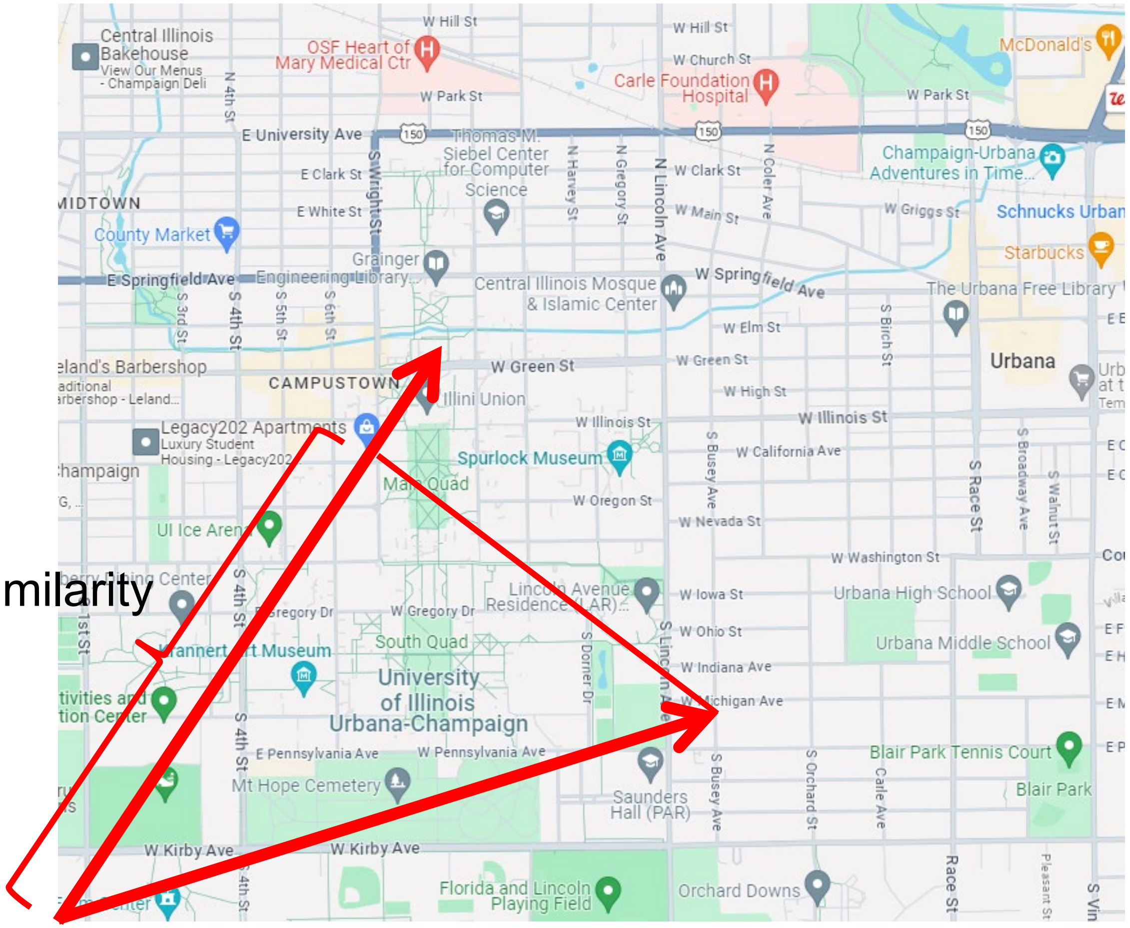
Dot product (or inner product)

$$s_{dot}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x}^T \boldsymbol{y} = \sum_i x_i y_i$$

Cosine similarity

$$s_{cos}(\boldsymbol{x}, \boldsymbol{y}) = \frac{\boldsymbol{x}^T \boldsymbol{y}}{\|\boldsymbol{x}\|_2 \|\boldsymbol{y}\|_2}$$

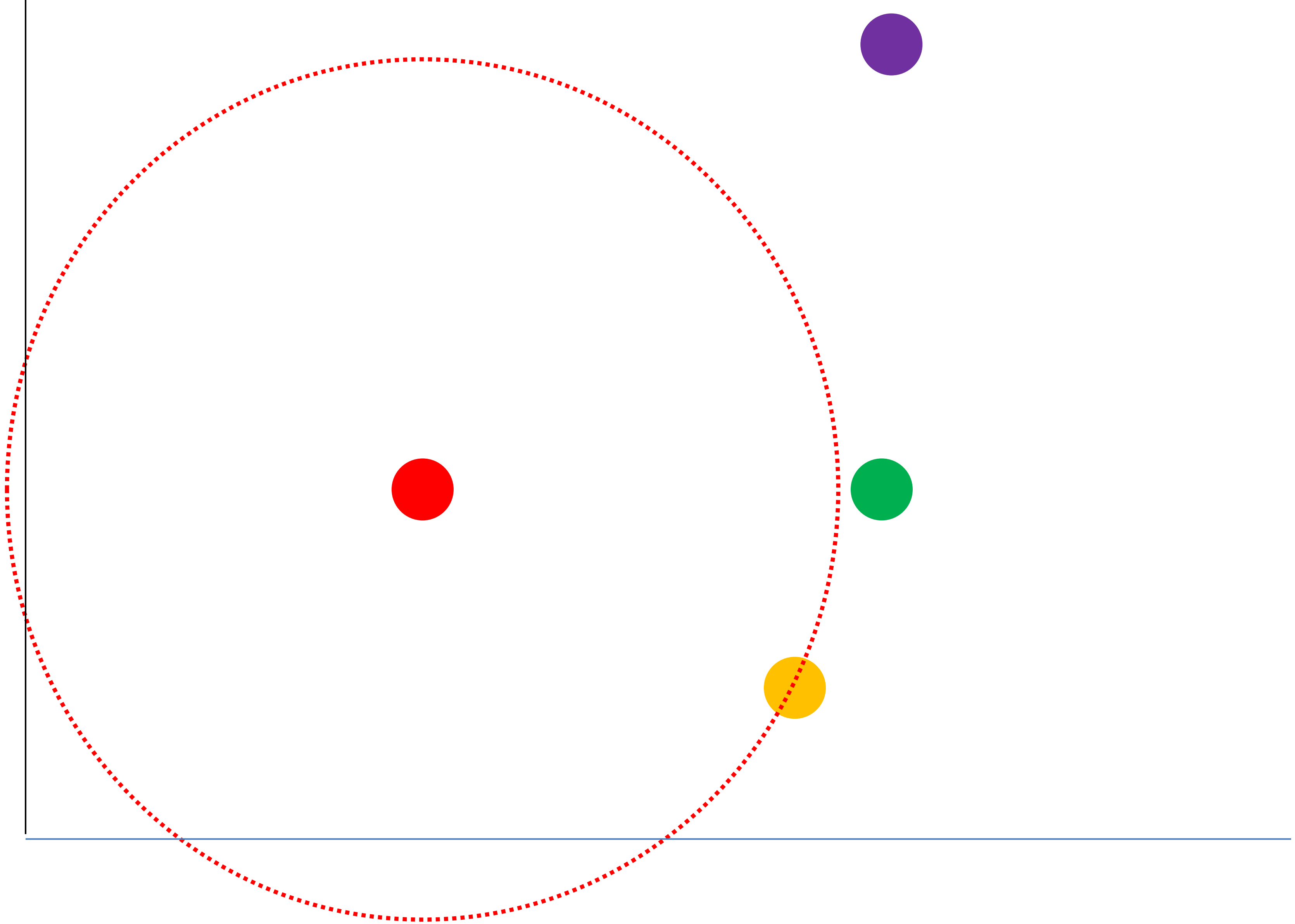
Cosine similarity



Dot product: how far does one vector go in the direction of the other vector

Cosine similarity: how similar are the two directions

Which is closest to the red circle under L1, L2, and cosine distance?



