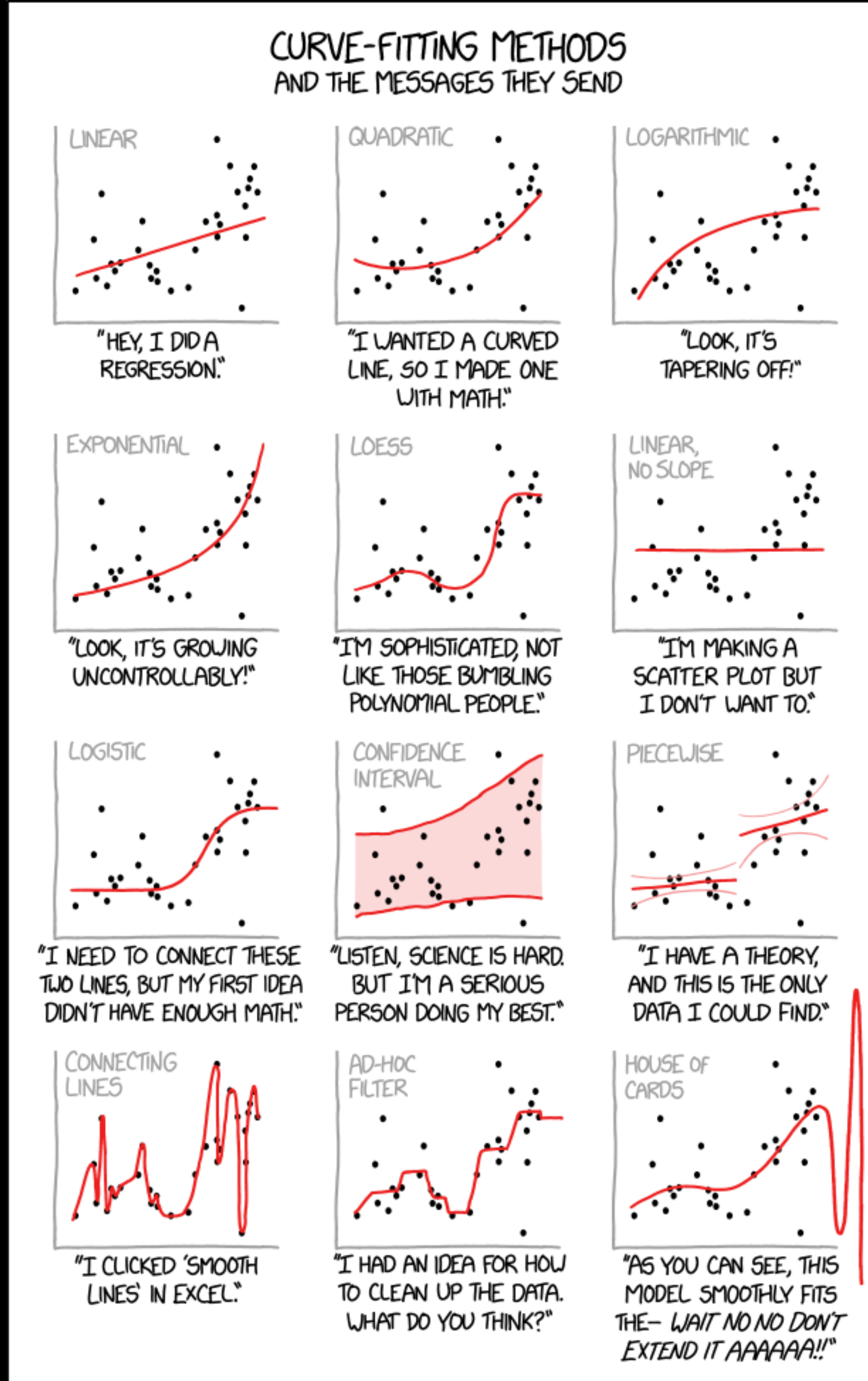
Welcome to Week #13!

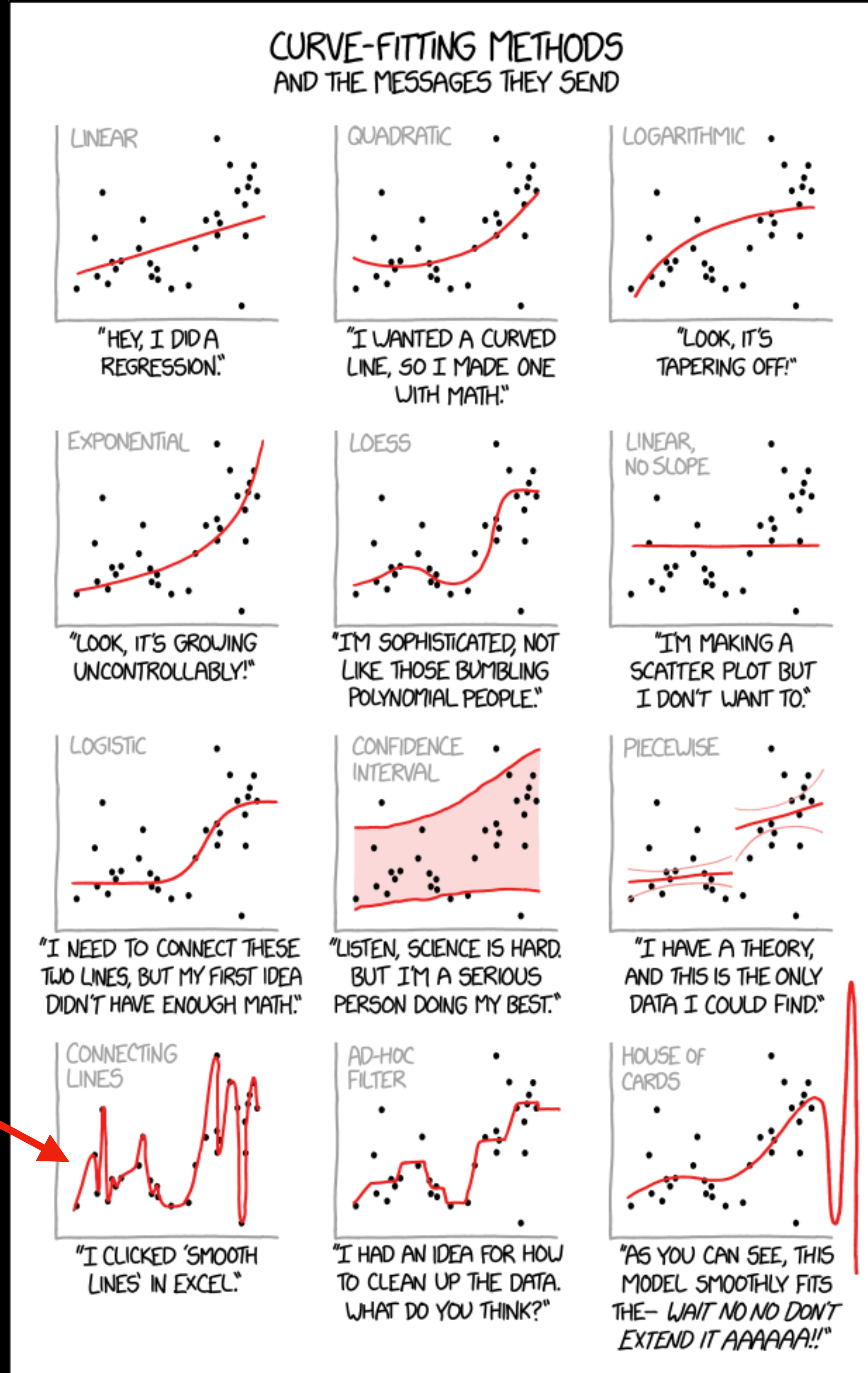
K-Nearest Neighbors

K-Nearest Neighbors

First: an intro to overfitting


CURVE-FITTING METHODS
AND THE MESSAGES THEY SEND
LINEAR
"HEY, I DID A REGRESSION."
QUADRATIC
"I WANTED A CURVED LINE, SO I MADE ONE WITH MATH."
LOGARITHMIC
"LOOK, IT'S TAPERING OFF!"
EXPONENTIAL
"LOOK, IT'S GROWING UNCONTROLLABLY!"
LOESS
"I'M SOPHISTICATED, NOT LIKE THOSE BUMBLING POLYNOMIAL PEOPLE."
LINEAR, NO SLOPE
"I'M MAKING A SCATTER PLOT BUT I DON'T WANT TO."
LOGISTIC
"I NEED TO CONNECT THESE TWO LINES, BUT MY FIRST IDEA DIDN'T HAVE ENOUGH MATH."
CONFIDENCE INTERVAL
"LISTEN, SCIENCE IS HARD. BUT I'M A SERIOUS PERSON DOING MY BEST."
PIECEWISE
"I HAVE A THEORY, AND THIS IS THE ONLY DATA I COULD FIND."
CONNECTING LINES
"I CLICKED 'SMOOTH LINES' IN EXCEL."
AD-HOC FILTER
"I HAD AN IDEA FOR HOW TO CLEAN UP THE DATA. WHAT DO YOU THINK?"
HOUSE OF CARDS
"AS YOU CAN SEE, THIS MODEL SMOOTHLY FITS THE– *WAIT NO NO DON'T EXTEND IT AAAAAA!!*"

Overfit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Overfit?

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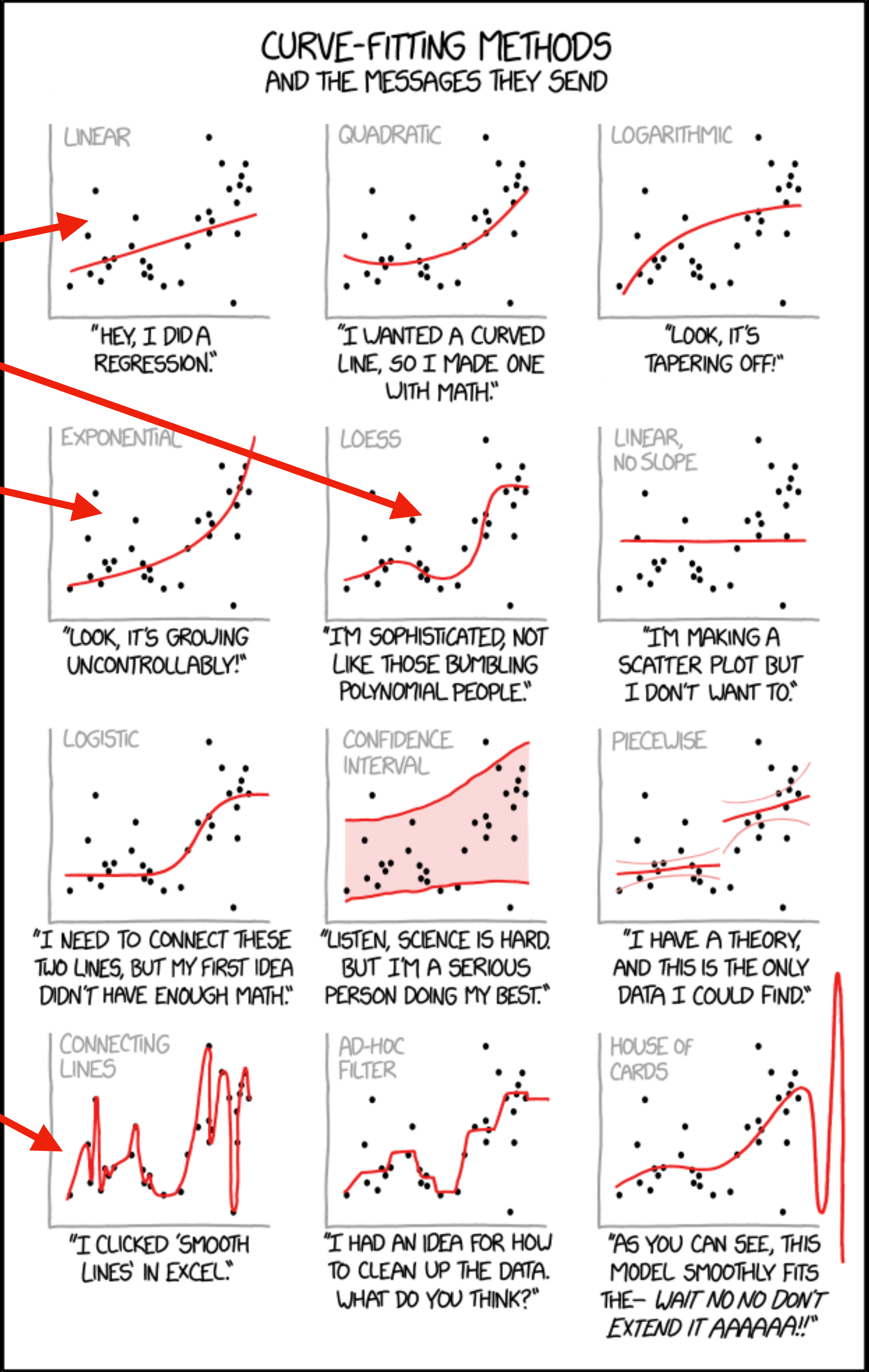

Overfit?

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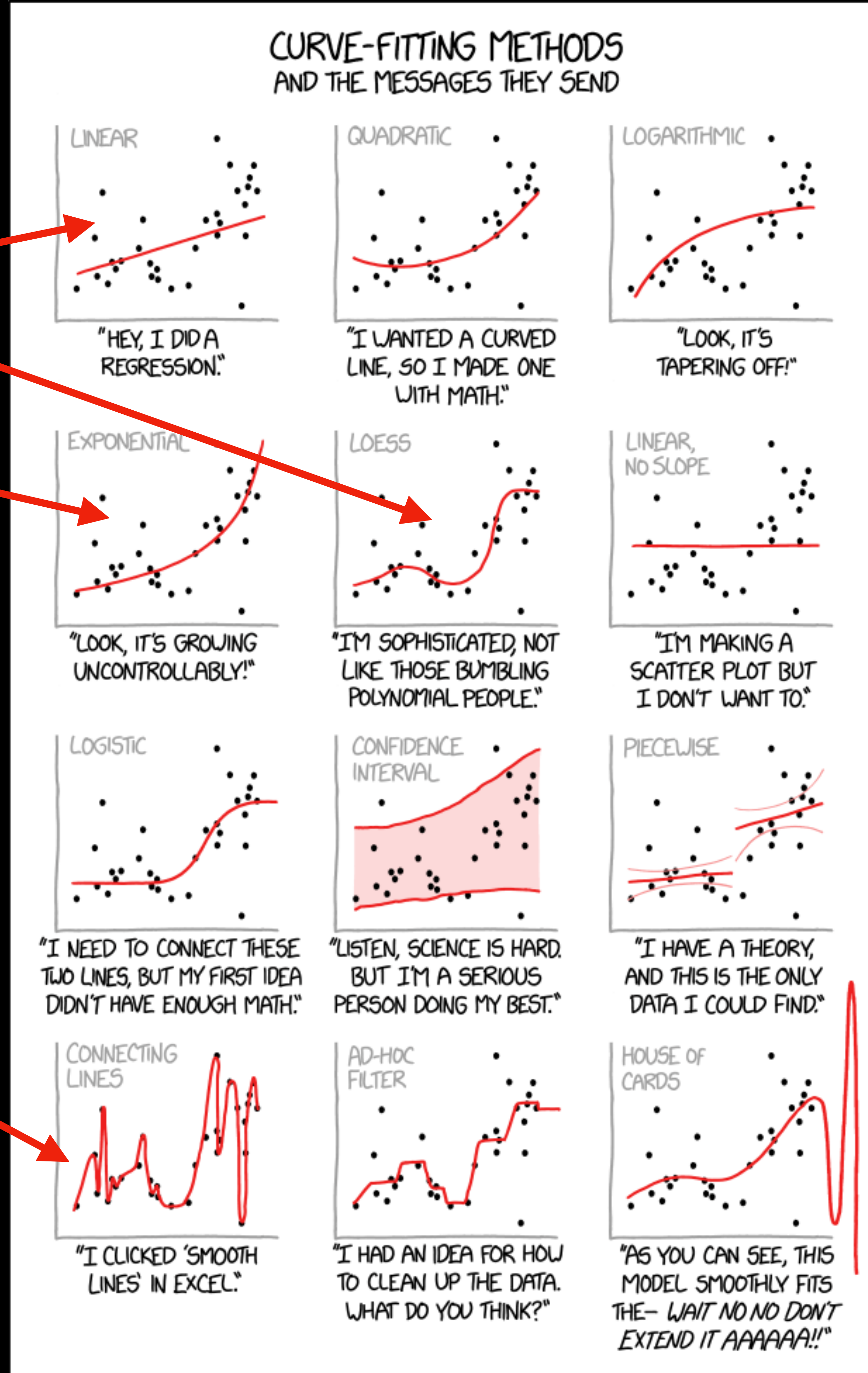