Comparing distance/similarity functions

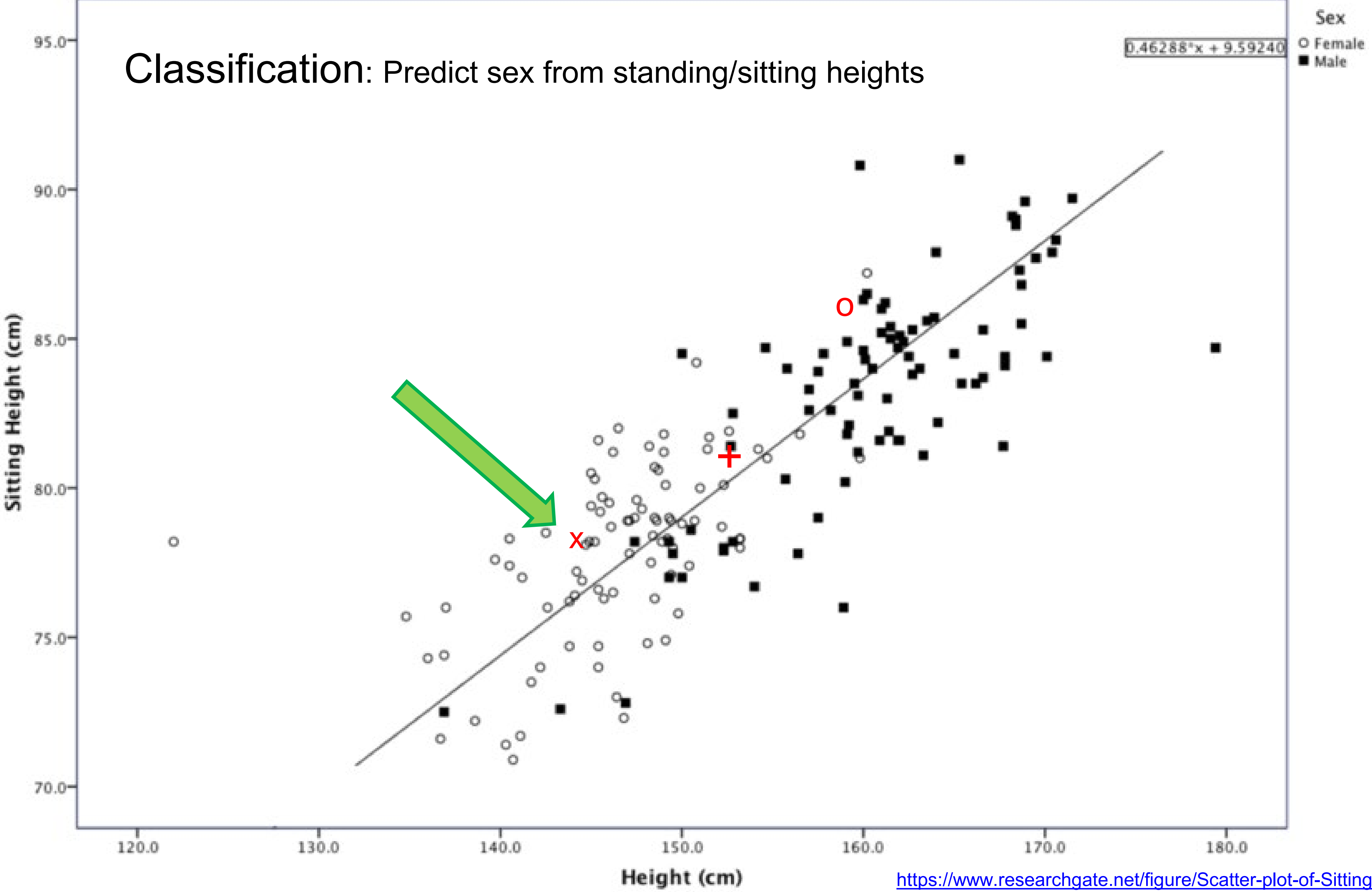
- L2 depends much more heavily than L1 on the coordinates with the biggest differences

$$d_2([0\ 100],[5\ 1]) = 99.1$$
$$d_1([0\ 100],[5\ 1]) = 104$$

- Cosine and L2 are equivalent if the vectors are unit length

$$\|\boldsymbol{x}-\boldsymbol{y}\|_2^2 = \underset{1}{\boldsymbol{x}^T\boldsymbol{x}} - 2\boldsymbol{x}^T\boldsymbol{y} + \underset{1}{\boldsymbol{y}^T\boldsymbol{y}} = 2(1 - s_{cos}(\boldsymbol{x},\boldsymbol{y}))$$

Classification: Predict sex from standing/sitting heights



https://www.researchgate.net/figure/Scatter-plot-of-Sitting-Height-over-Height-for-males-and-females_fig3_301724988

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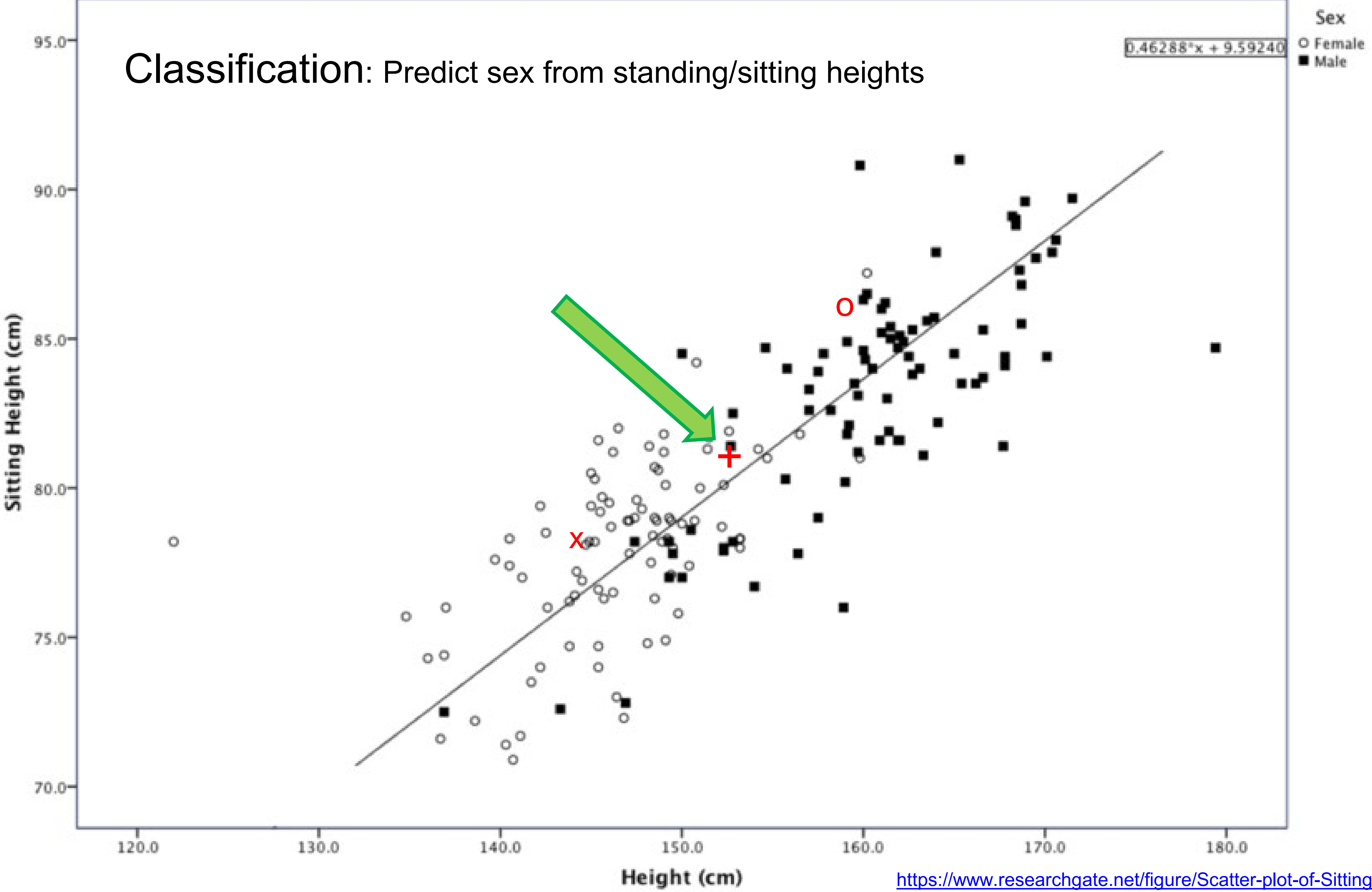

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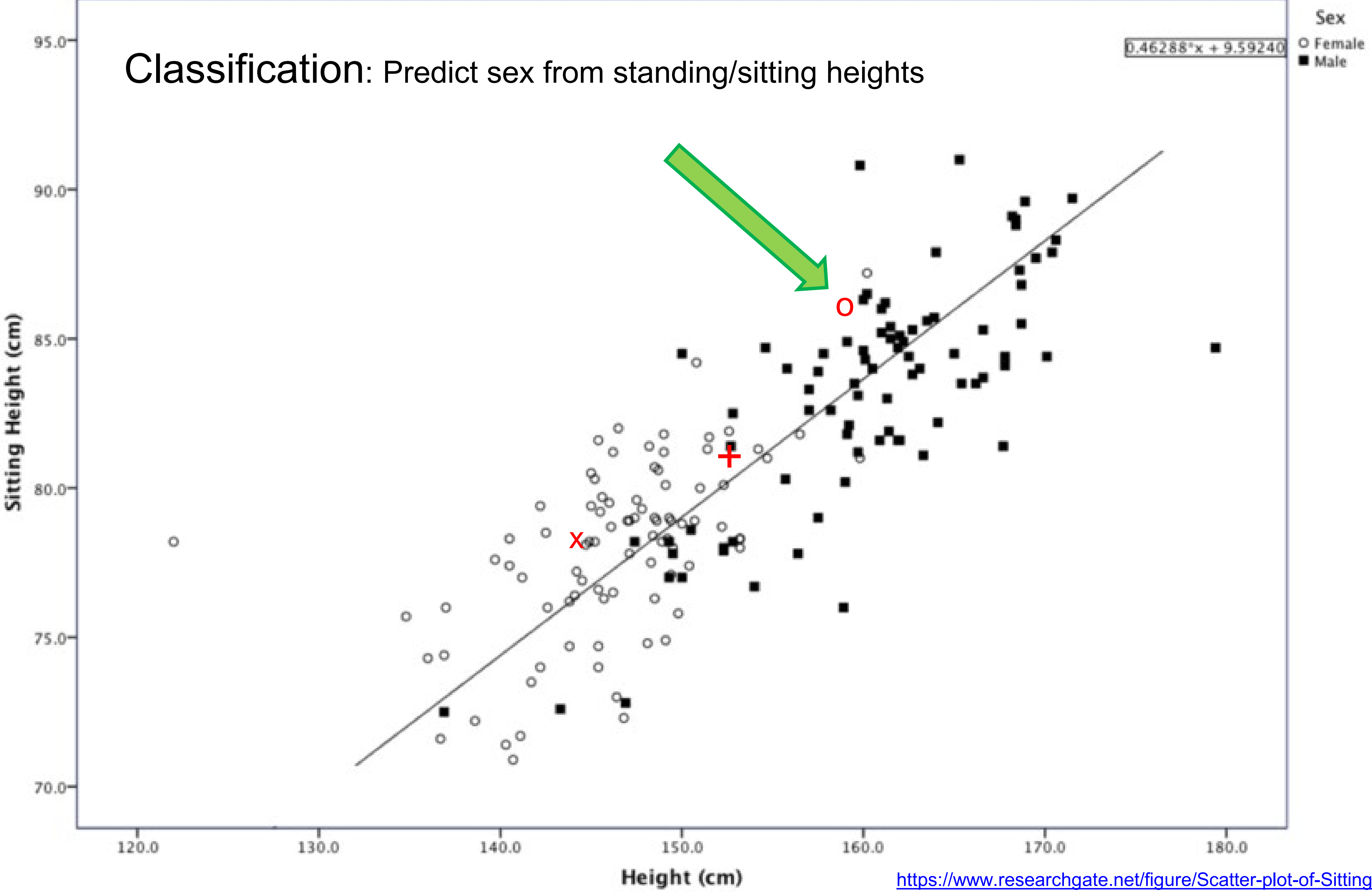

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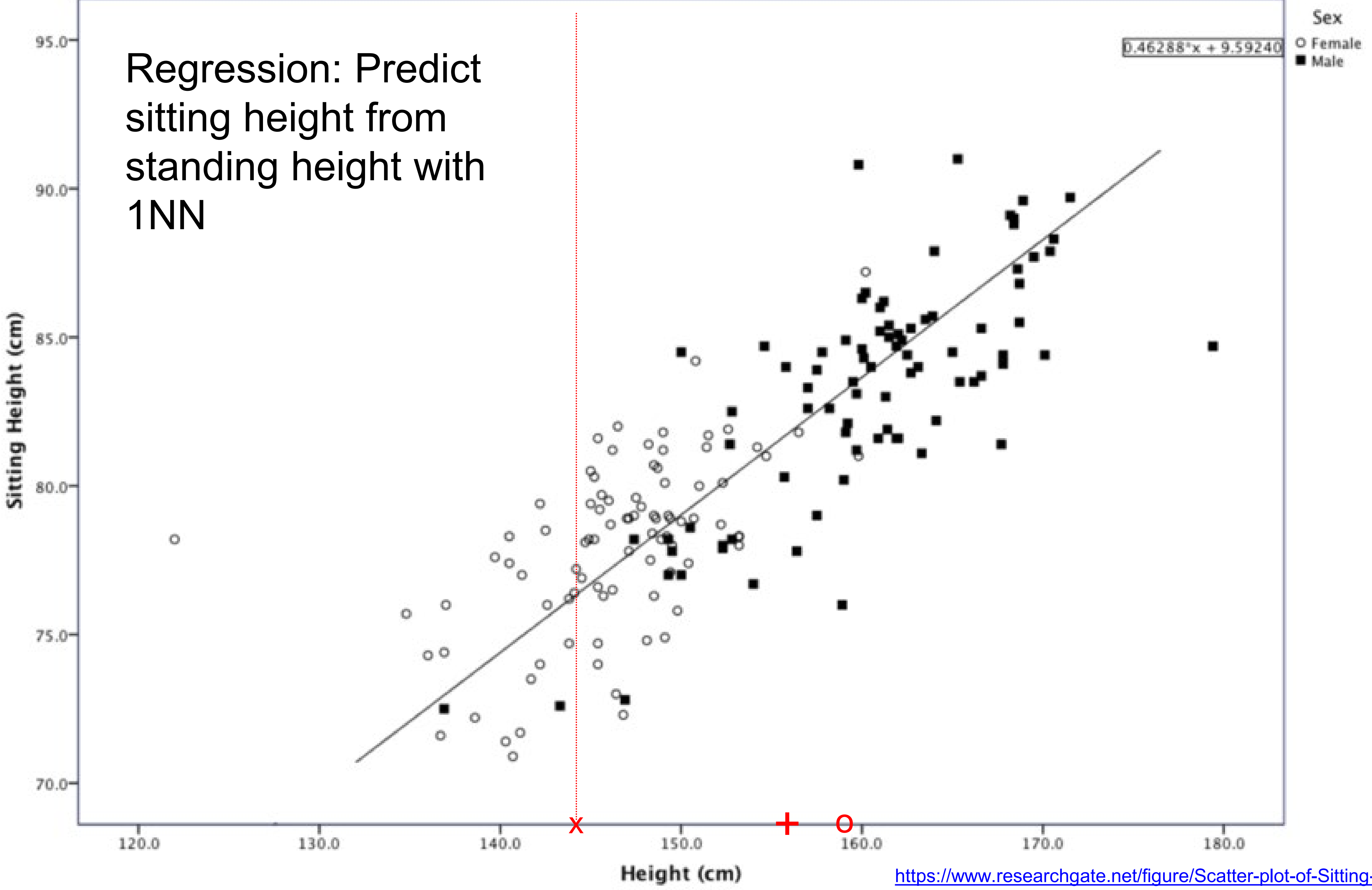
KNN Regression

- Also retrieve the K-nearest neighbors
- But, instead of predicting the most common retrieved label, predict the average of the returned values

Regression: Predict sitting height from standing height with 1NN



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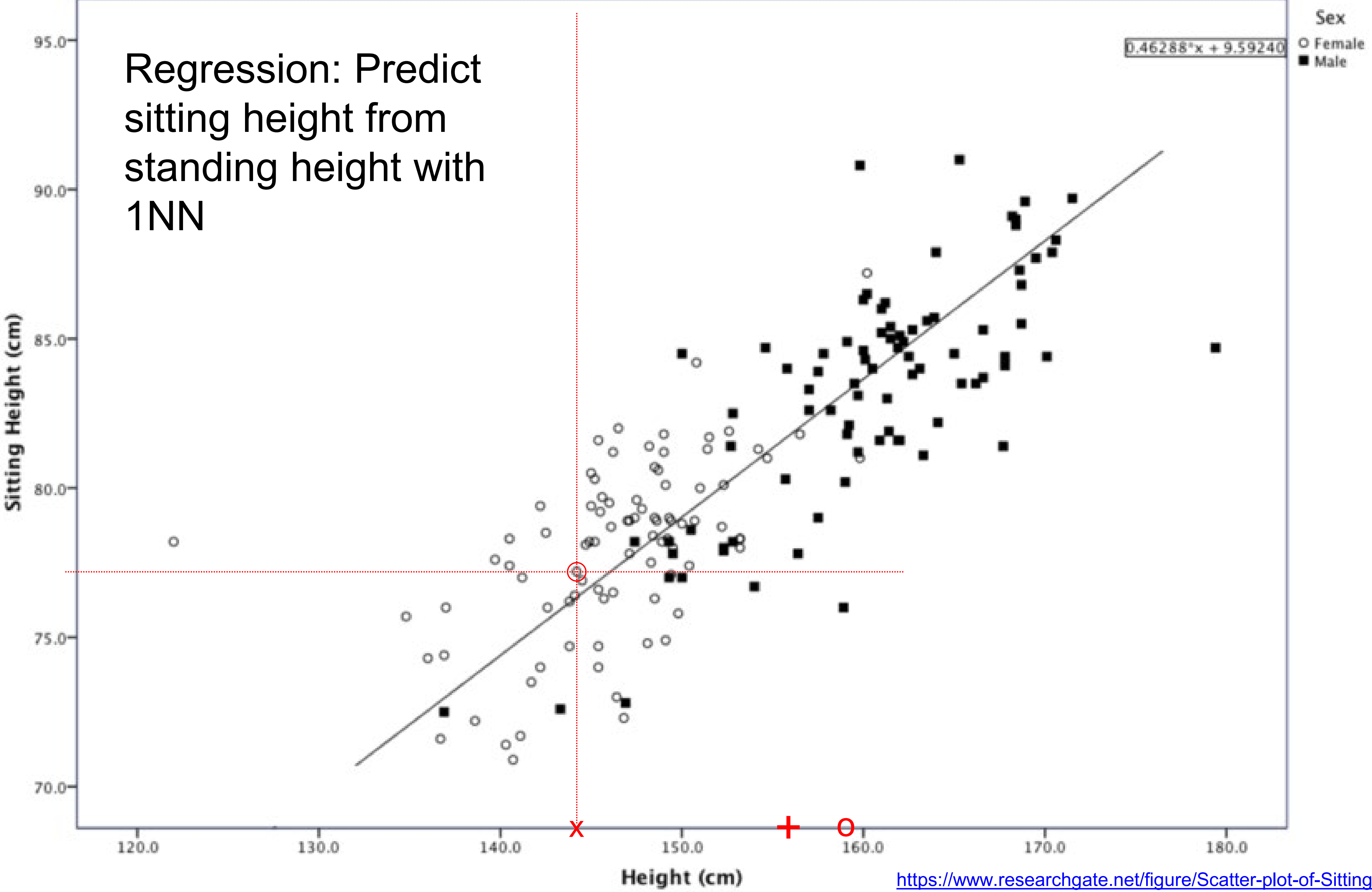