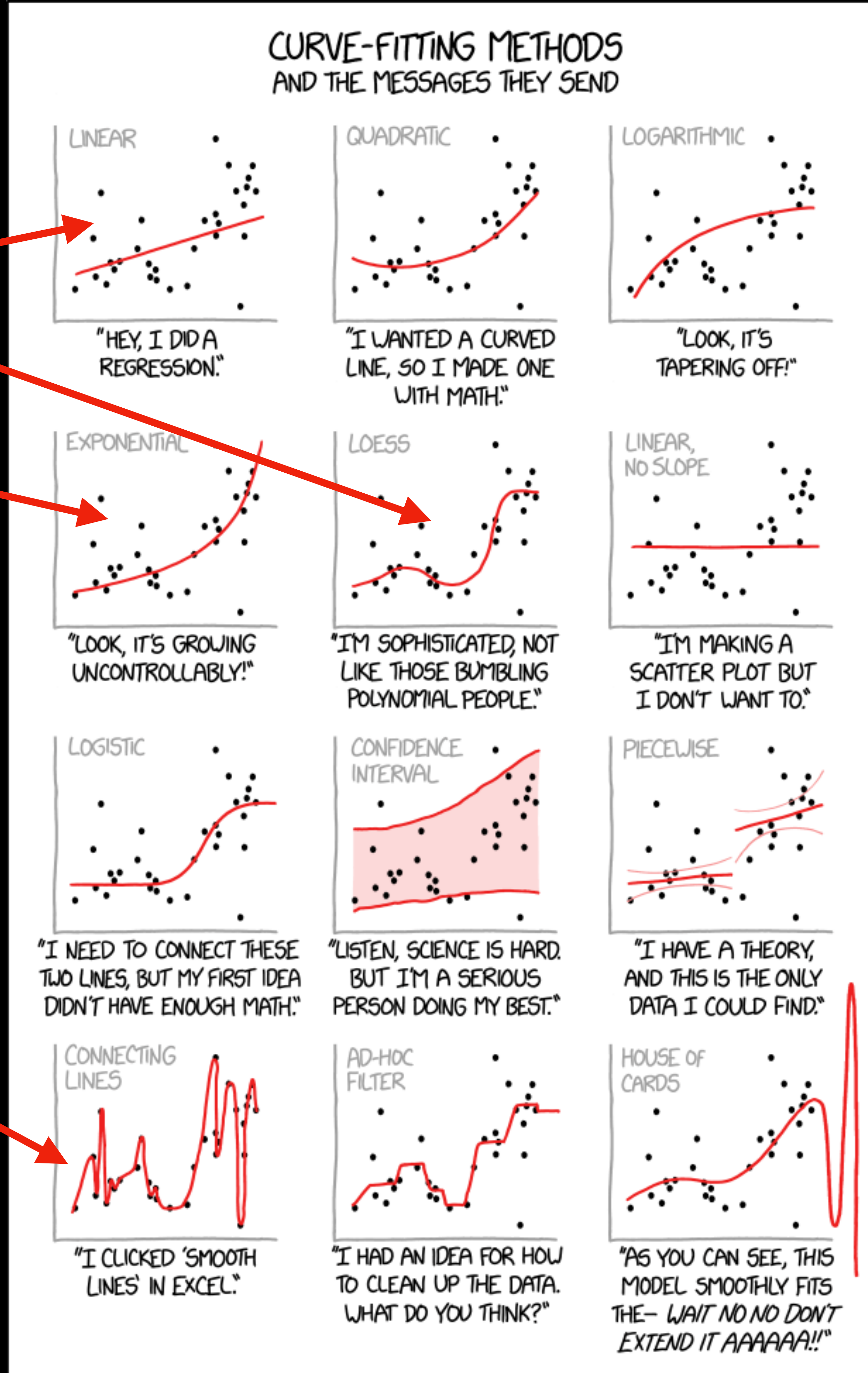
Underfit?

Overfit?

Overfit?

Underfit?

Overfit



Is overfitting or underfitting worse?

Bias-Variance Trade-Off (First Glance)

$$E\left(y_0 - \hat{f}(x_0)\right)^2 = \text{Var}(\hat{f}(x_0)) + [\text{Bias}(\hat{f}(x_0))]^2 + \text{Var}(\epsilon)$$

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mean square error if we kept estimating response variable y by our fitted function of our explanatory variables, f(x) with different sample datasets at point x_0

MSE

“how good is our fit?”

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how much our function, f, changes if we use a different random sample (variance)

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Inherent error (bias) in the fact that any model is only an approximation to reality

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Inherent error in our measurements

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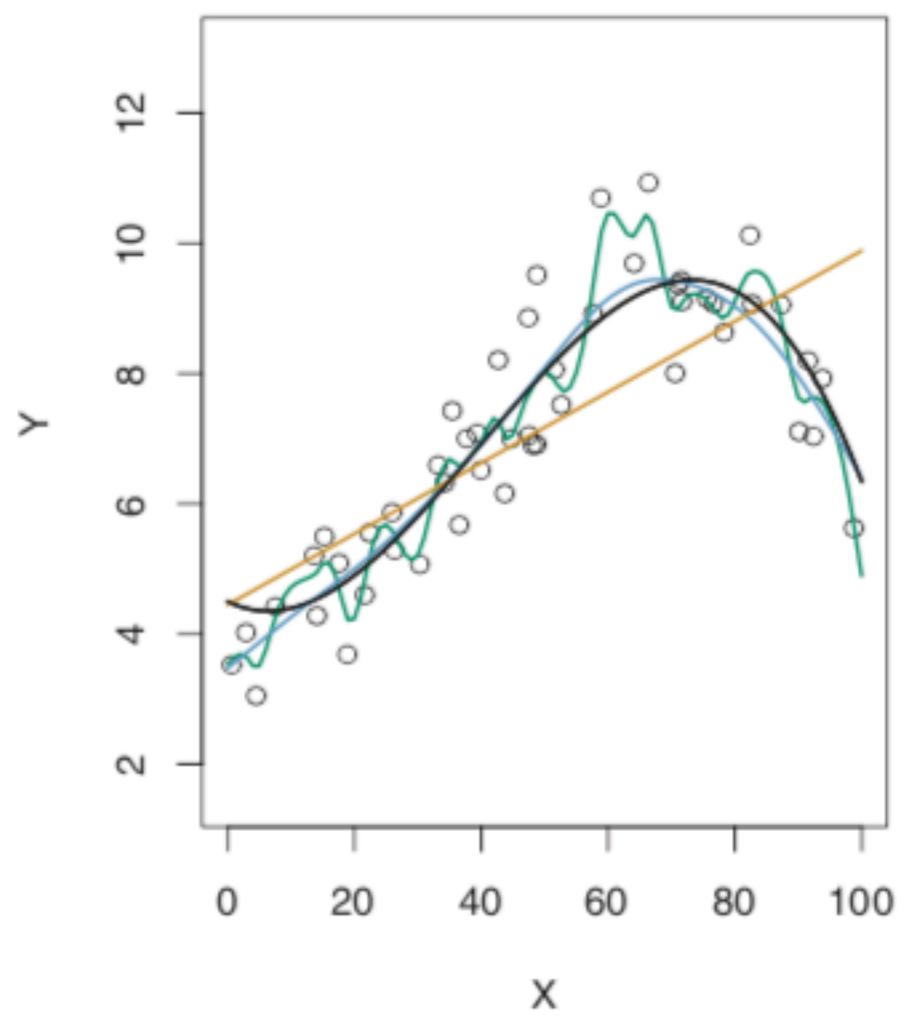

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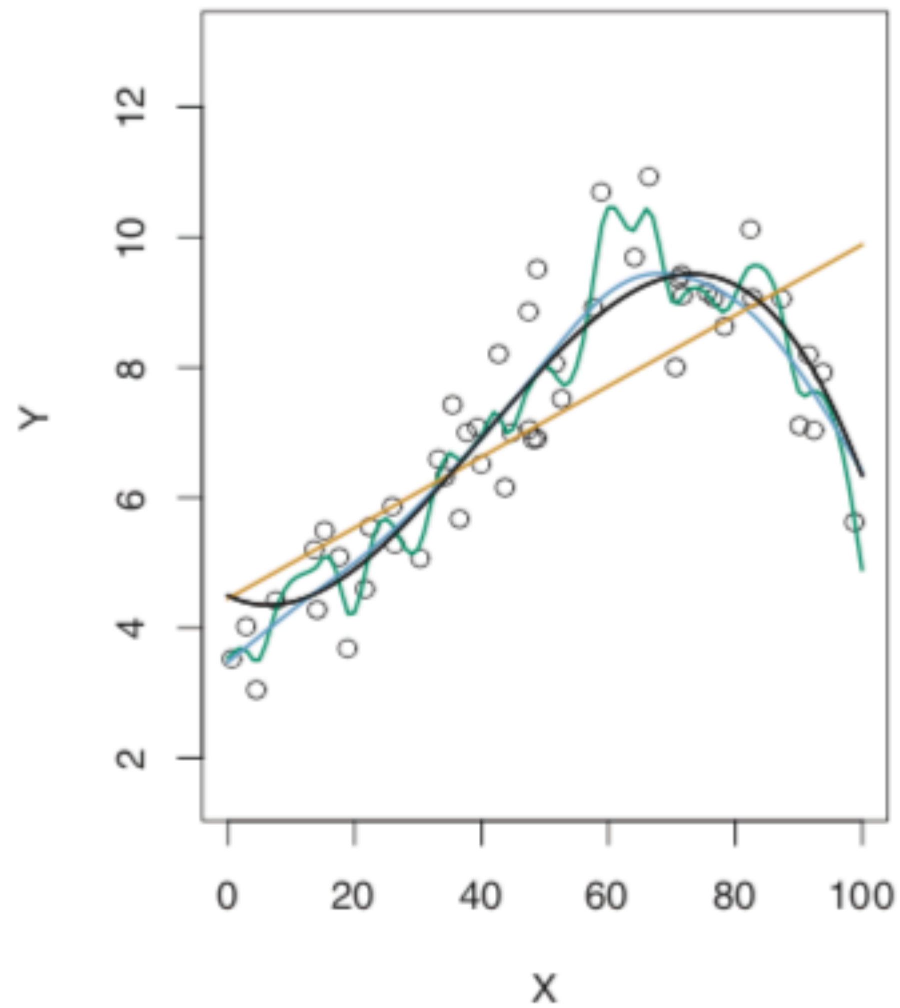

Actual underlying function - y

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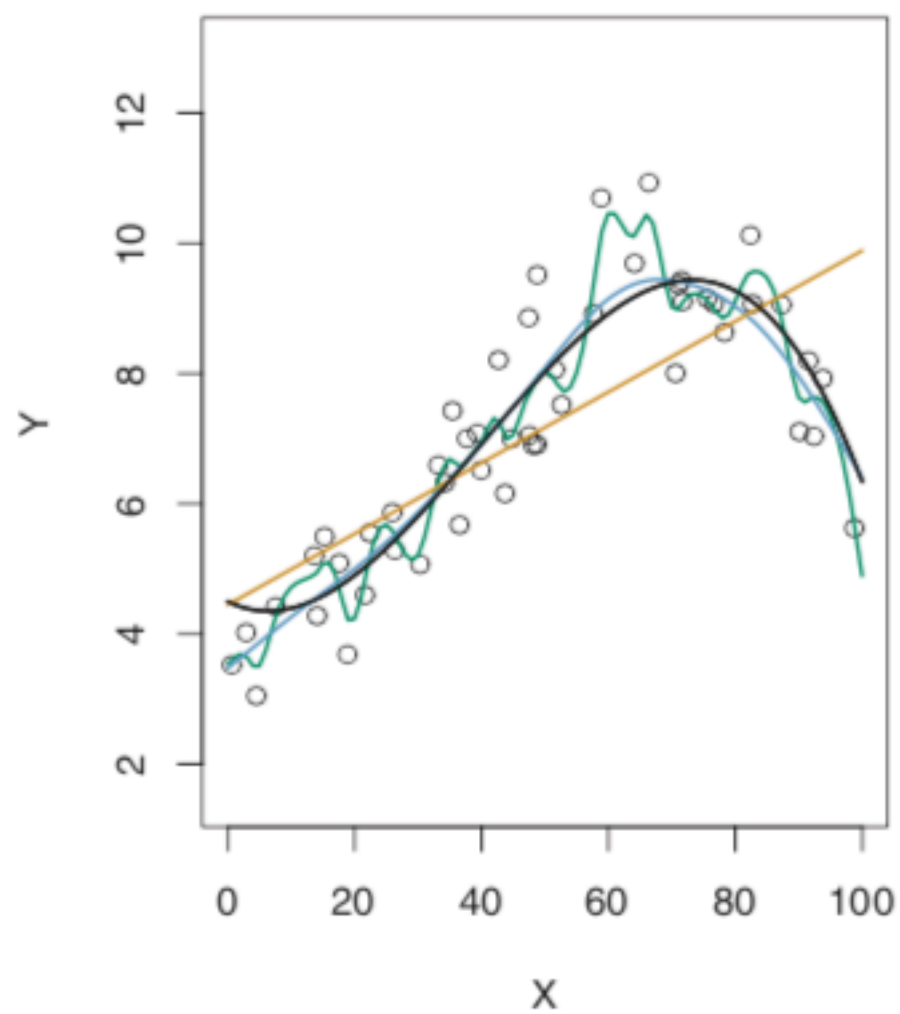

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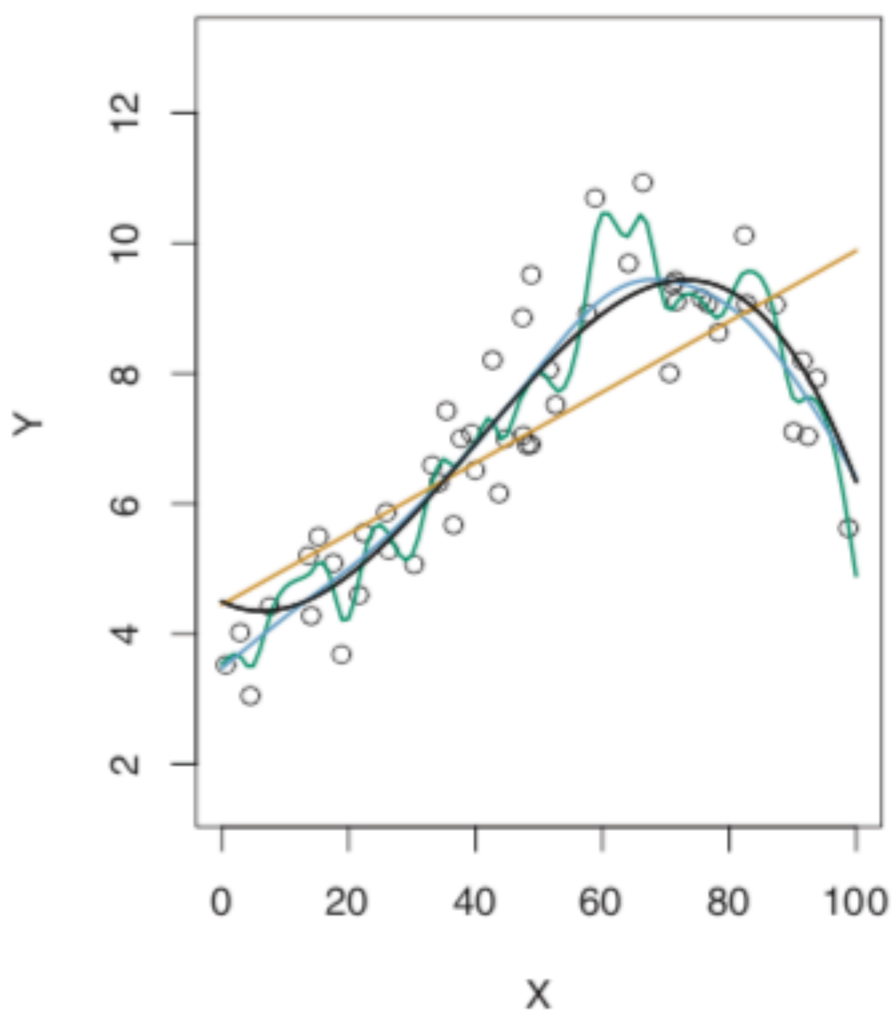