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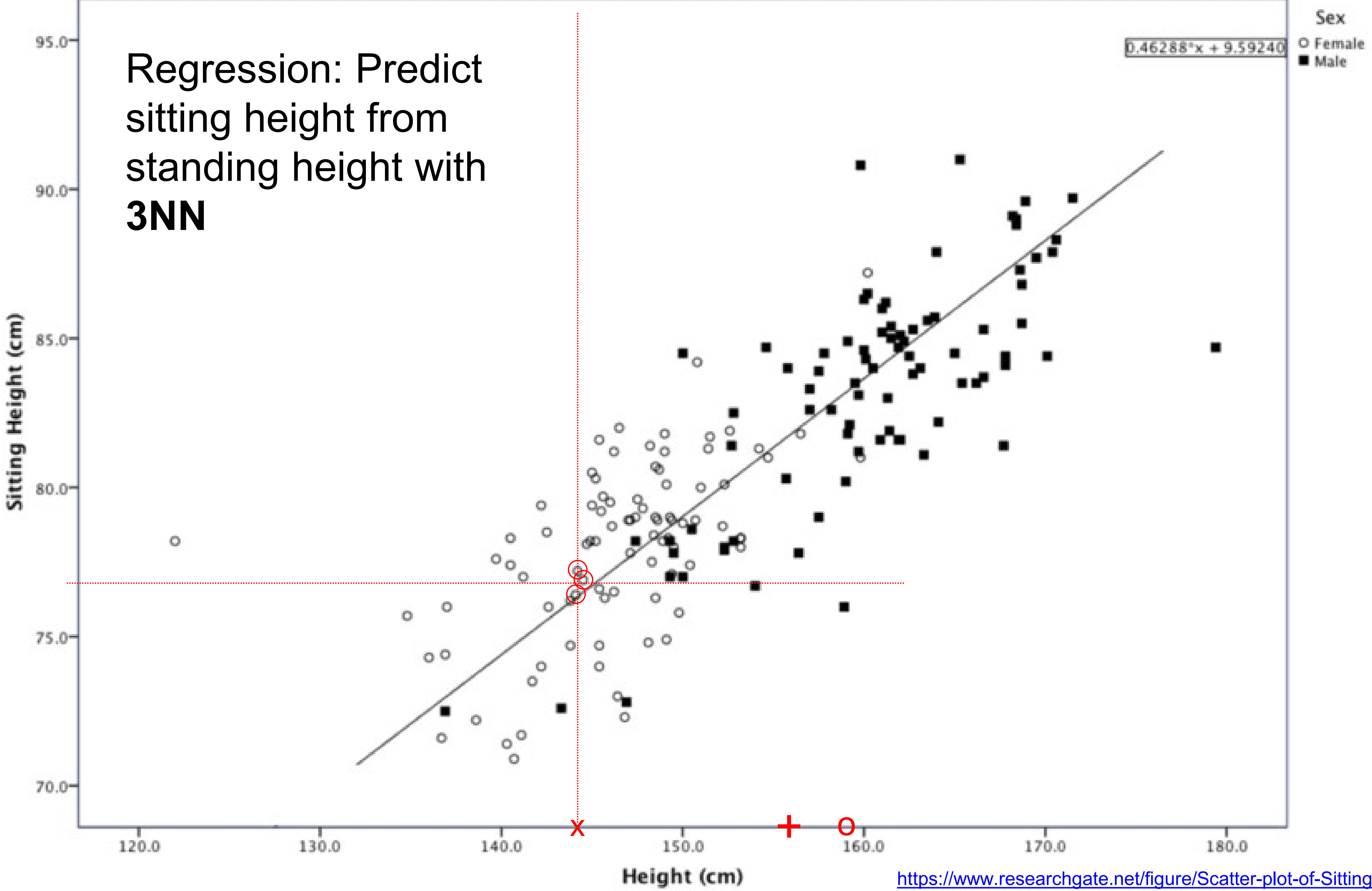

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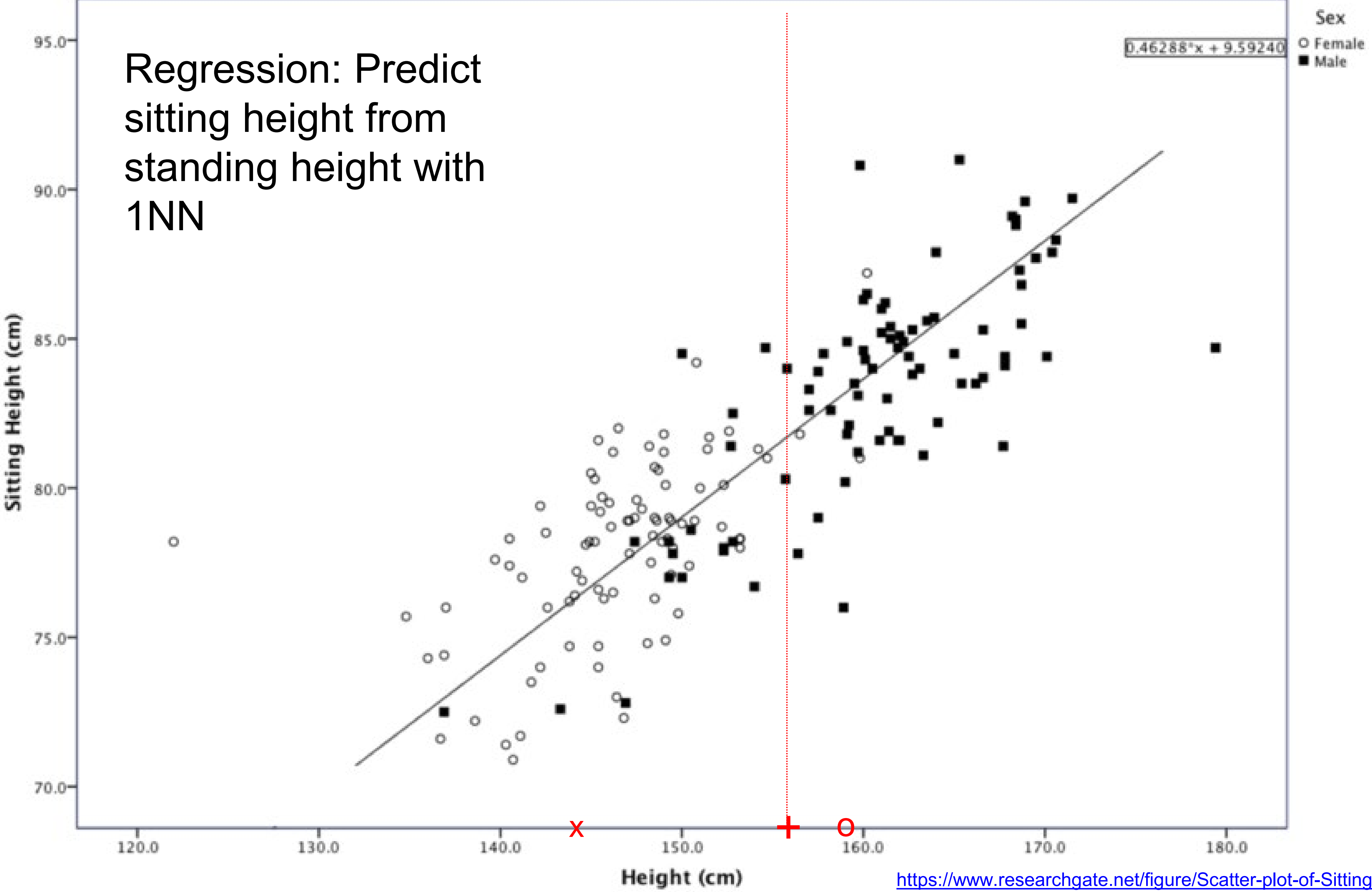

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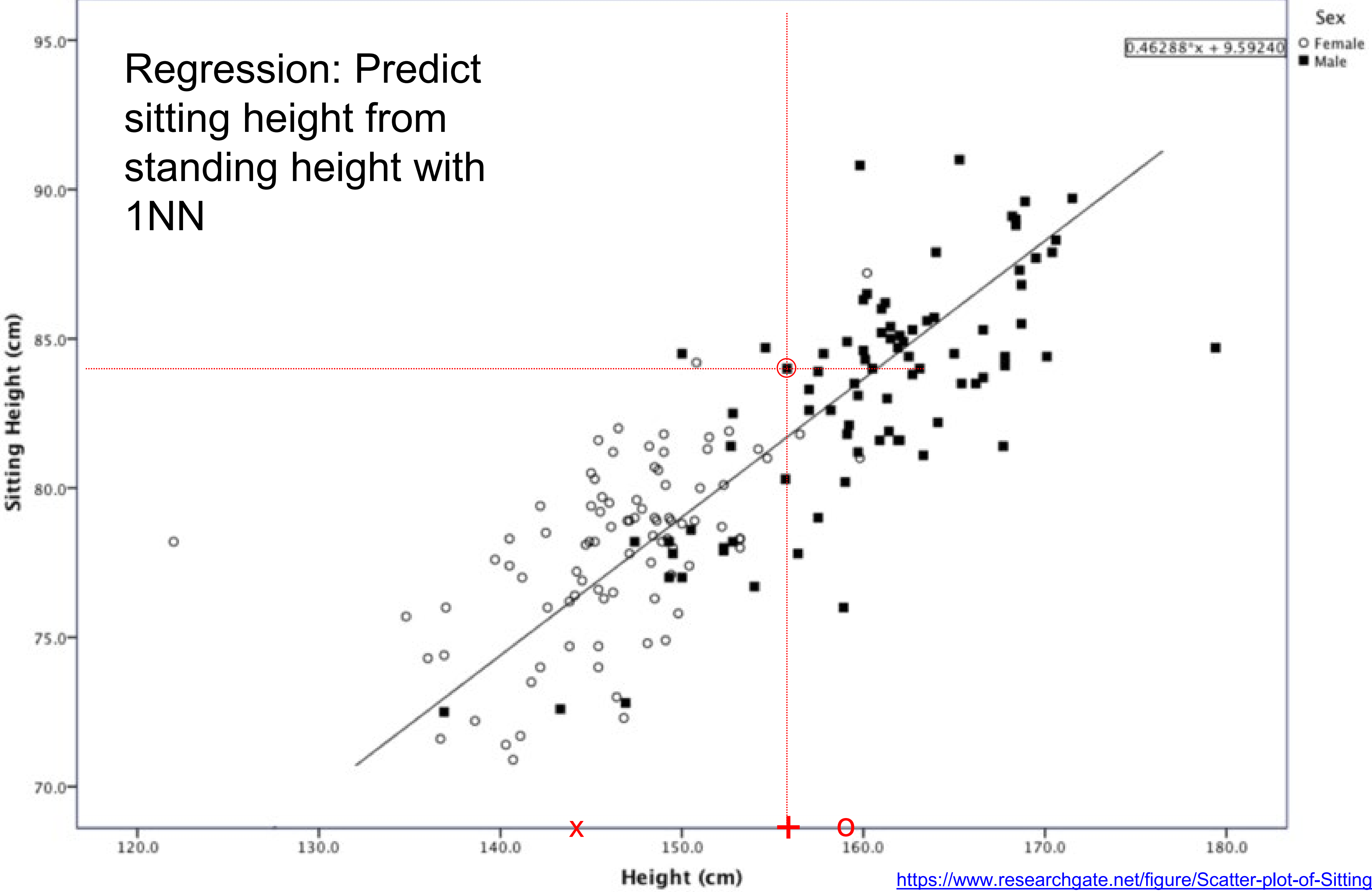