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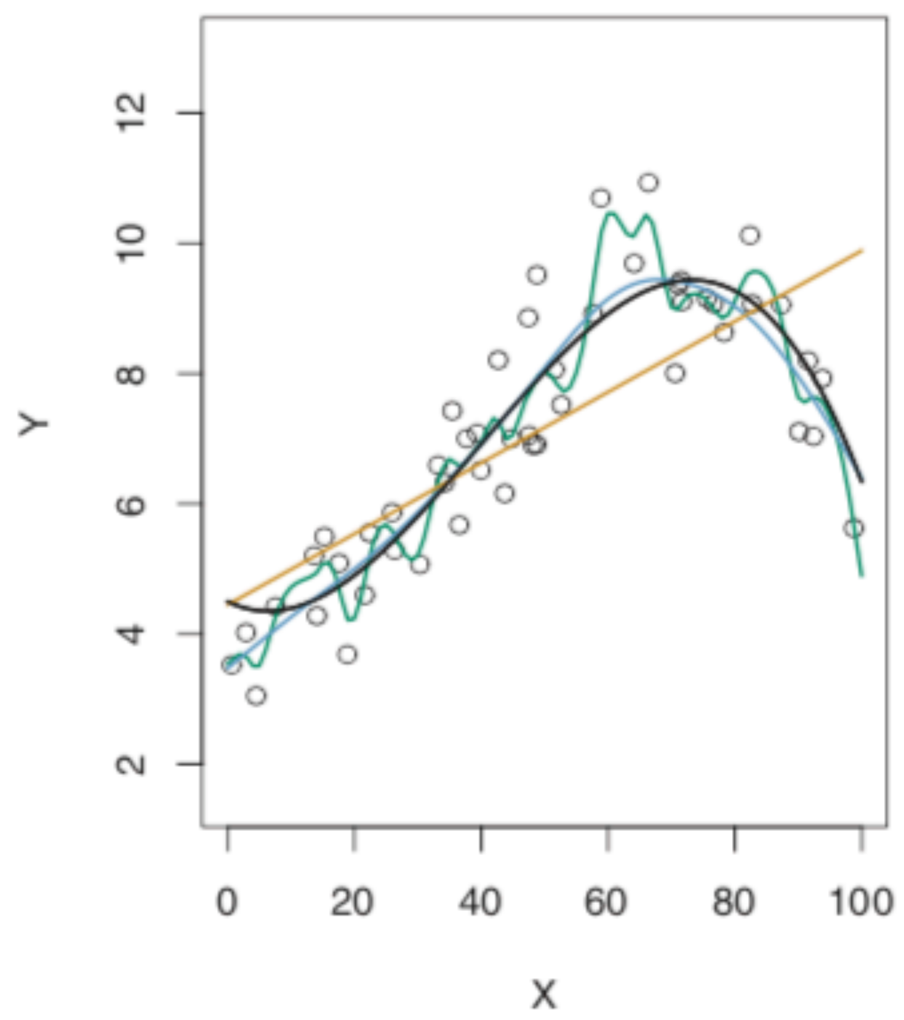

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Low "flexibility" smooth spline

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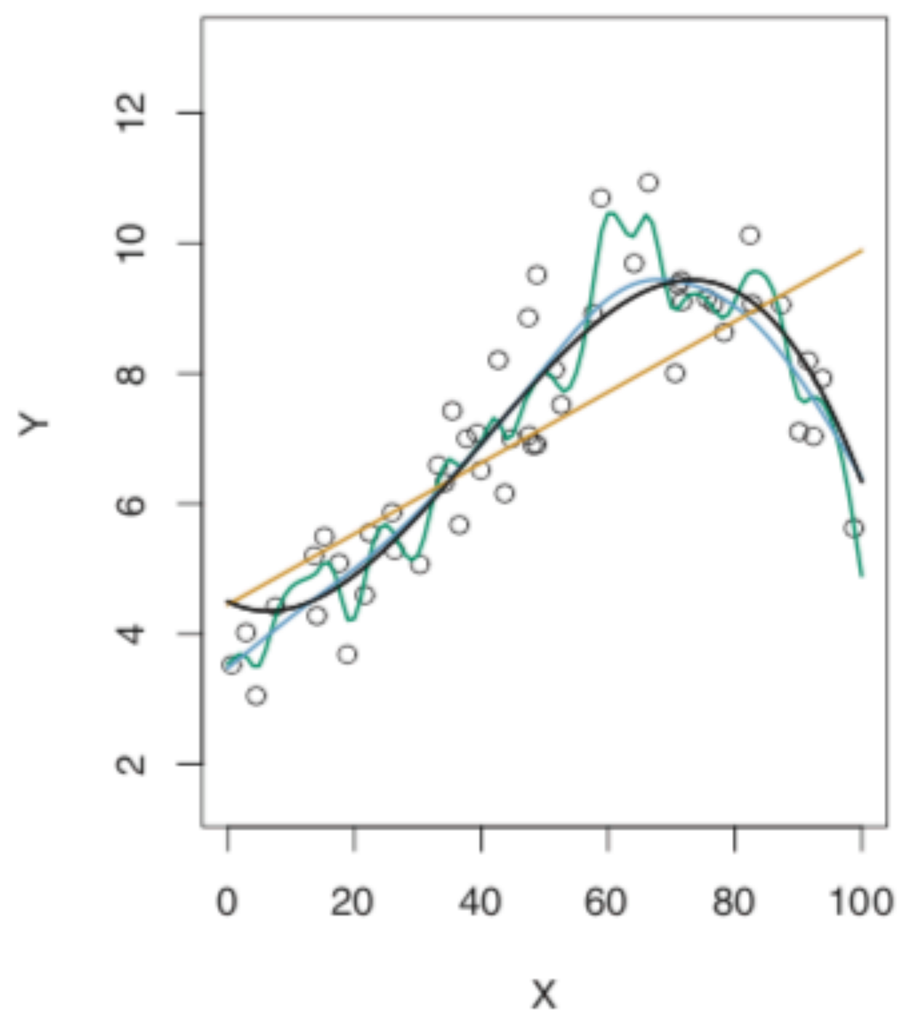

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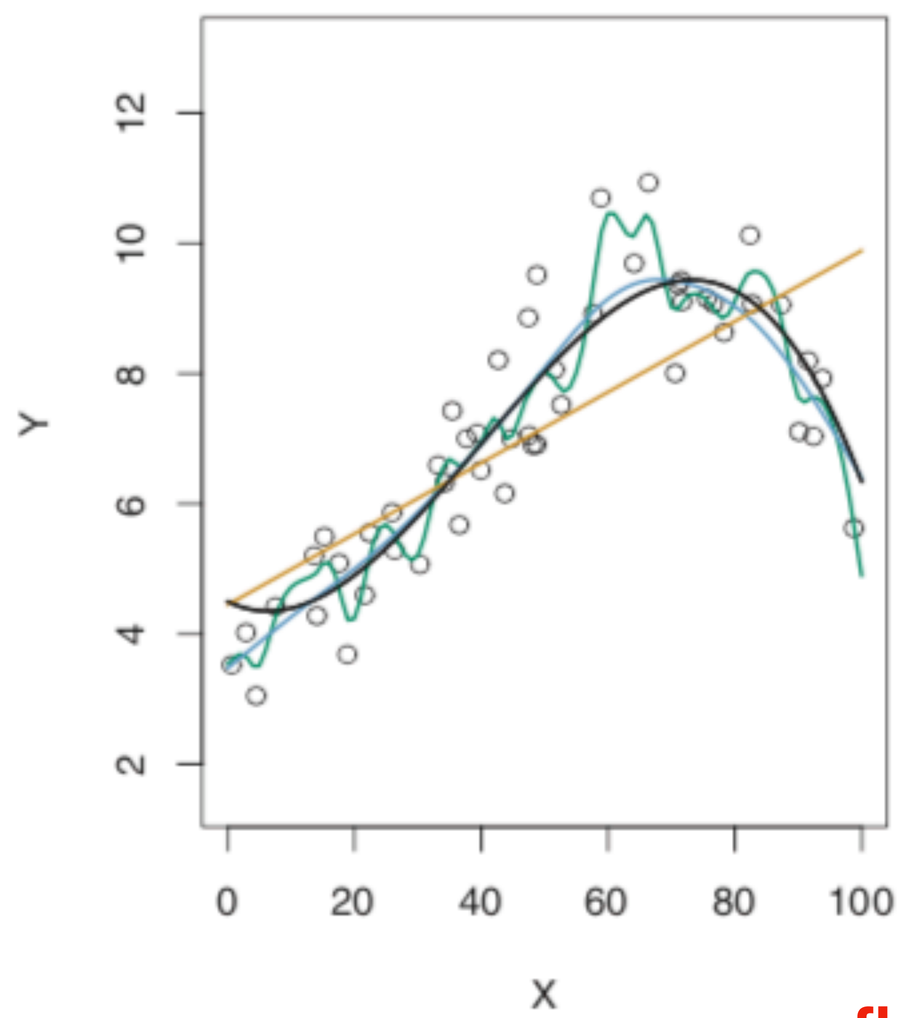

flexibility = DOF ~ how “wiggly” a line is

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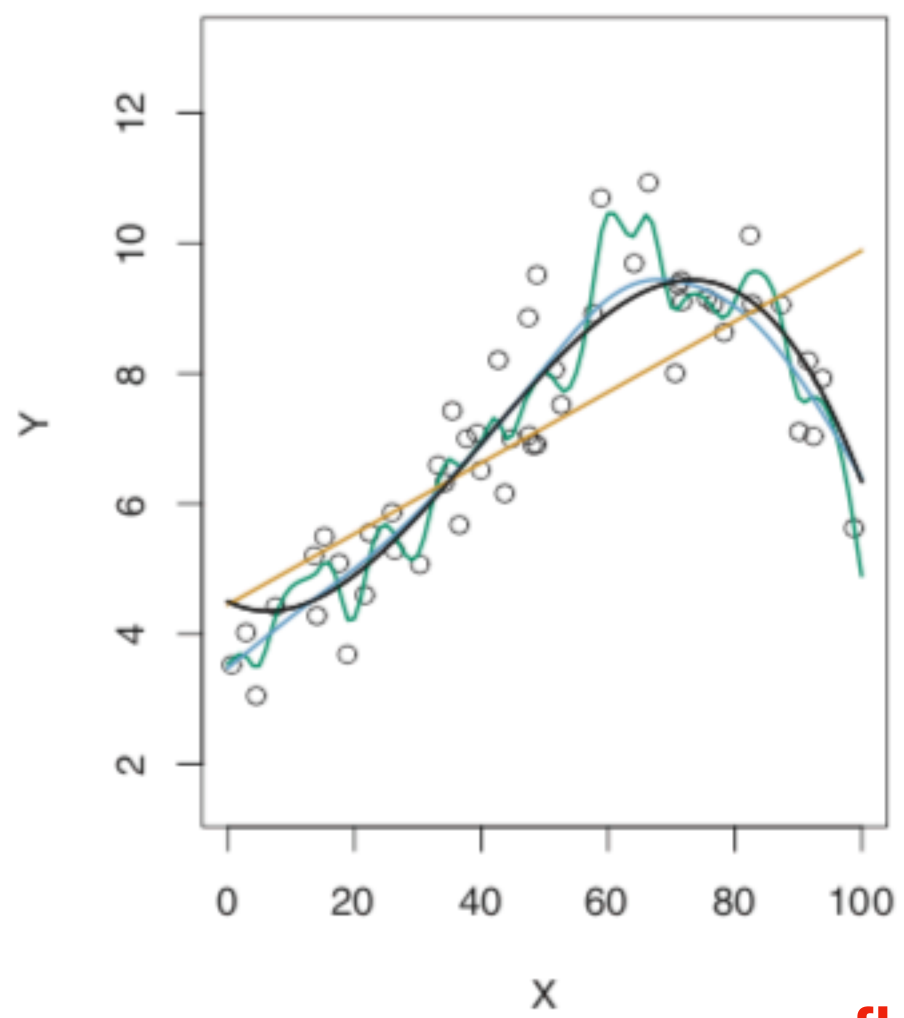

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fits data well, but underlying model badly

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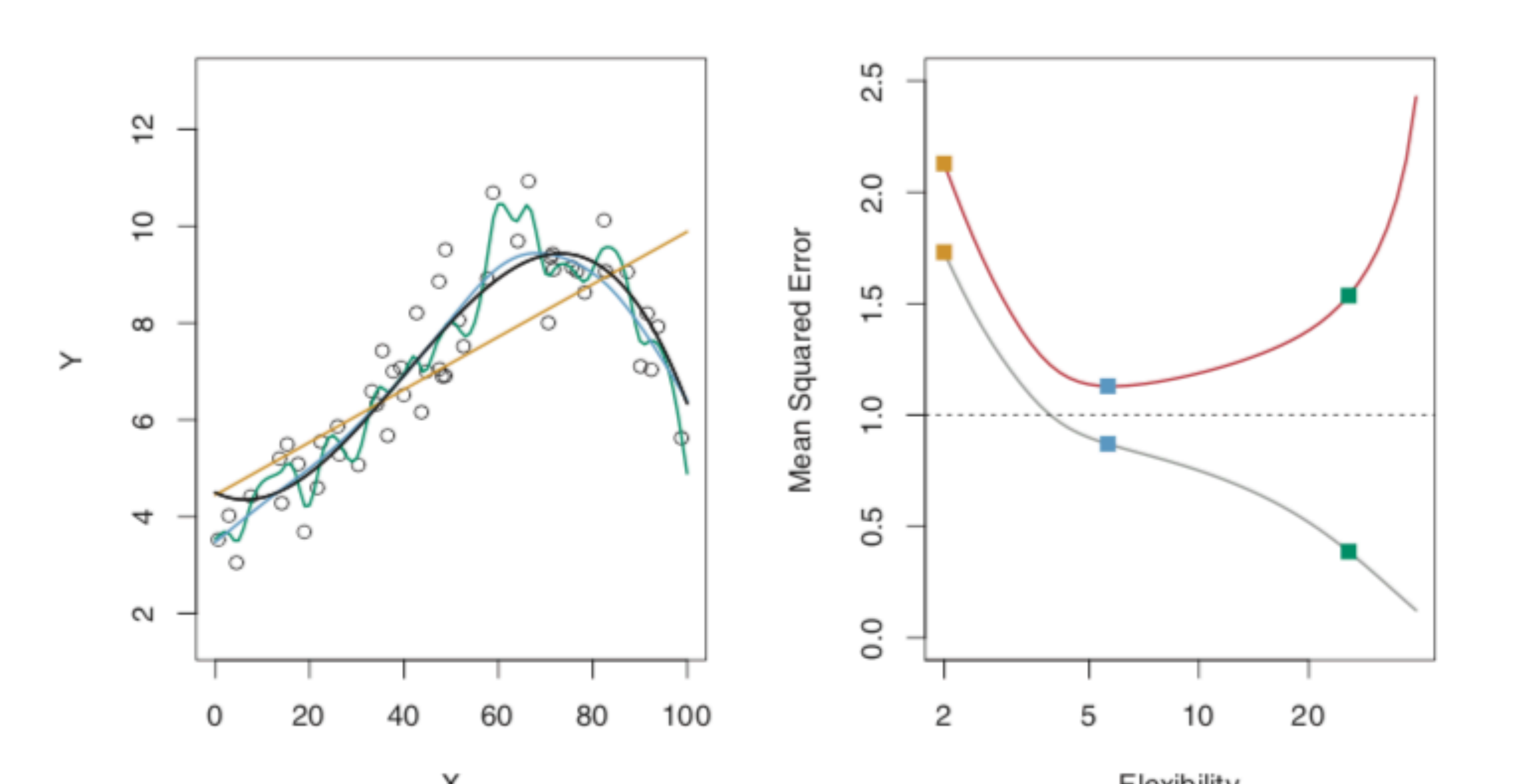