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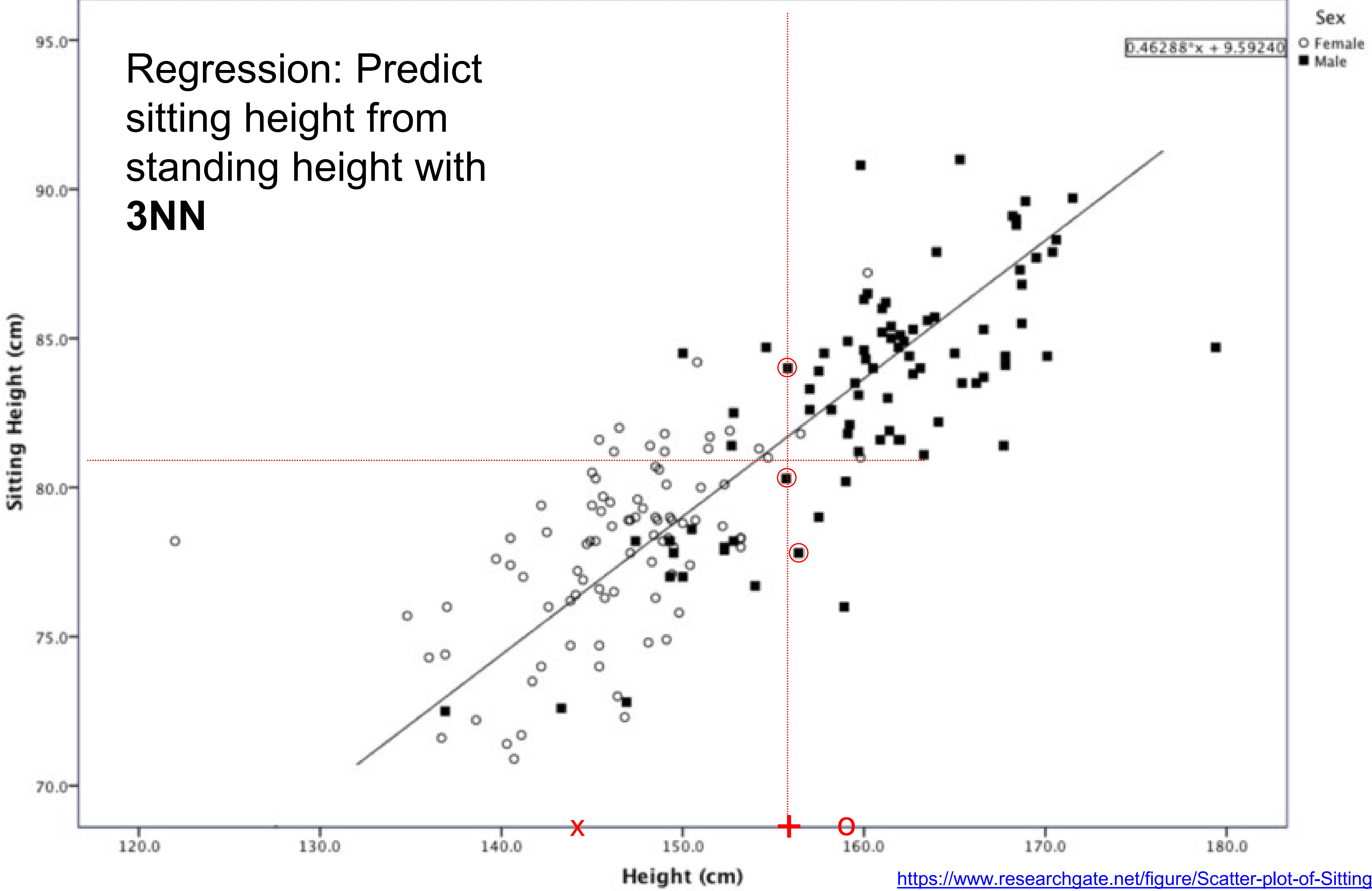

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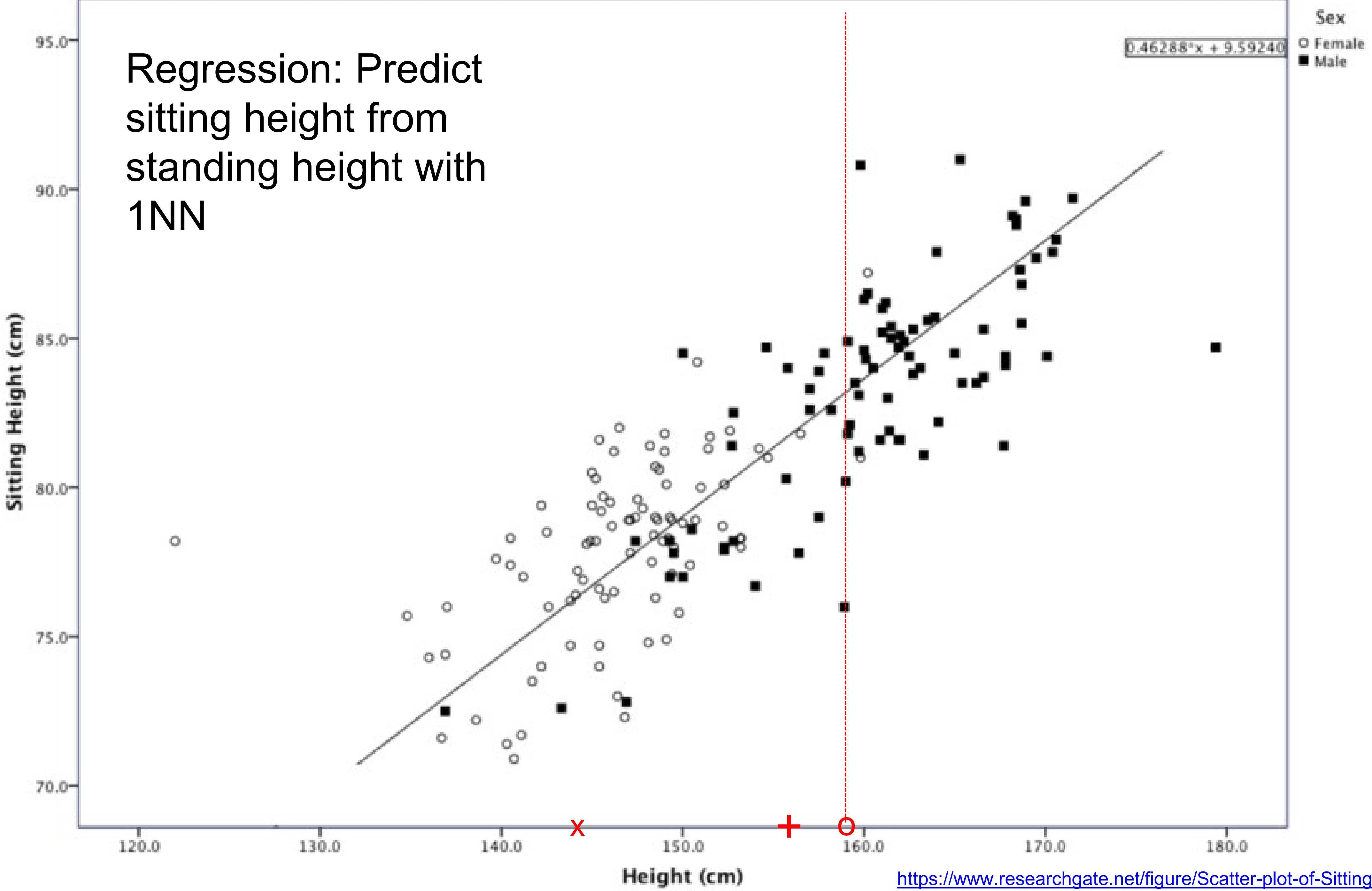