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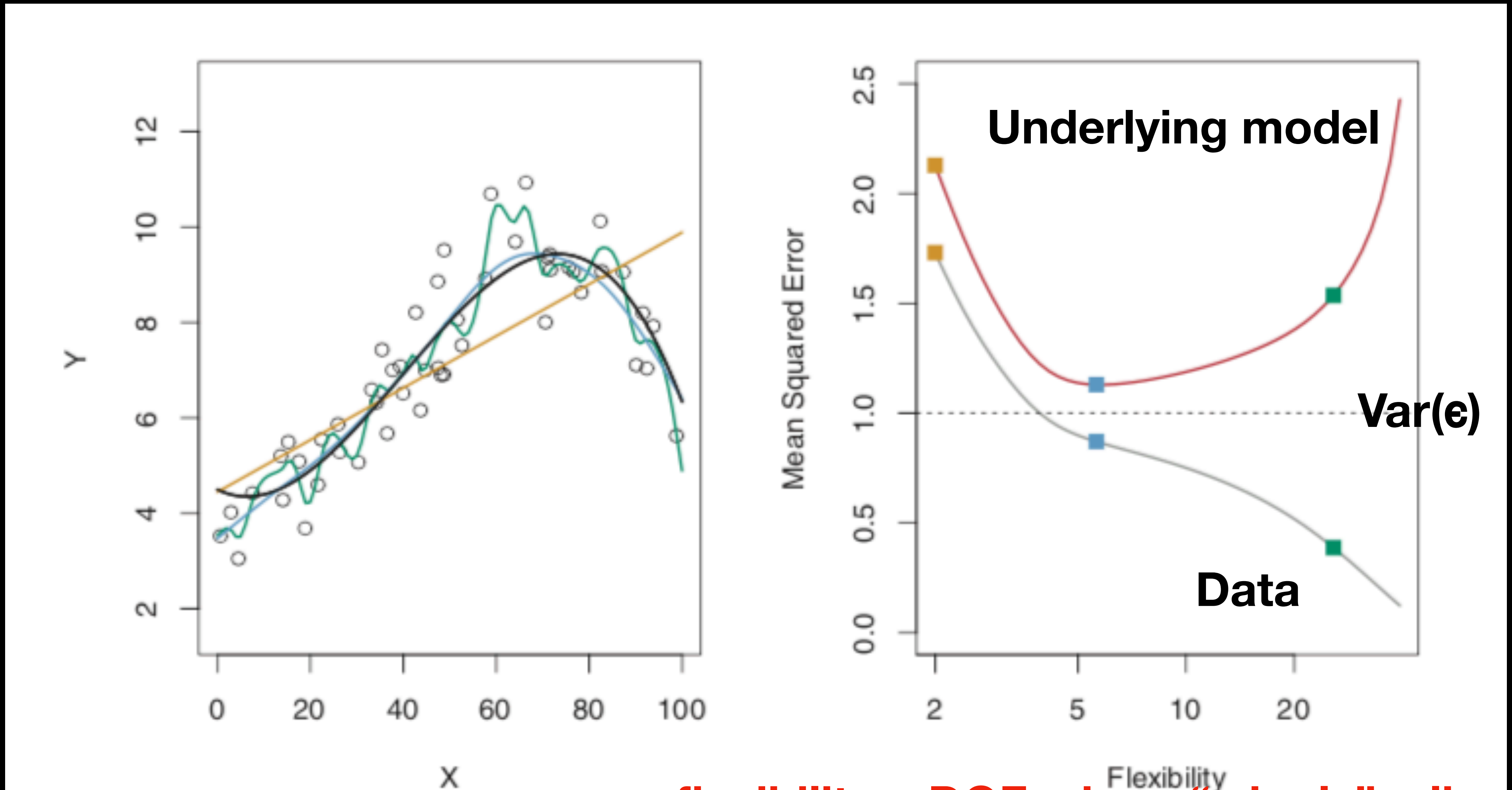

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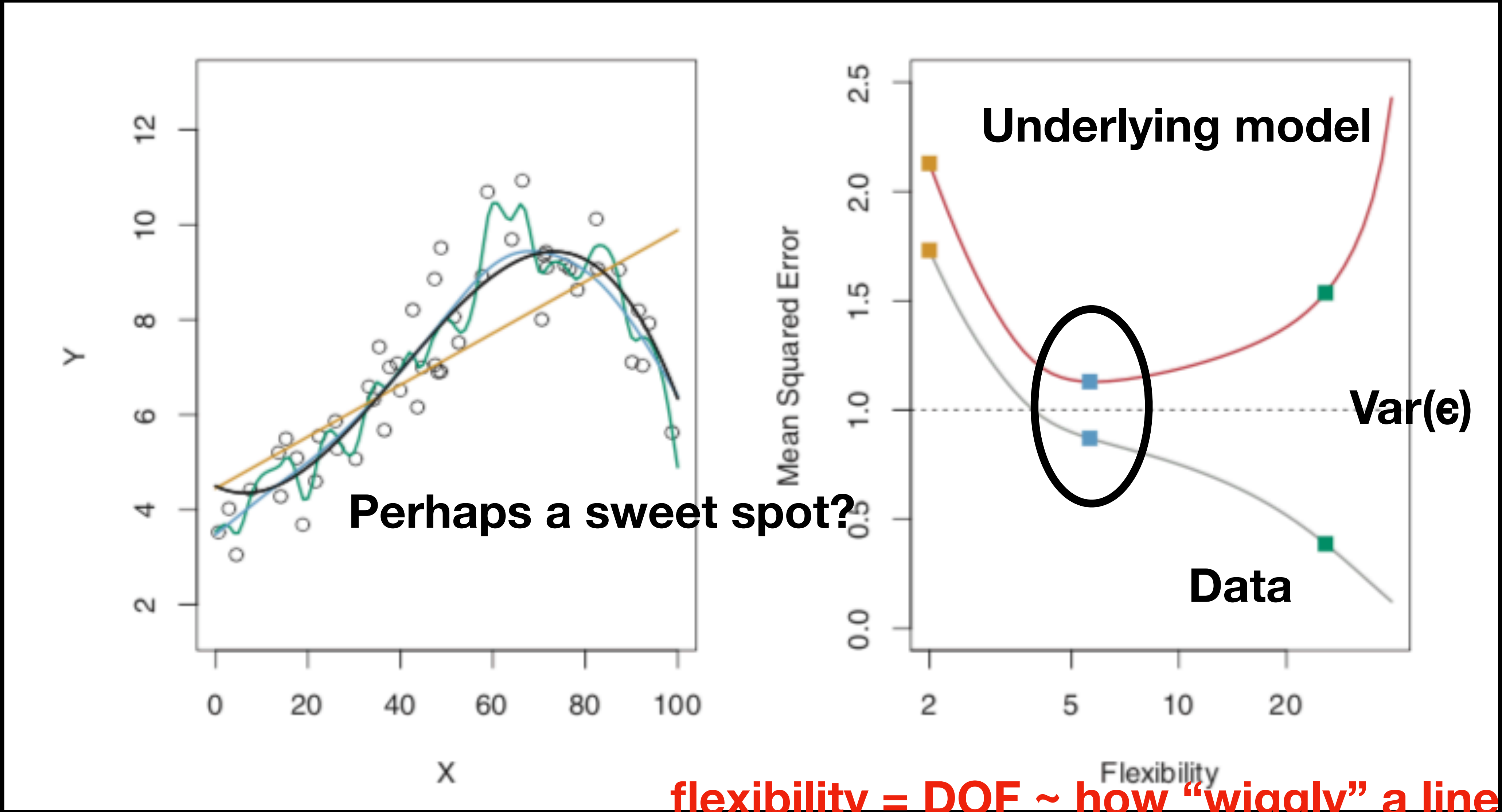

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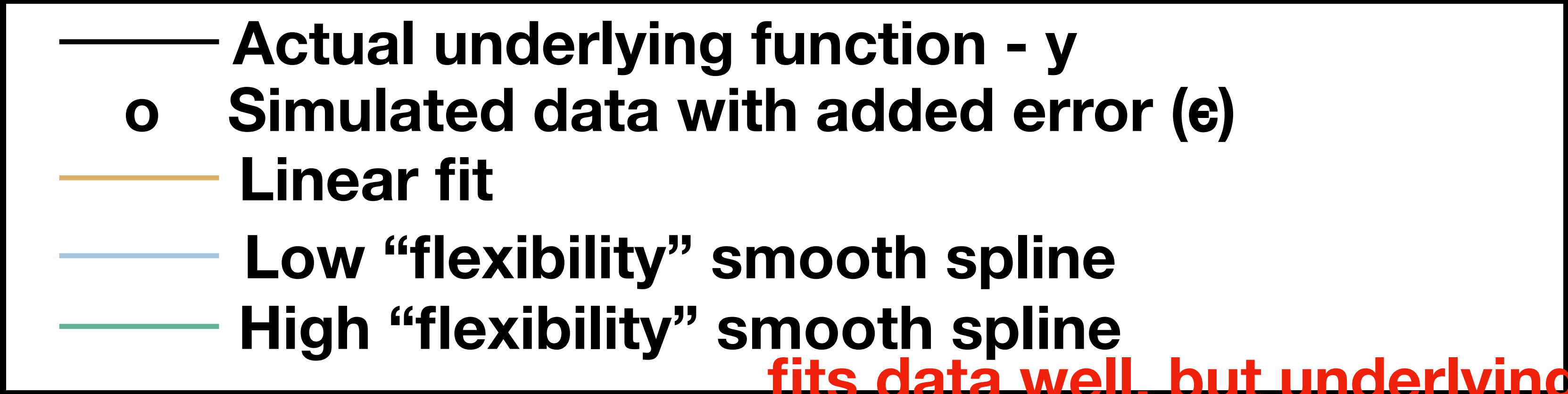

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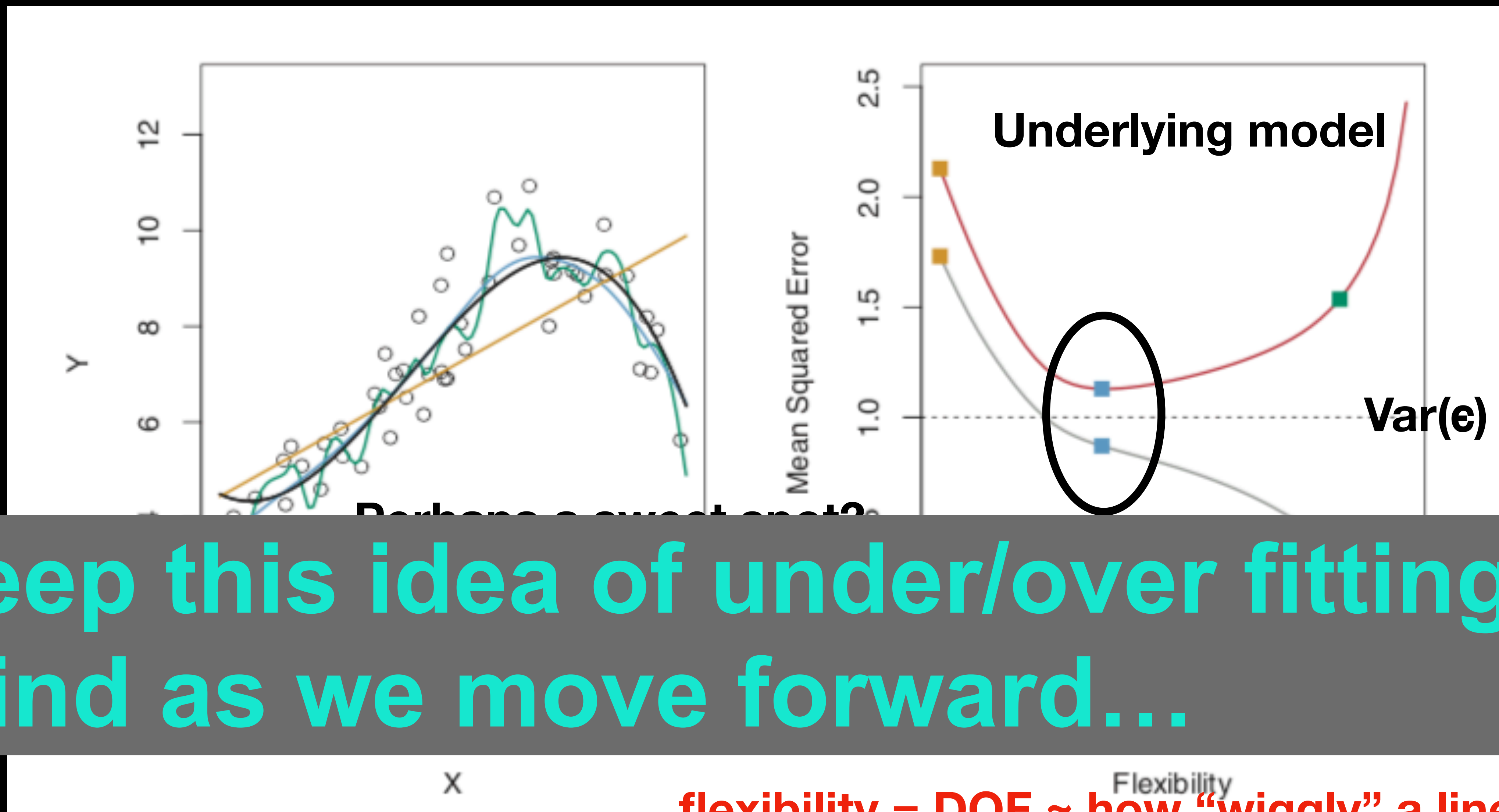

Keep this idea of under/over fitting in mind as we move forward…

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K-Nearest Neighbors

~~First: an intro to overfitting~~

So far…

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \ldots + \beta_n x_n$$

predicted y

intercept

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"I have a basic idea of what the functional form of y looks like (a line or a logit) - computer go find the parameters of that functional form.

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This is nice because we have some hope of gaining intuition from our models.

So far…

$$\underbrace{\hat{y}}_{\text{predicted } y} = \underbrace{\beta_0}_{\text{intercept}} + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \ldots + \beta_n x_n$$

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Now we classify…

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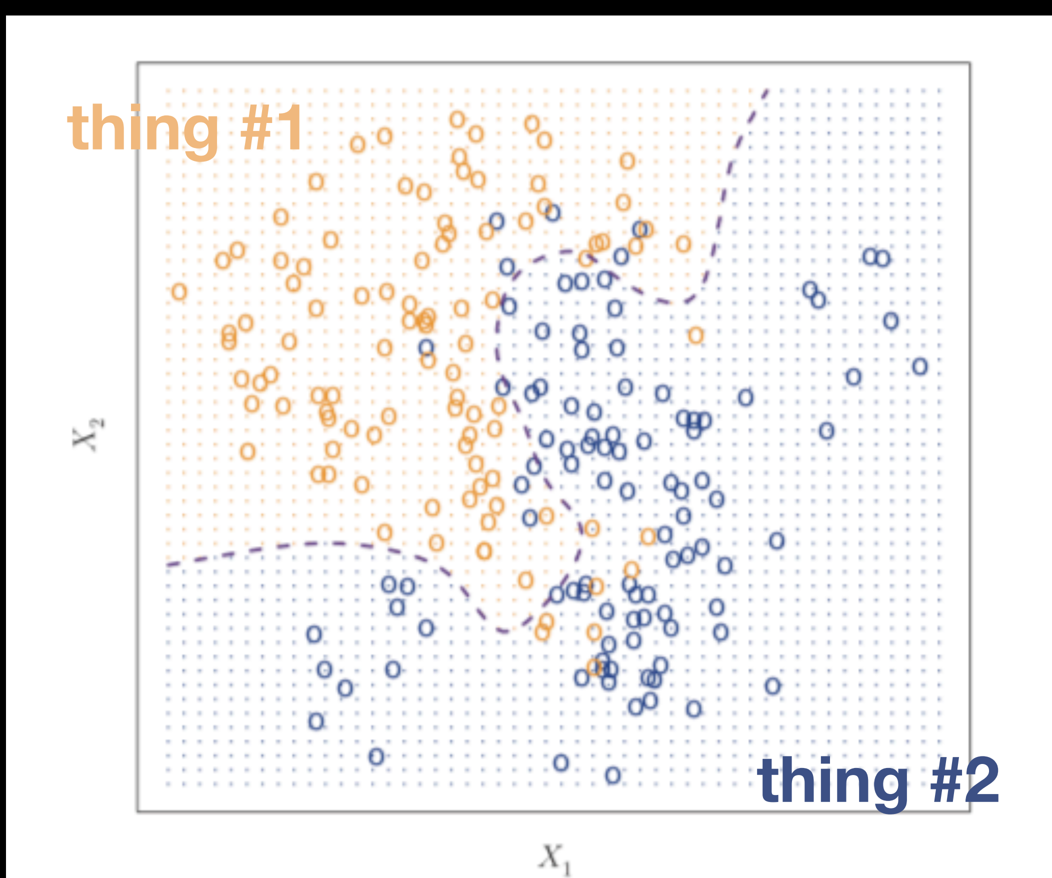