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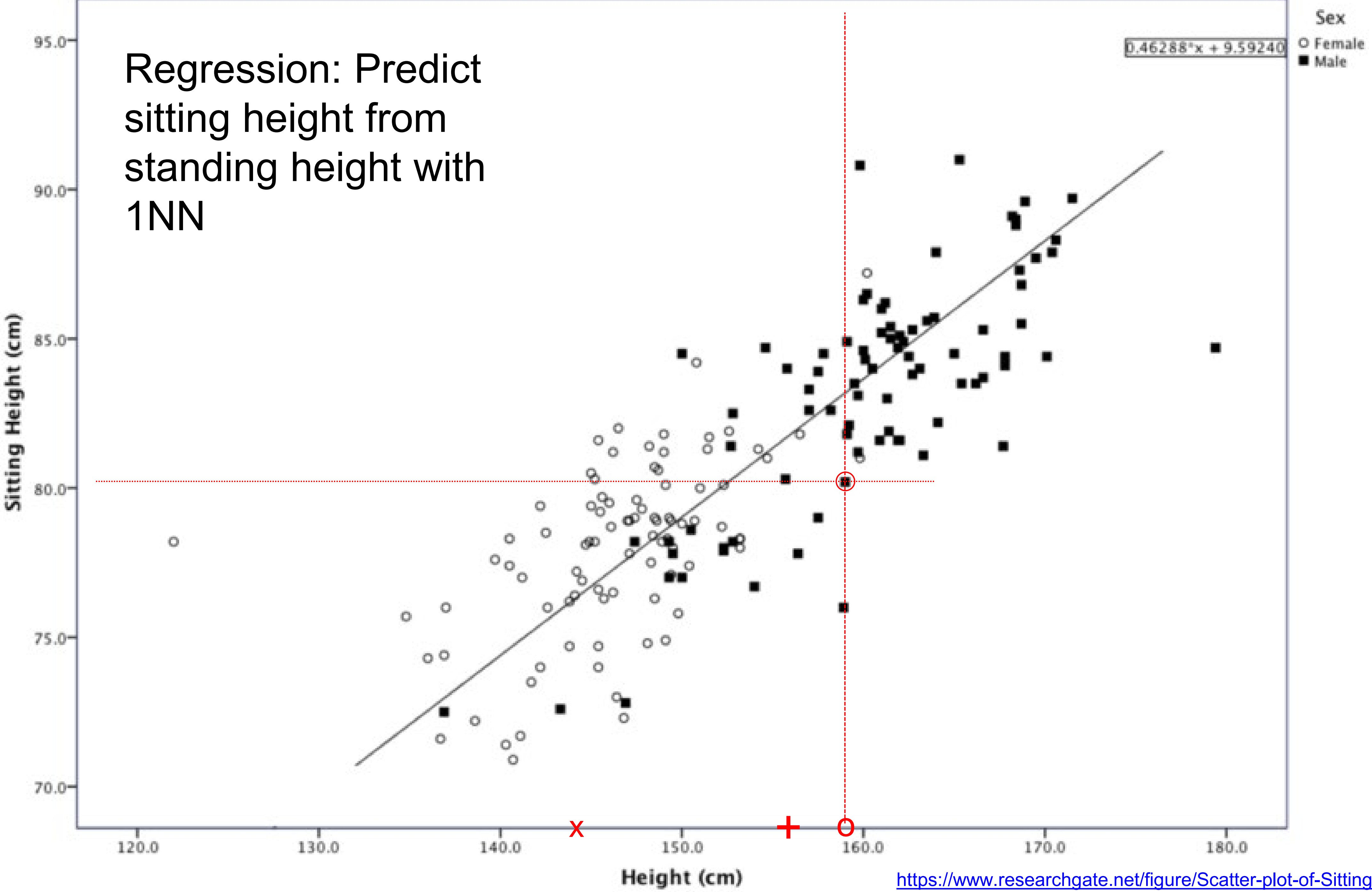

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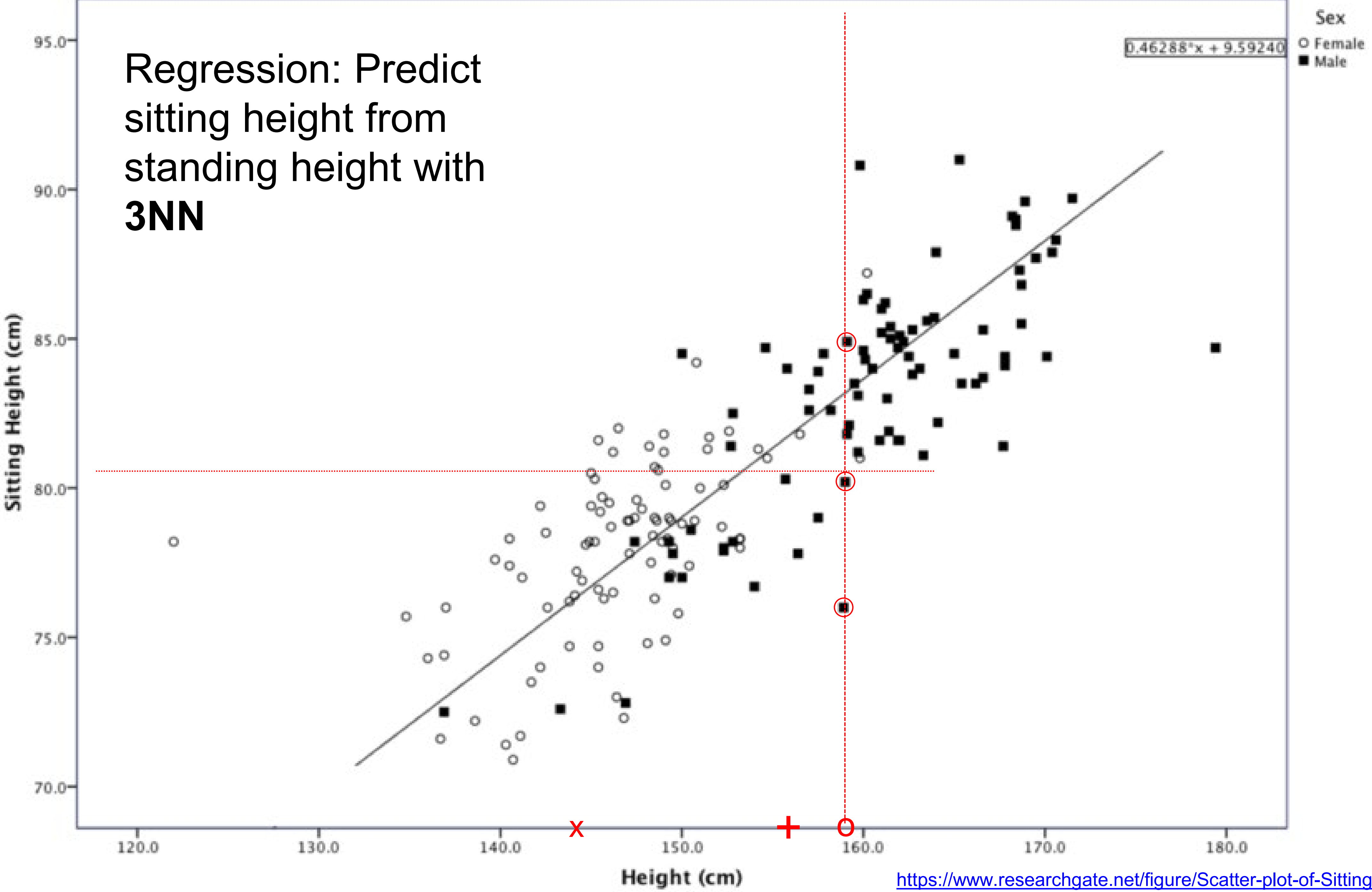

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How do we measure and analyze regression error?

- Root mean squared error
  $\sqrt{\frac{1}{\mathrm{N}}\sum_i (f(X_i) - y_i)^2}$

- Mean absolute error $\frac{1}{\mathrm{N}}\sum_i |f(X_i) - y_i|$

- R^2: $1 - \frac{\sum_i (f(X_i) - y_i)^2}{\sum_i (y_i - \bar{y})^2}$ (unexplained variance) / (total variance)

- RMSE/MAE are unit-dependent measures of accuracy, while R^2 is a unitless measure of the fraction of explained variance

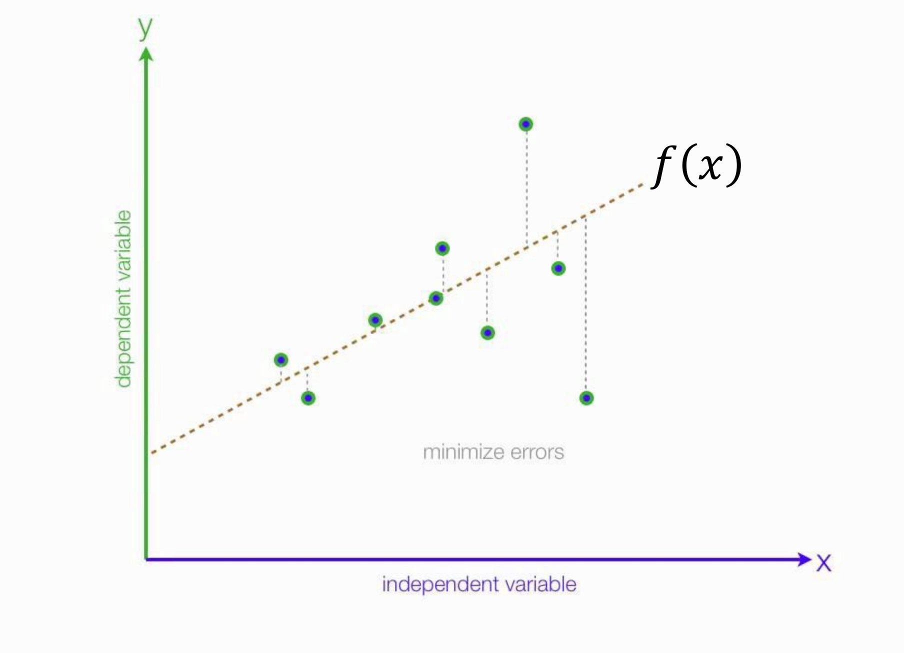


Fig: https://medium.com/analytics-vidhya/mae-mse-rmse-coefficient-of-determination-adjusted-r-squared-which-metric-is-better-cd0326a5697e

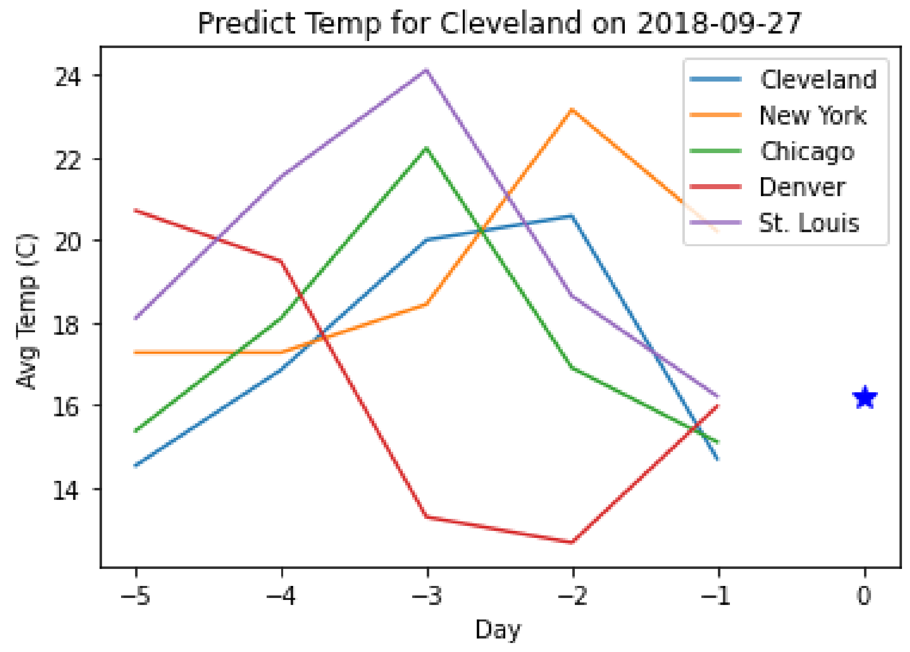
Q1-Q3

https://tinyurl.com/441-fa24-L3

Introducing the Temperature Regression Dataset

- Input: temperature (C) from 83 US cities for each of previous 5 days
  – Total of $415 = 83 \times 5$ features
- Target: temperature of Cleveland for next day

- Datasets
  – Train: 2555 samples (7 years of data, starting 2011-09-29)
  – Val: 365 samples (next 1 year of data)
  – Test: 365 samples (next 1 year of data)



KNN for Temperature Regression

```
def regress_KNN(X_query, X_train, y_train, K):

        # (1) Compute distances between X_query and each
        sample in X_train

        # (2) Get the K_smallest_idx: K indices
        corresponding to smallest   distances(e.g. use
        np.argsort)

        # (3) Return the mean of y_train[K_smallest_idx]


def RMSE(y_pred, y_true):
        return np.sqrt(np.mean((y_pred-y_true)**2))
```

Testing procedure:

```
        # Get y_pred[i] = regressKNN(X_test[i], X_train,
        y_train, K) for each ith sample in X_test

        # measure error: err = RMSE(y_pred, y_test)
```

Some things to consider

- The temperatures will vary a lot over the year, which will reduce the number of examples with similar temperatures
  - What can we do?

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- The temperatures will vary a lot over the year, which will reduce the number of examples with similar temperatures
  - What can we do?
  - Reframe the problem by making all of the temperatures relative to previous day’s Cleveland temperature

- How do we choose K?

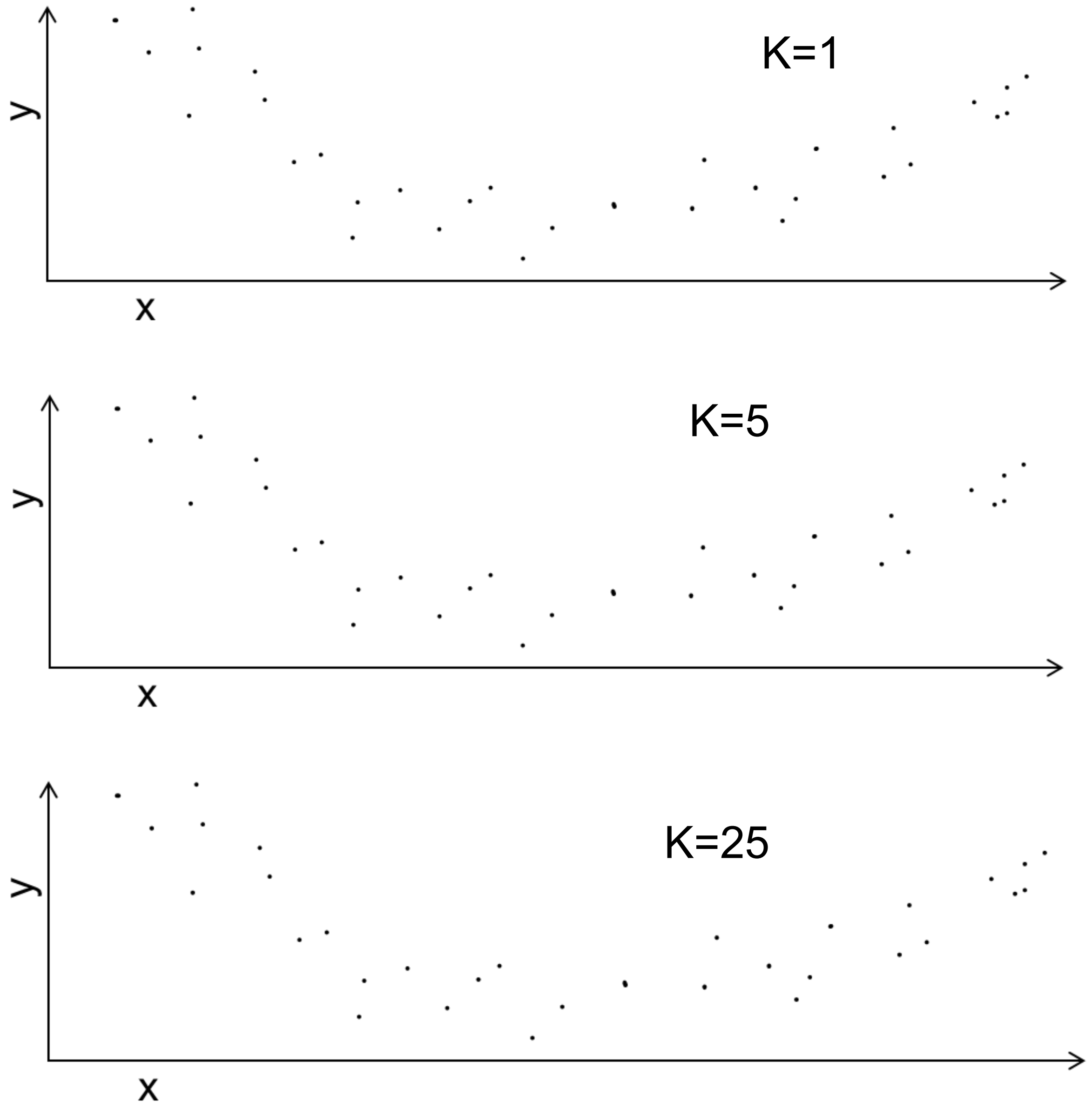
Choosing K Using a Validation Set

For each candidate K, e.g. K=1, 3, 5, 9, 11, 25:

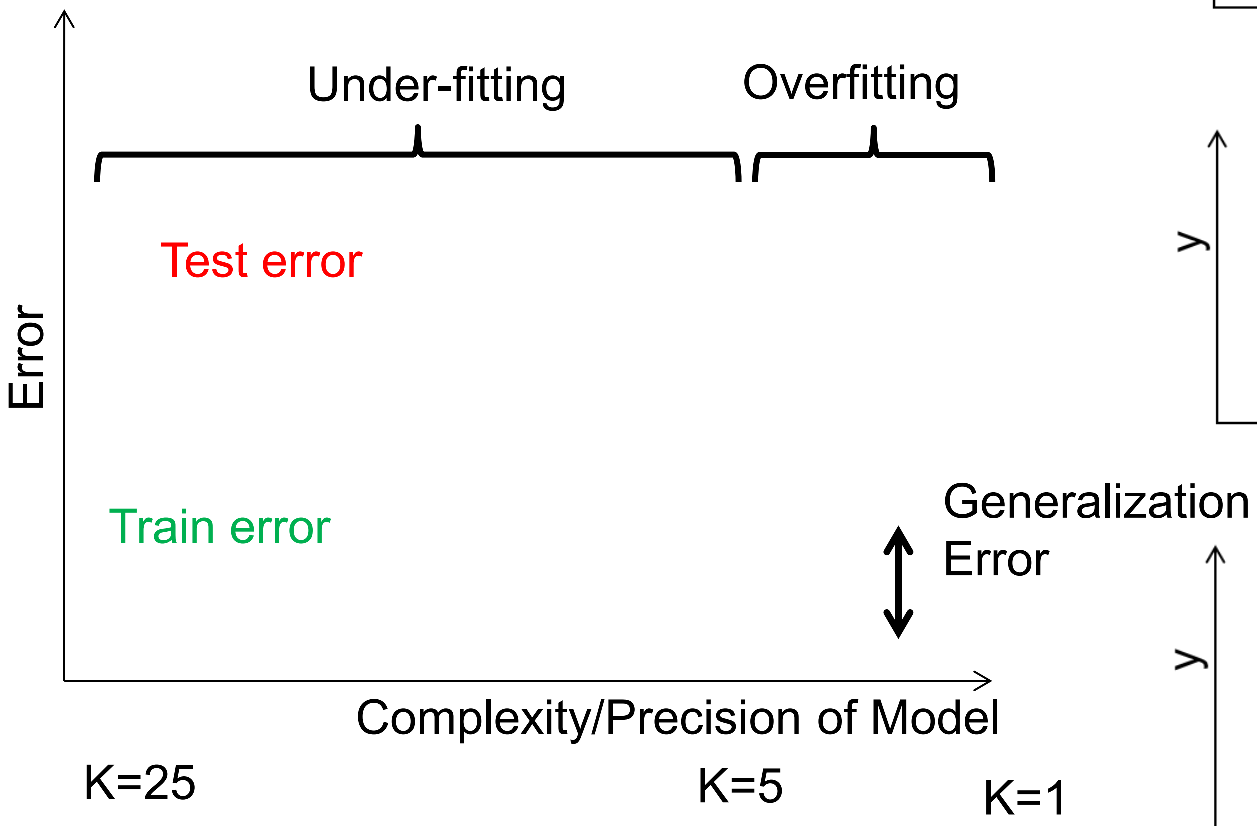
- Evaluate error using the validation set