"I want to know where thing #1 and thing #2 live in some 2D space - computer, go figure out the boundary between these two things and let me know"

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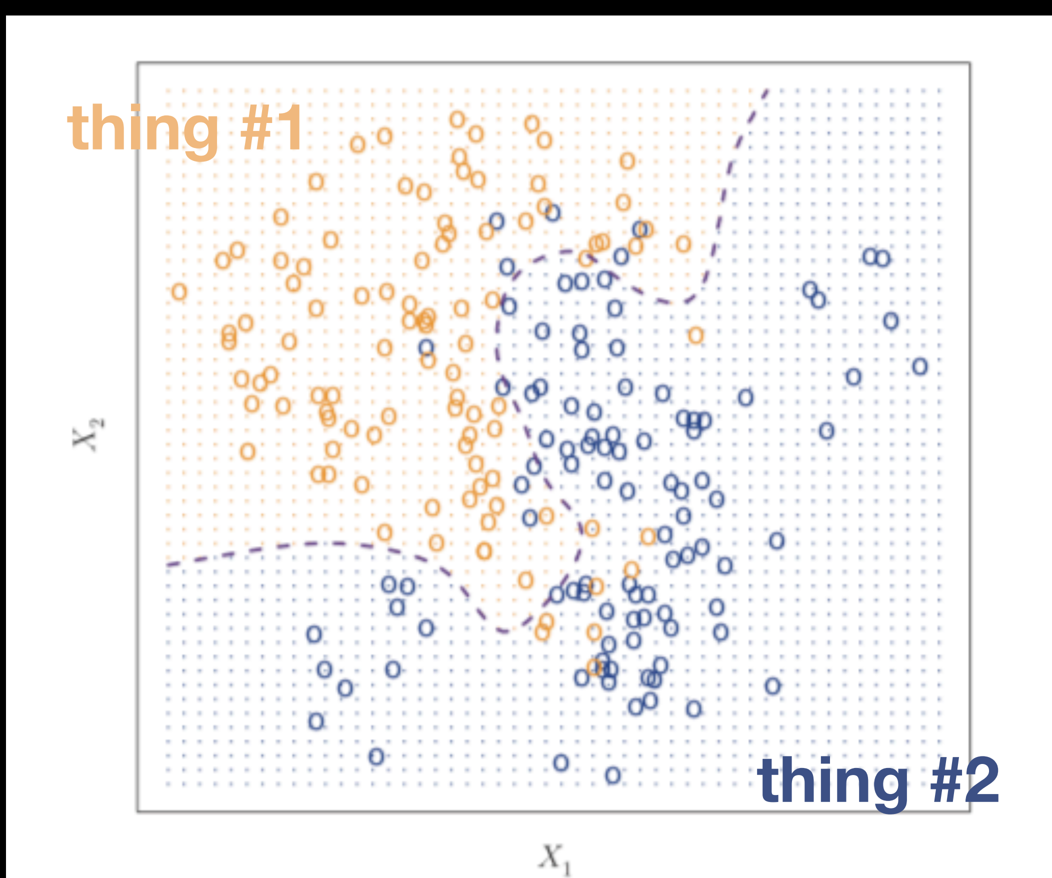

"I want to know where thing #1 and thing #2 live in some 2D space - computer, go figure out the boundary between these two things and let me know"

This is nice because we don't have to assume some model beforehand.

K Nearest Neighbors, in pictures

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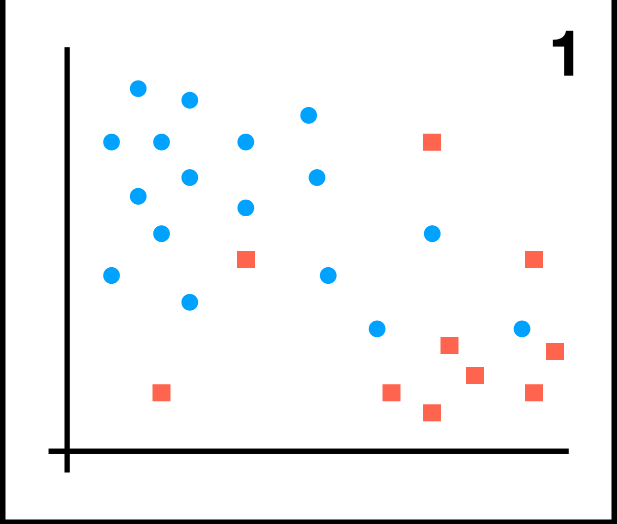

Sample (training) data representing underlying population

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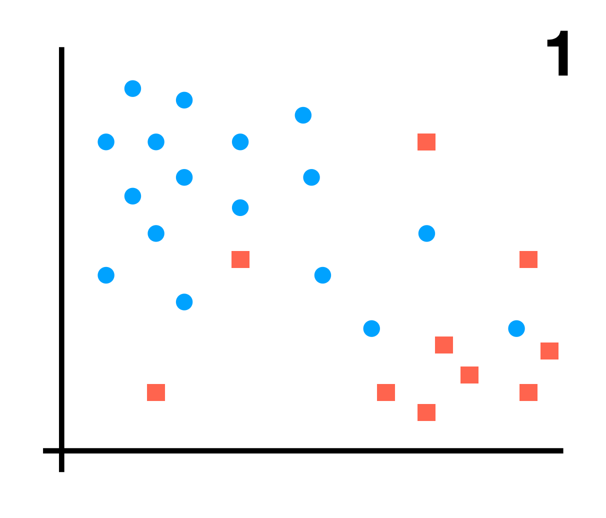

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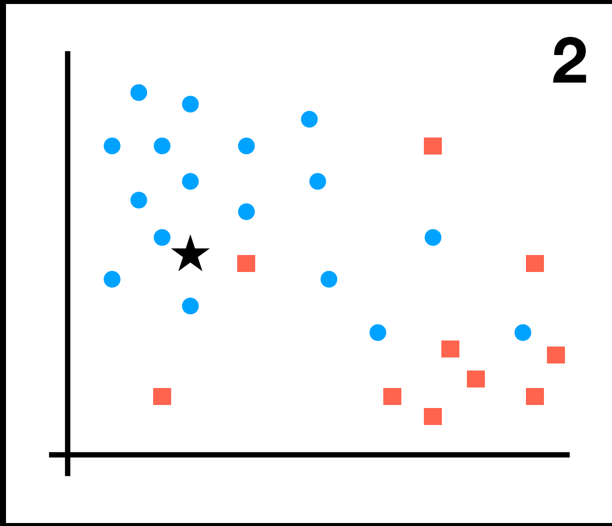

New point of interest

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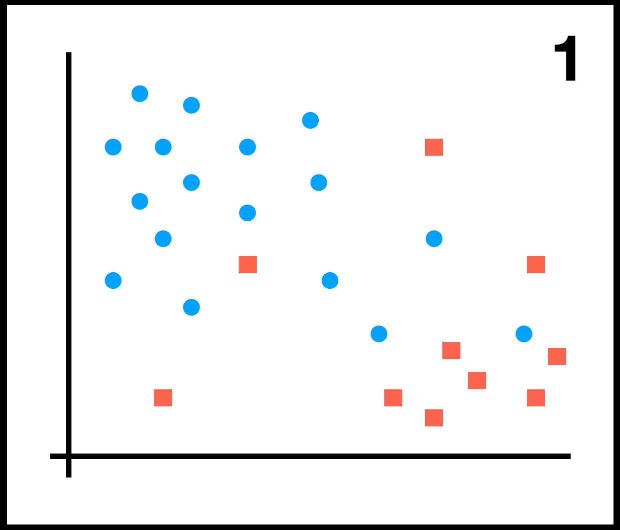

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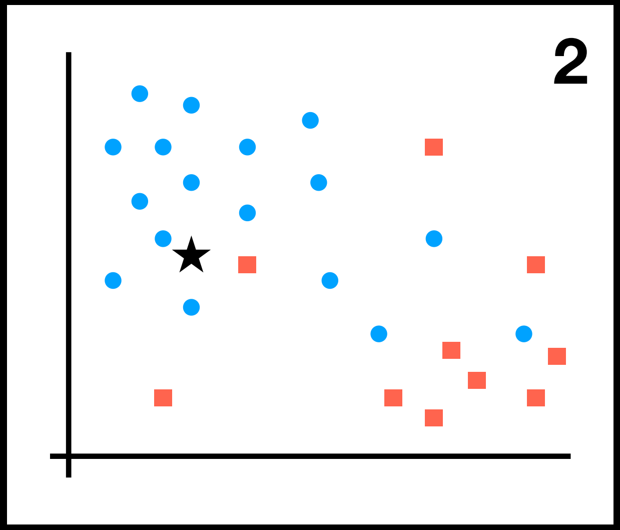

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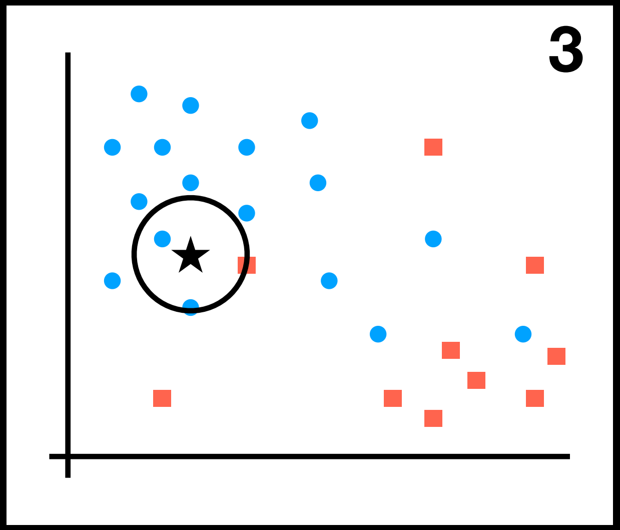
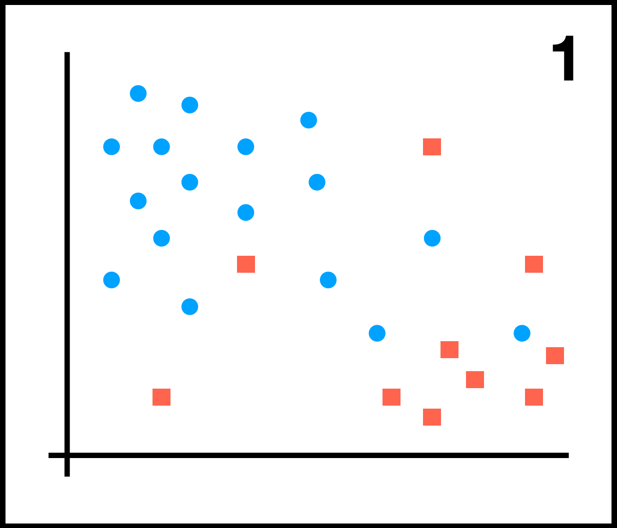


Find k nearest neighbors (here k = 3)

K Nearest Neighbors, in pictures



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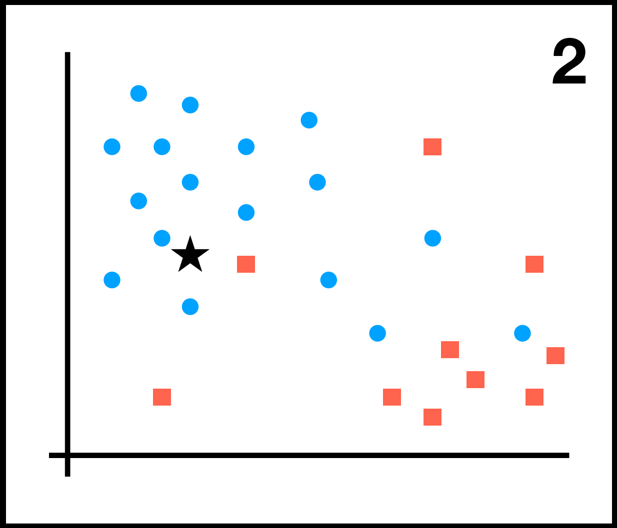

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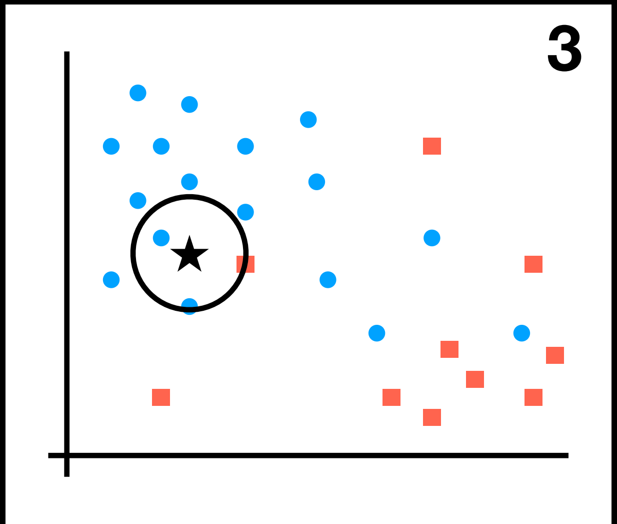

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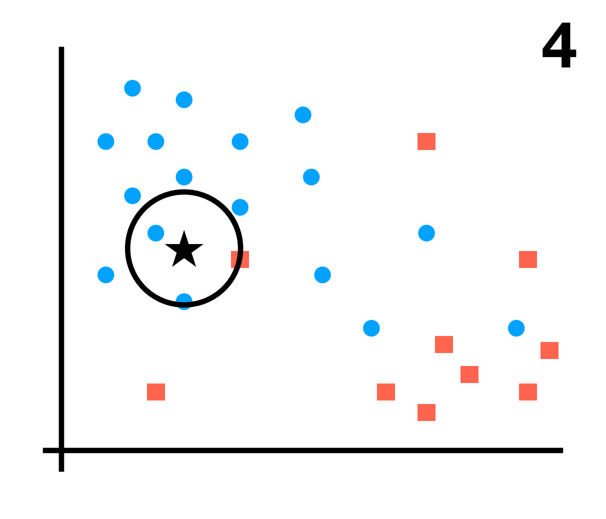
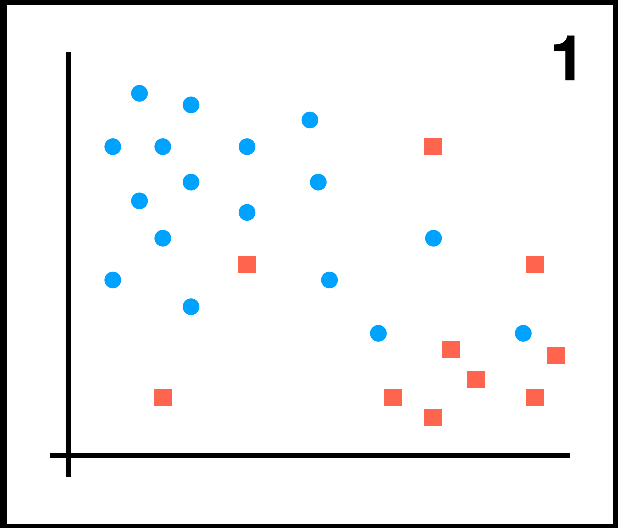


count “types” - here 2/3 points are blue
P(blue) = 2/3
P(red) = 1/3

K Nearest Neighbors, in pictures



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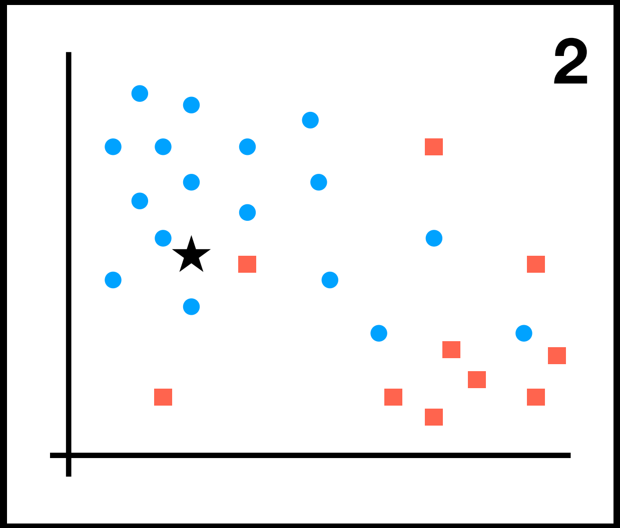

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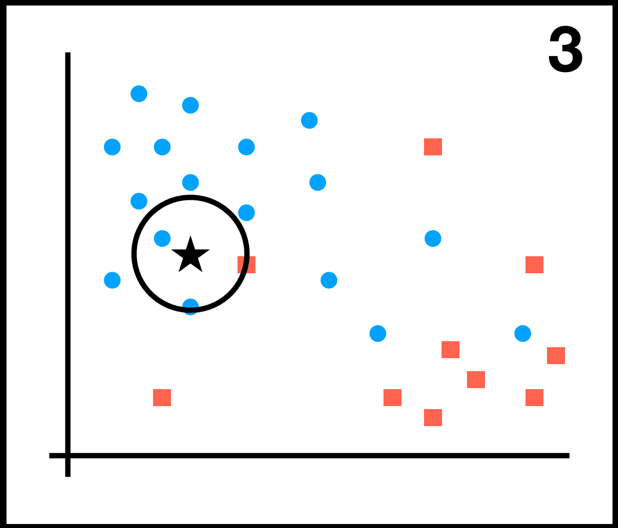

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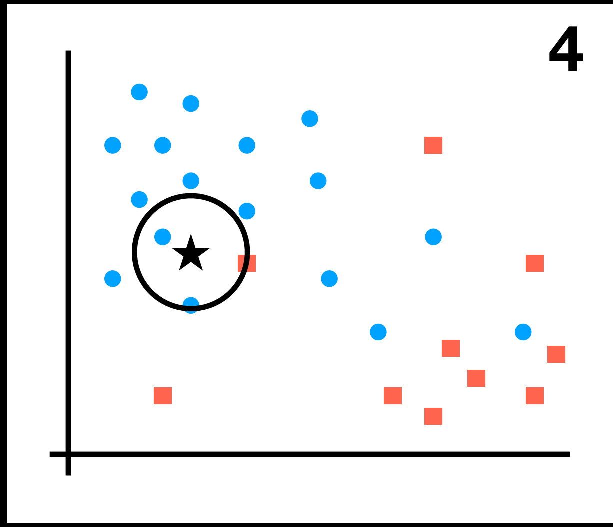

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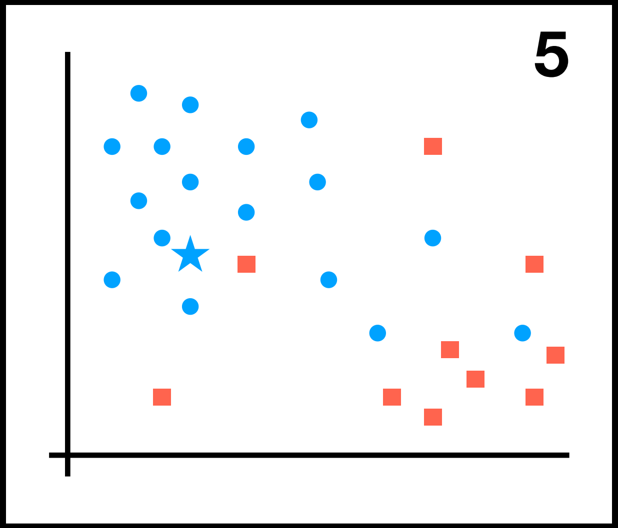
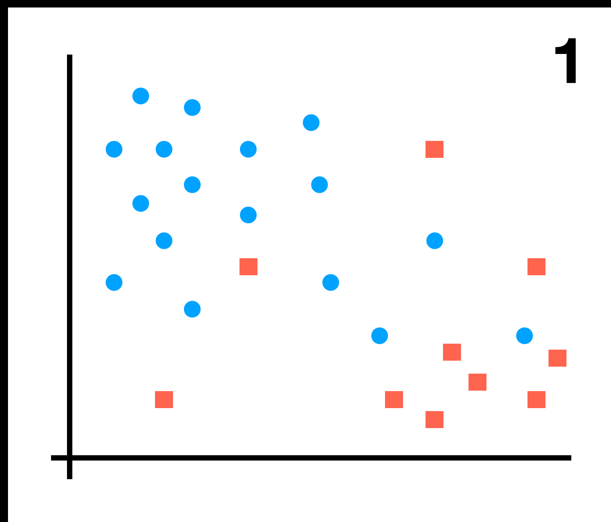


if P > cut off say new point is in that group
here: P(blue) > 0.5

K Nearest Neighbors, in pictures



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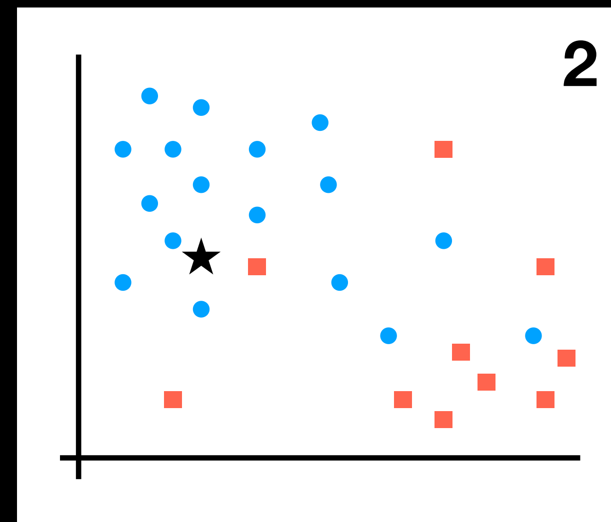

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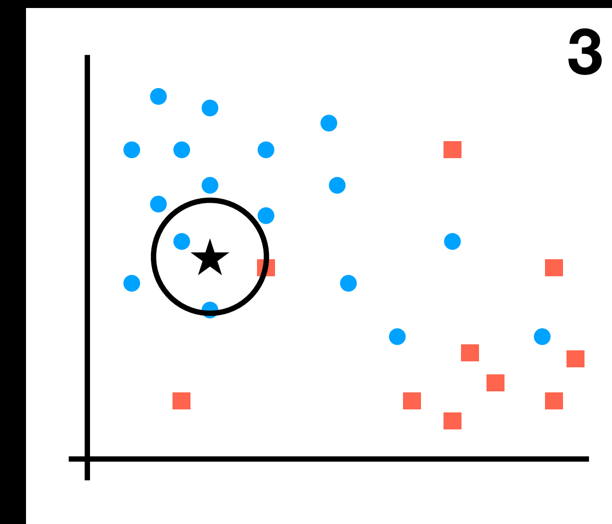

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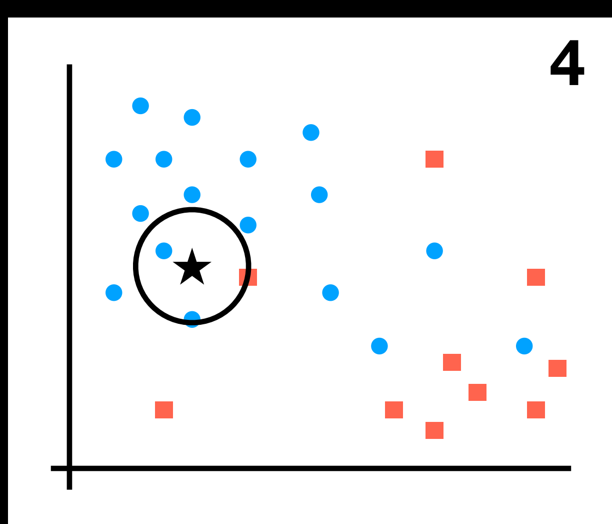

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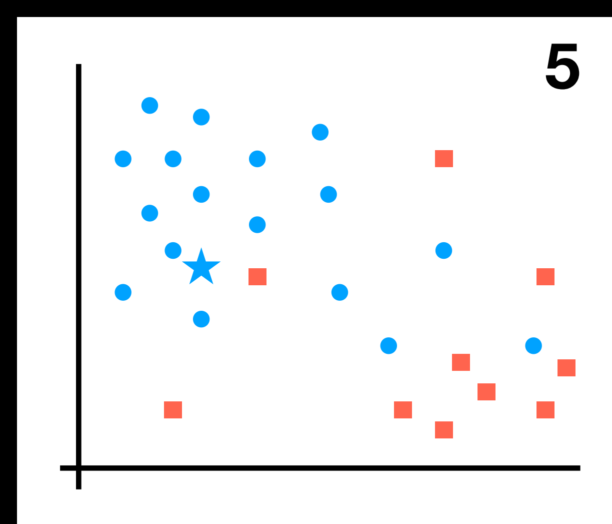
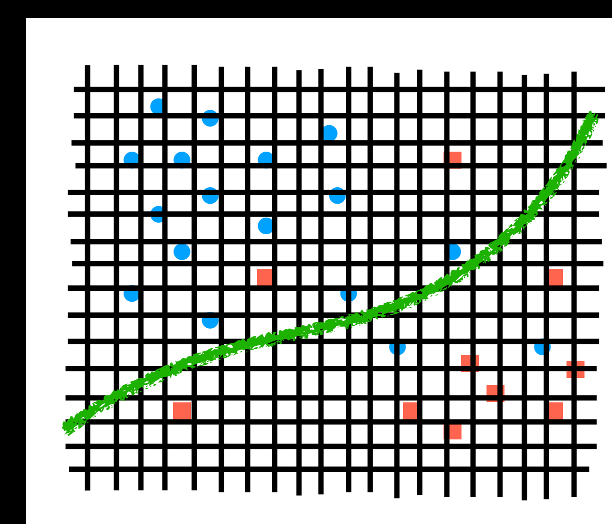
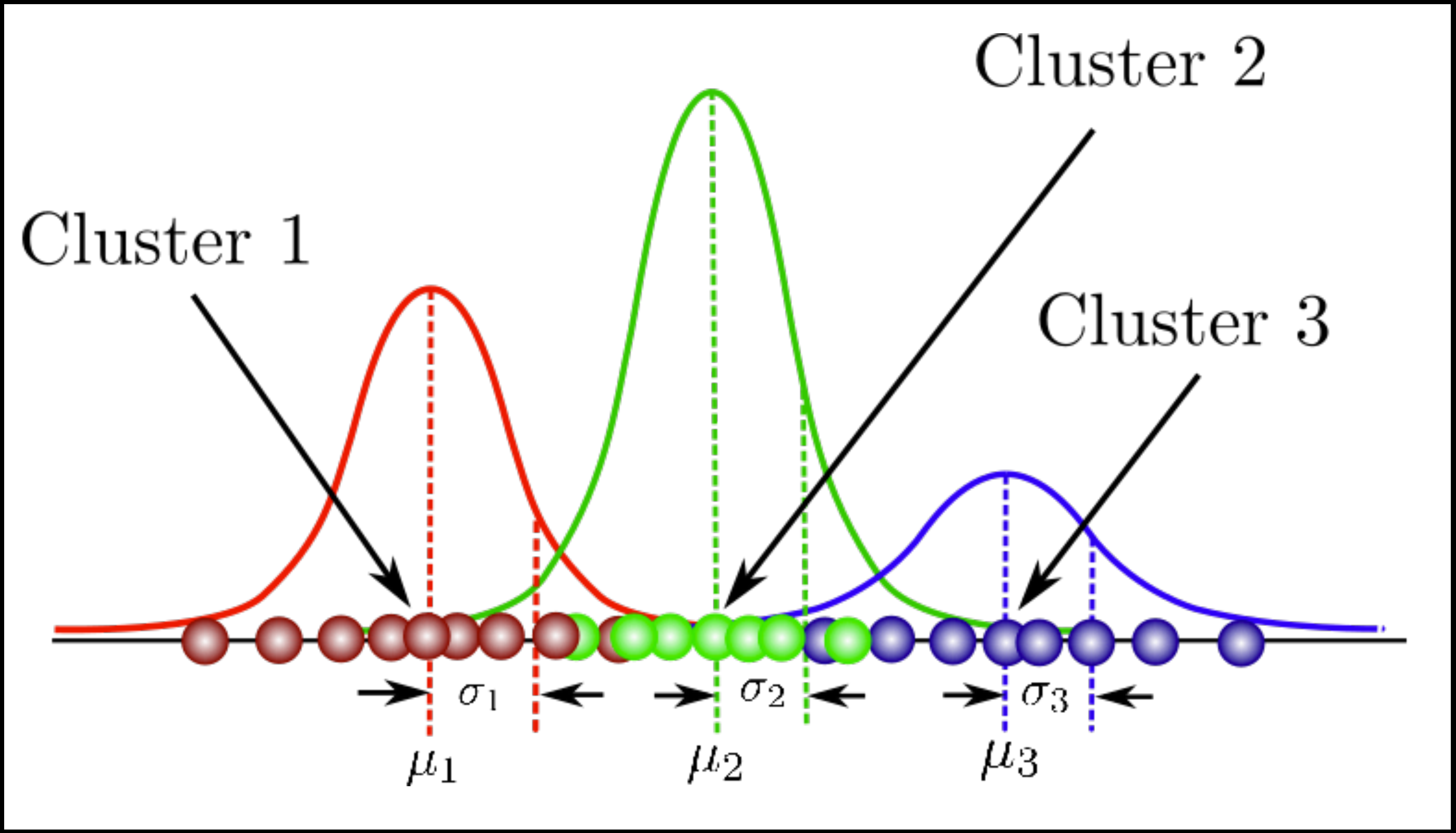


if P > cut off say new point is in that group
here: P(blue) > 0.5



Repeat 2-3 on a grid & draw a separating line

K Nearest Neighbors - with Gaussian Mixture Models.



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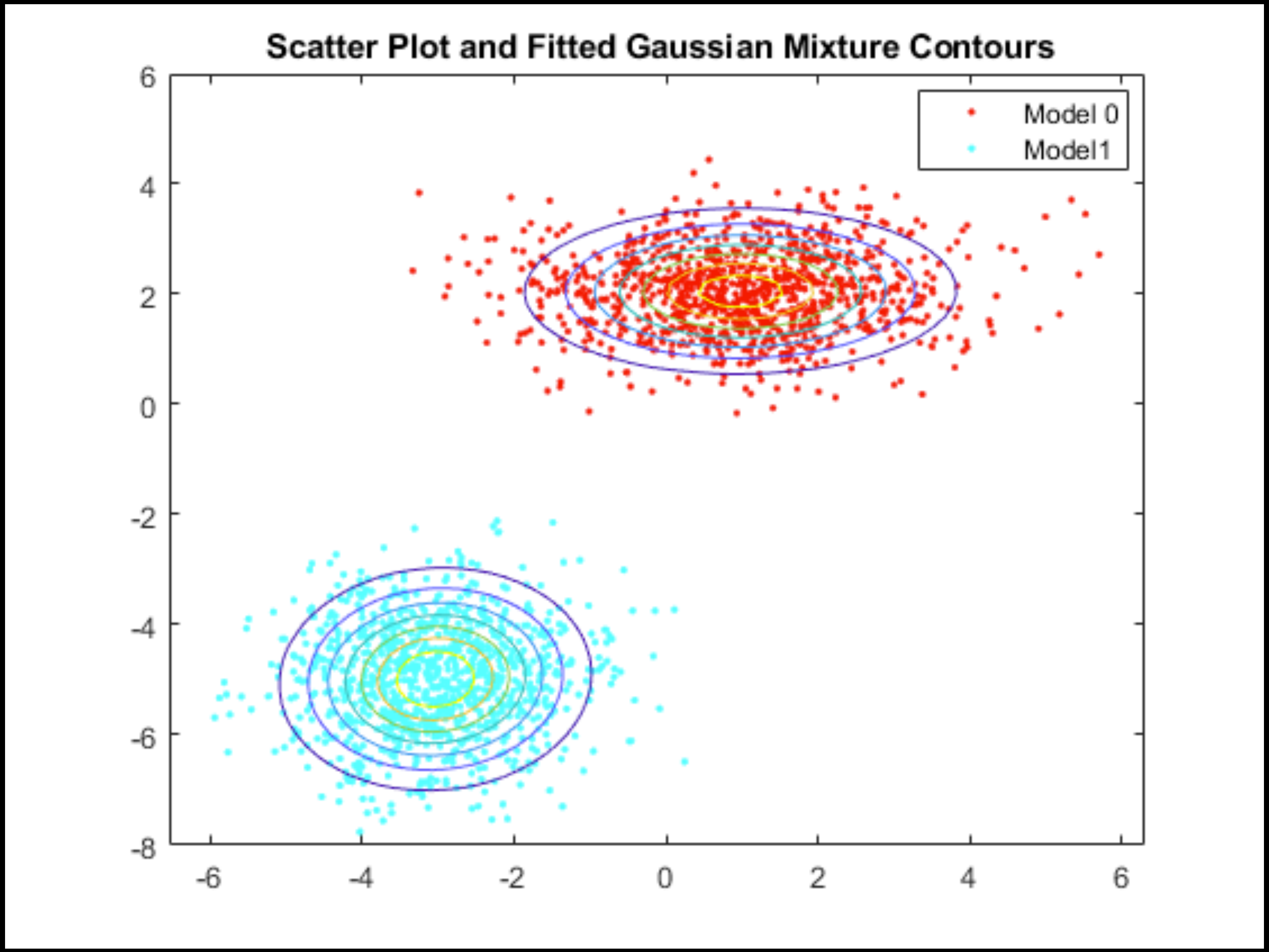