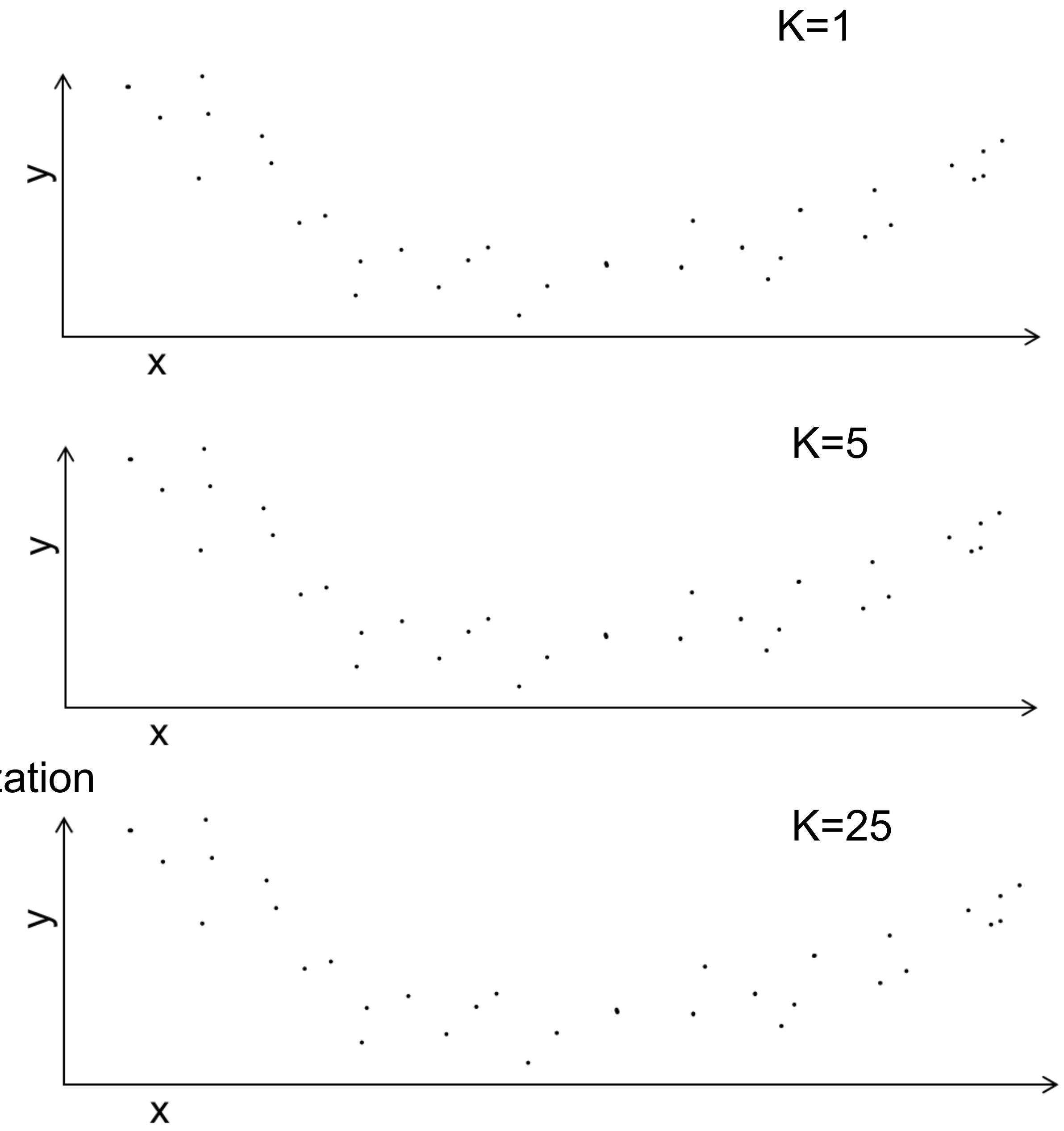
Select the K with the lowest validation error

Small K may “overfit” data, while large K may not be able to fit the true trend



Error and Bias Variance Trade-off





Error and Bias Variance Trade-off

When model parameters are fit to a *training set* and evaluated on a *test set*

- **Training error**: The error on the training set
- **Test error**: The error on the test set
- **Generalization error**: test error – training error

Test error has three important sources in common ML settings:

- **Intrinsic**: sometimes it is not possible to achieve zero error given available features (e.g. handwriting, weather prediction)
  - Bayes optimal error: The error if the true function $P(y|x)$ is known
- **Model Bias**: the model is limited so that it can't fit perfectly to the true data distribution (e.g. there will be error, even if you have infinite training data)
- **Model Variance**: given finite training data, different parameters and predictions would result from different samplings of data

A more complex or specific model is expected to have

- Lower bias: better fit to training set
- Higher variance: more uncertainty in best parameters, so higher generalization error
- Could have higher or lower test error

Q4-Q7

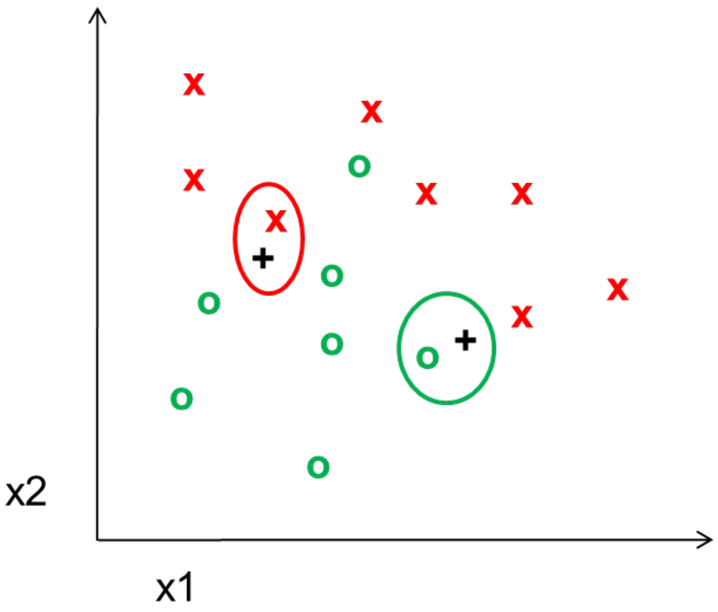
https://tinyurl.com/441-fa24-L3

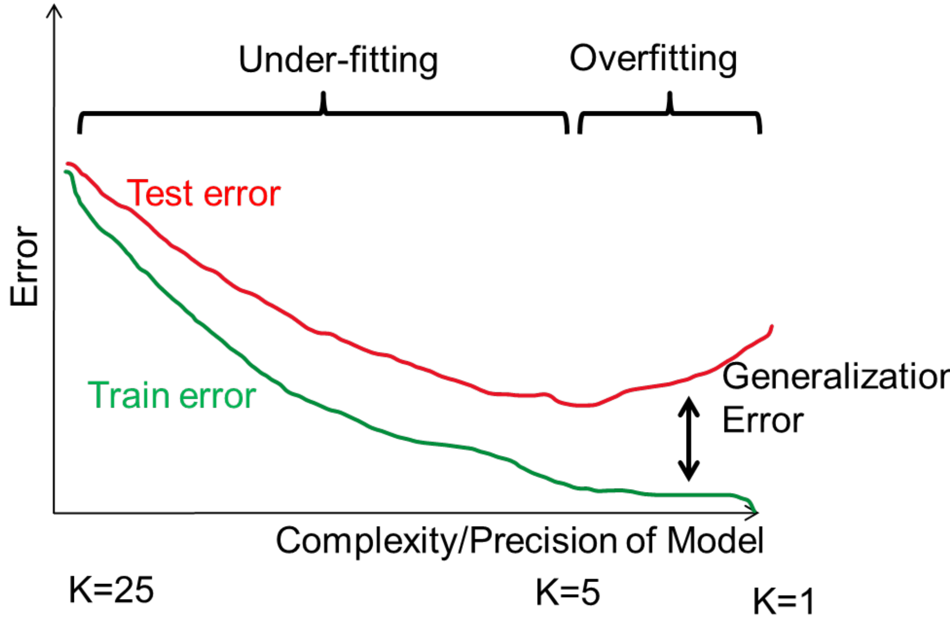
Things to remember

- Similarity/distance measures: L1, L2, cosine

- KNN can be used for either classification (return most common label) or regression (return average target value)

- Test error is composed of
  - **Irreducible error** (perfect prediction not possible given features)
  - **Bias** (model cannot perfectly fit the true function)
  - **Variance** (parameters cannot be perfectly learned from training data)





Thursday

- Retrieval and clustering