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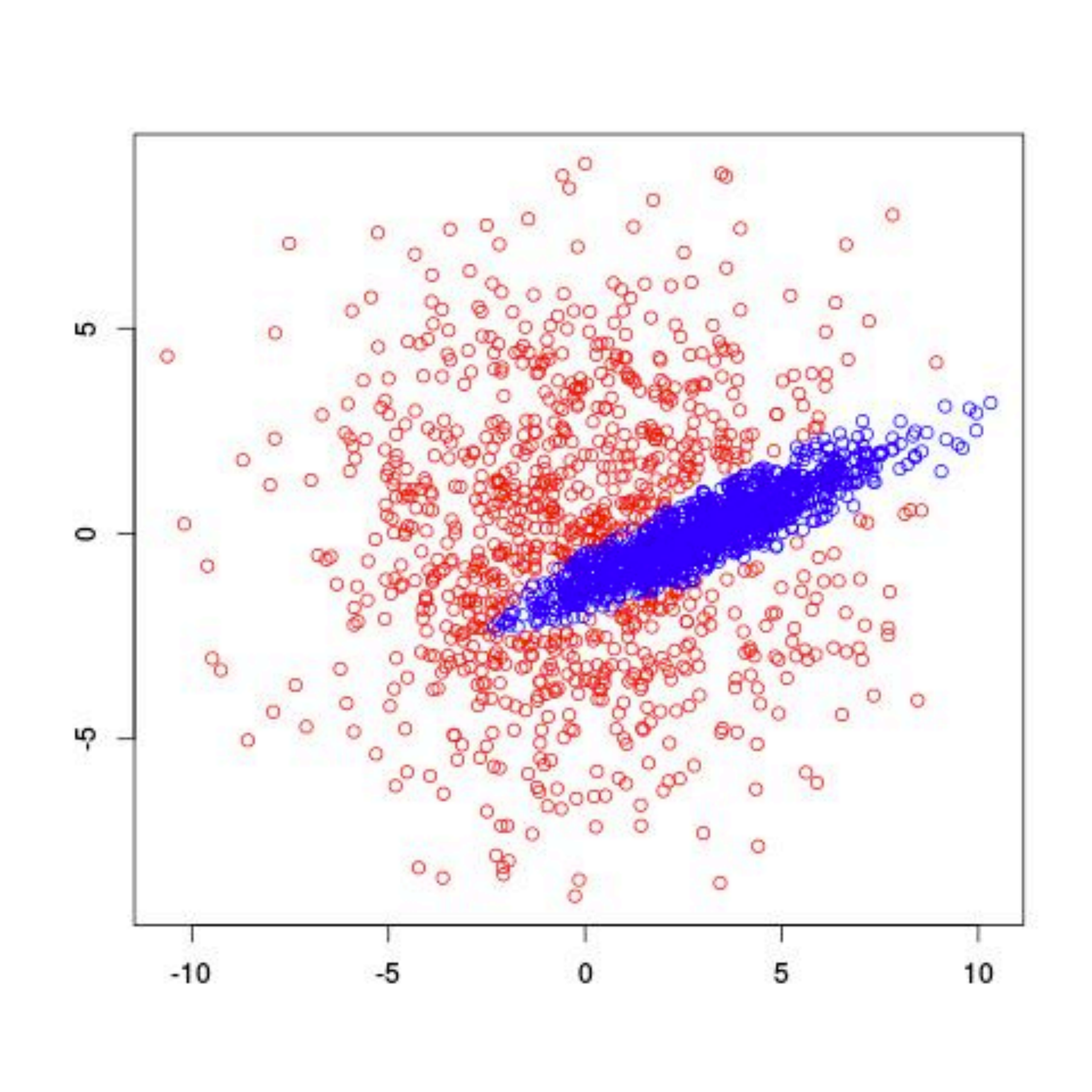
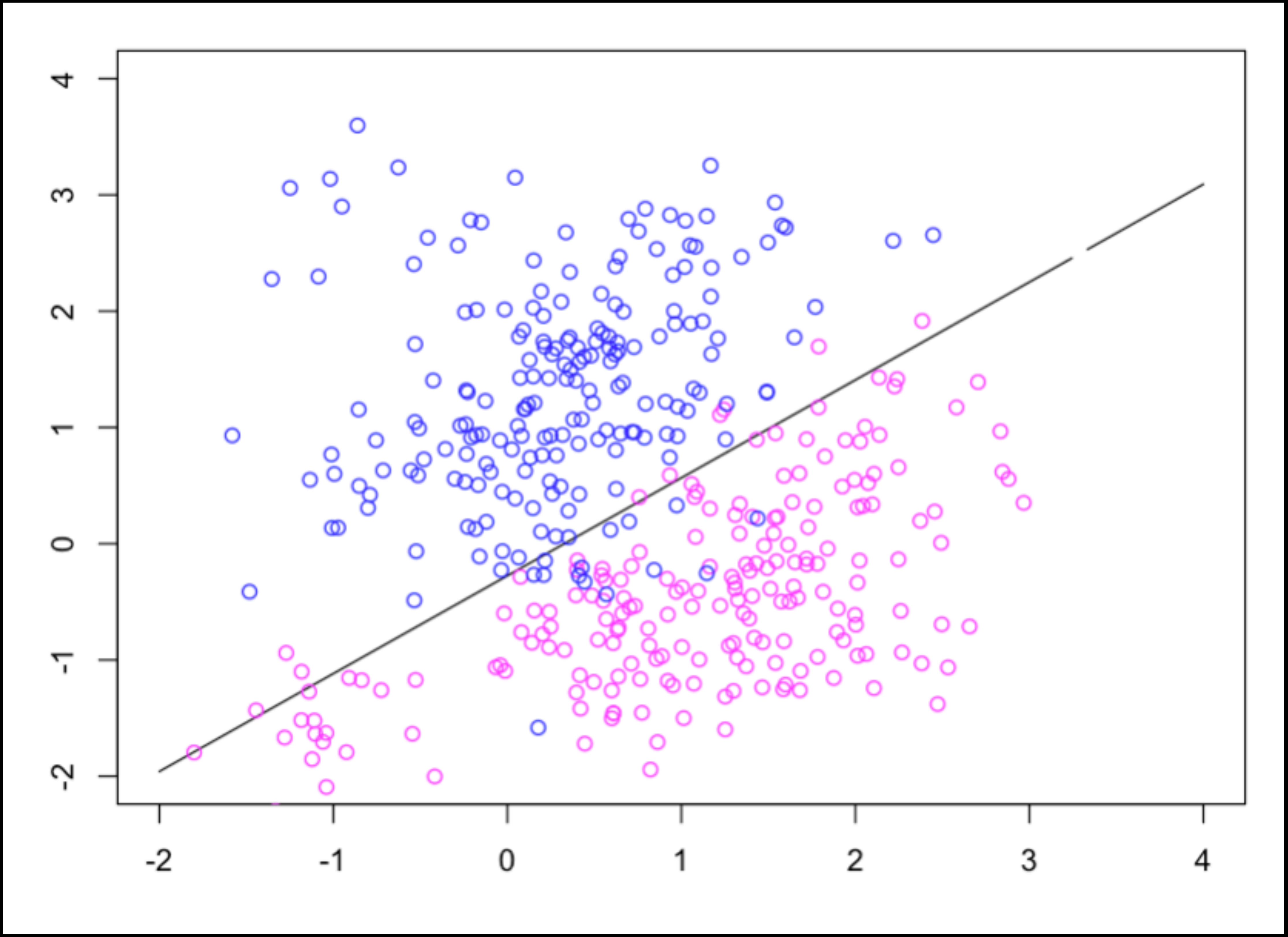
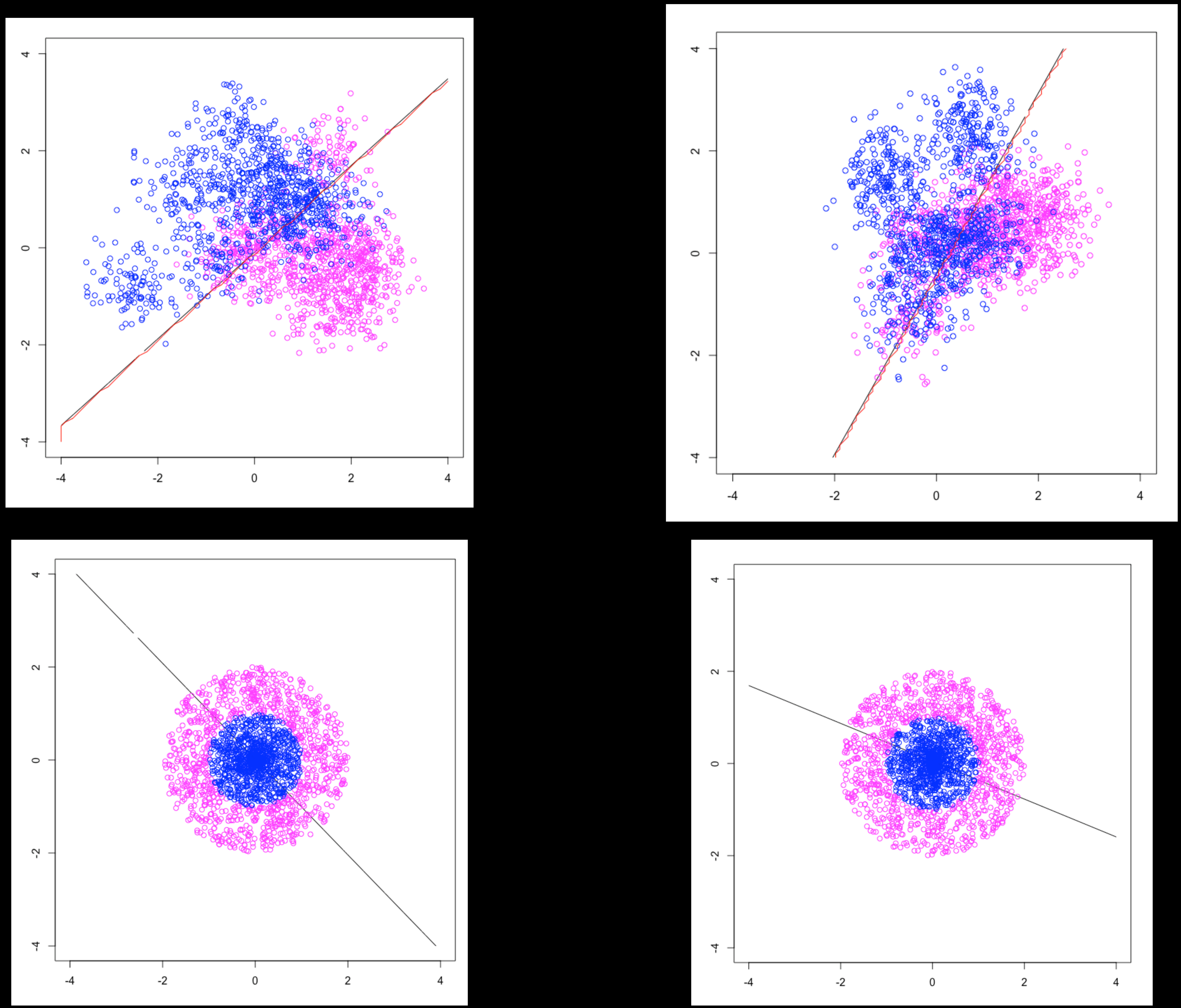


K Nearest Neighbors, in R!

K Nearest Neighbors, in R!
- just kidding logistic regression



GLM is clearly getting something wrong



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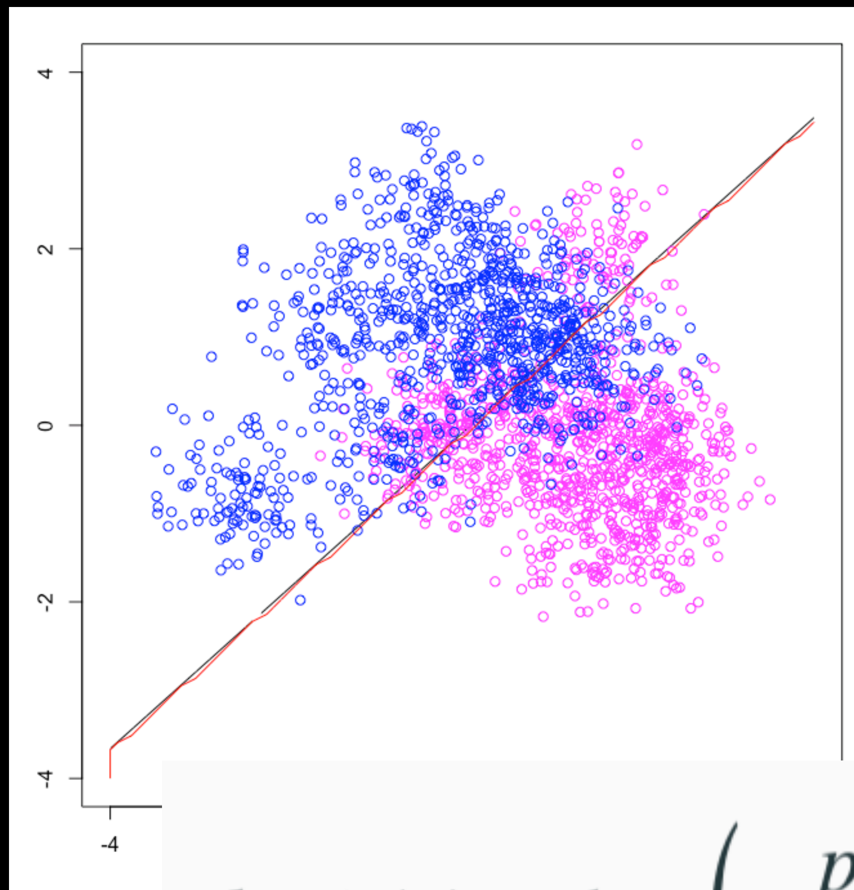
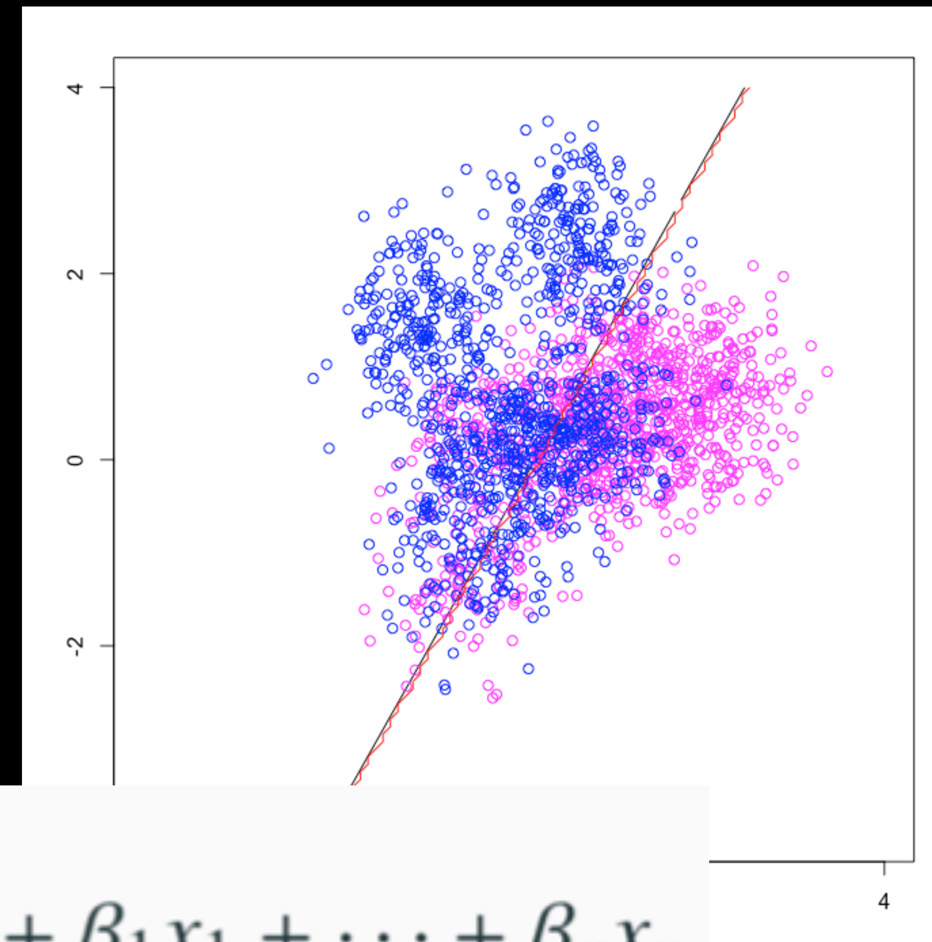
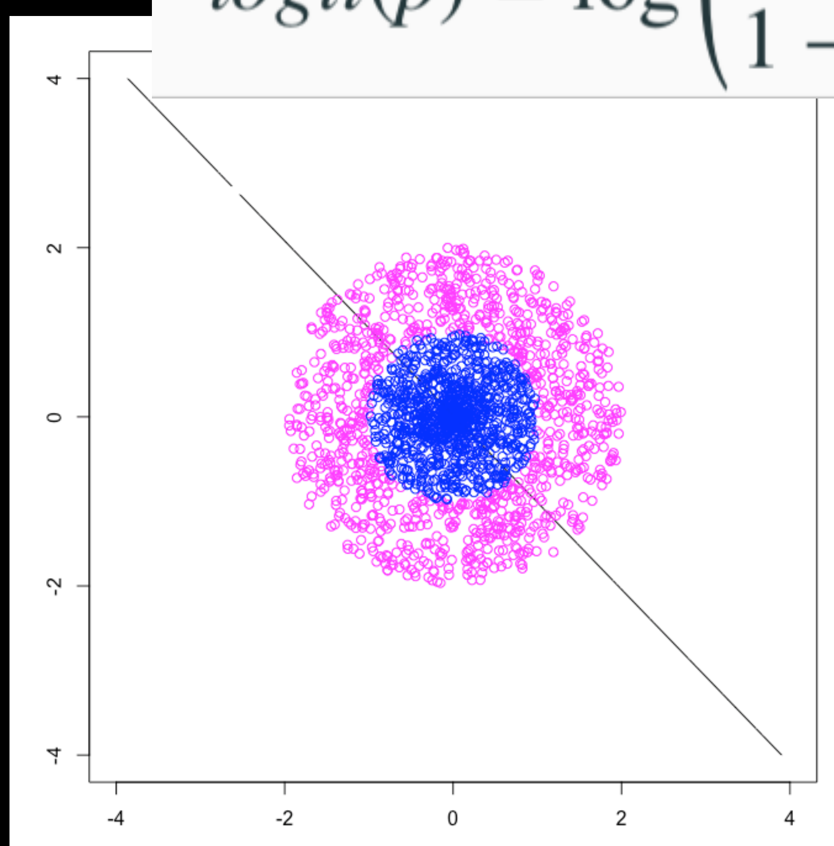
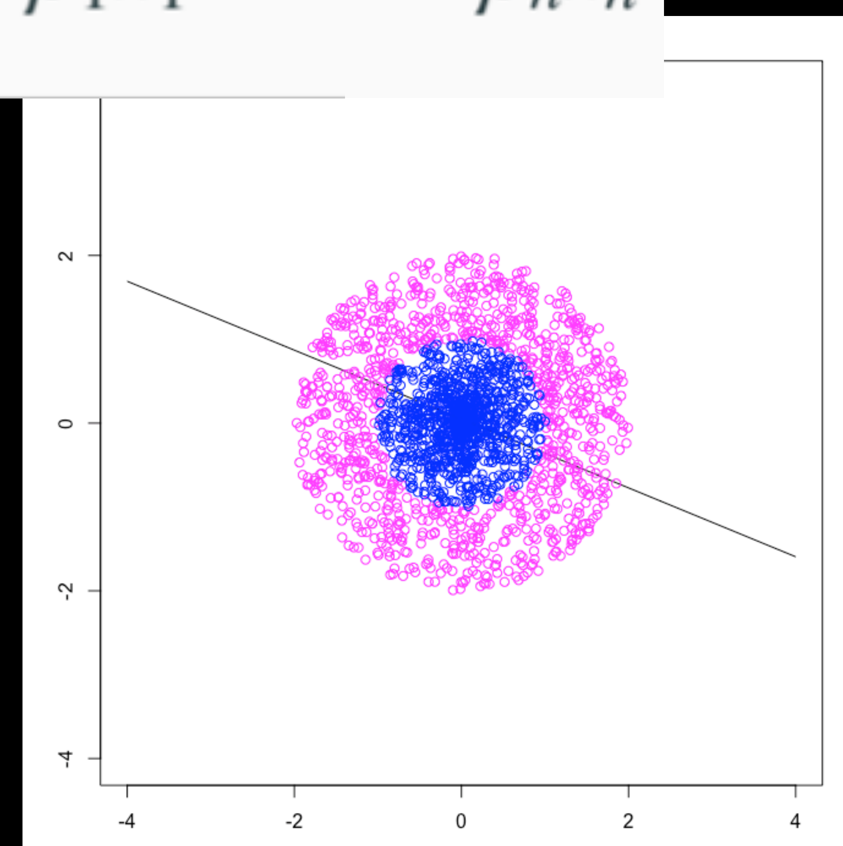


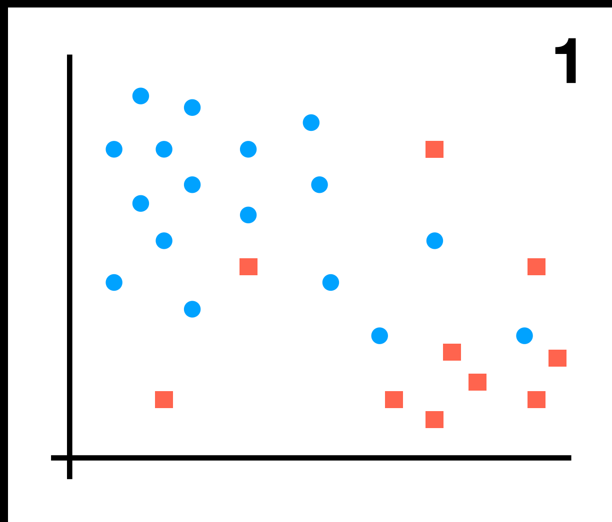


$$logit(p) = \log\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 x_1 + \cdots + \beta_n x_n$$

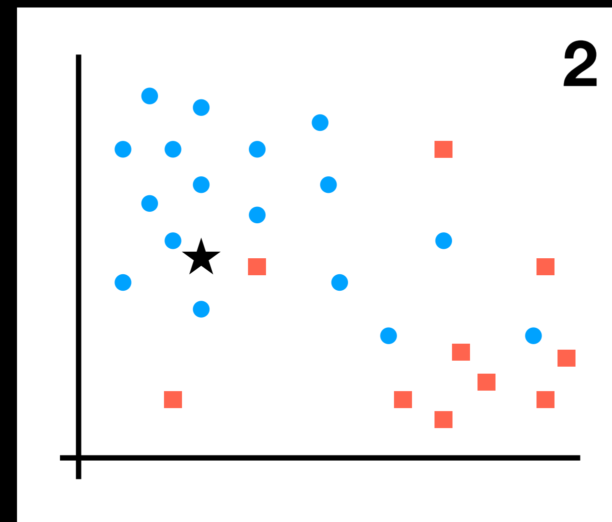




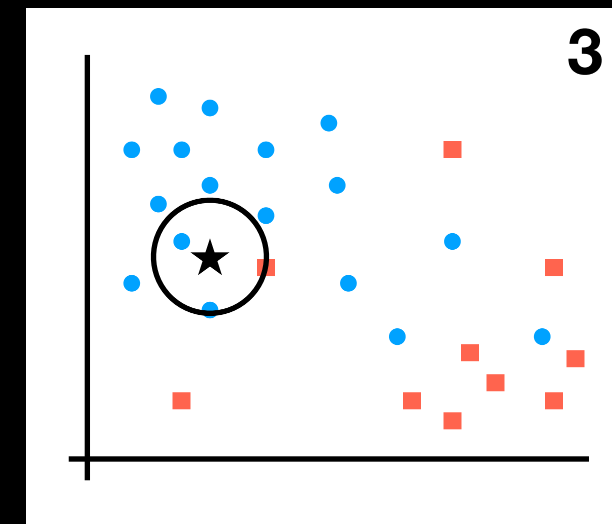
K Nearest Neighbors, in pictures



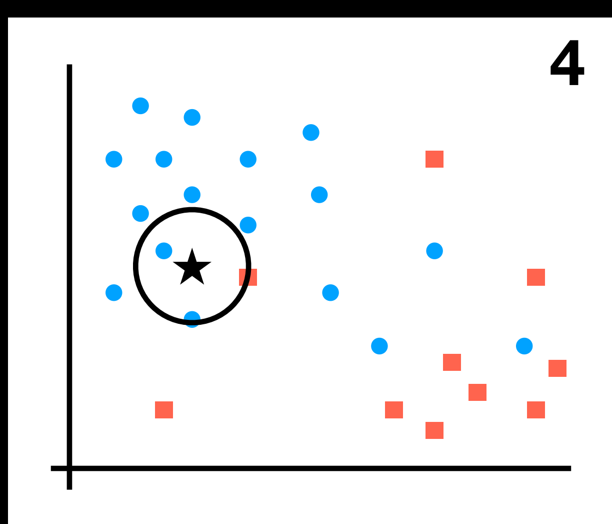
Sample (training) data representing underlying population



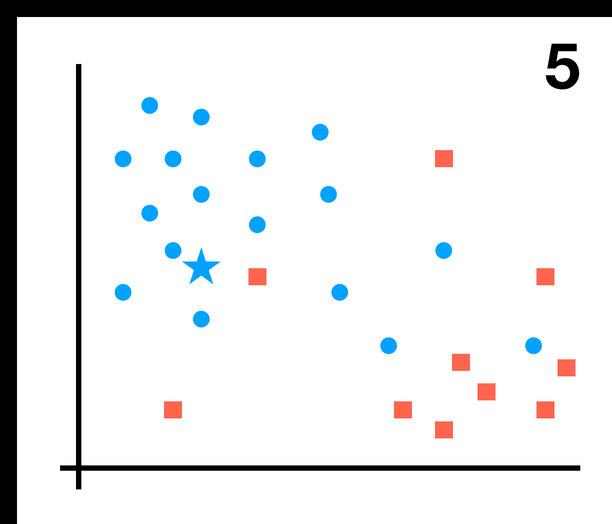
New point of interest



Find k nearest neighbors (here k = 3)



count “types” - here 2/3 points are blue
P(blue) = 2/3
P(red) = 1/3



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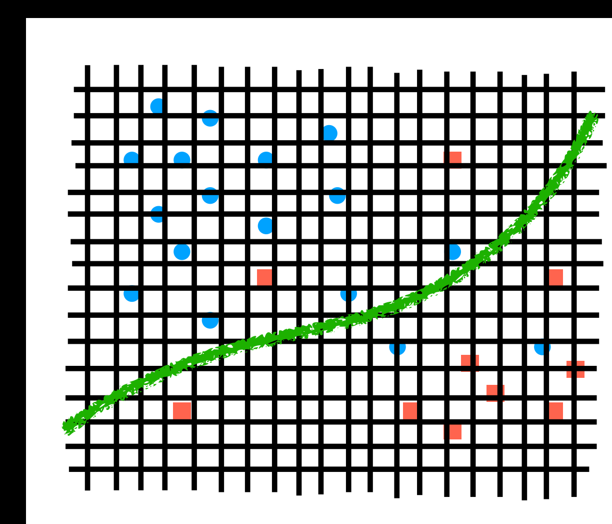


Repeat 2-3 on a grid & draw a separating line

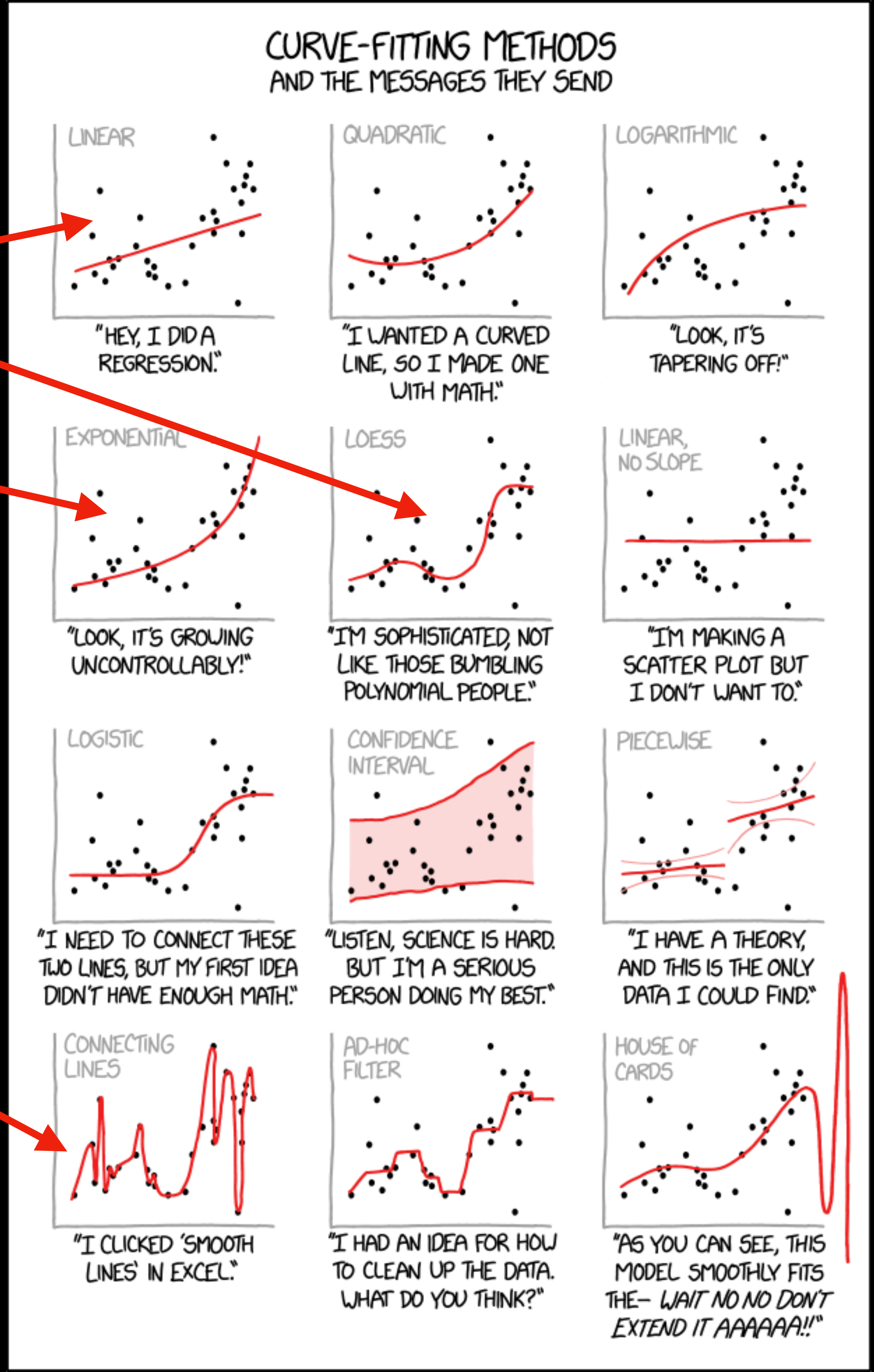
K Nearest Neighbors, in R!
For real this time!

Over/Under fitting - Quantifying how good your model is

Overfit?

Overfit?

Overfit

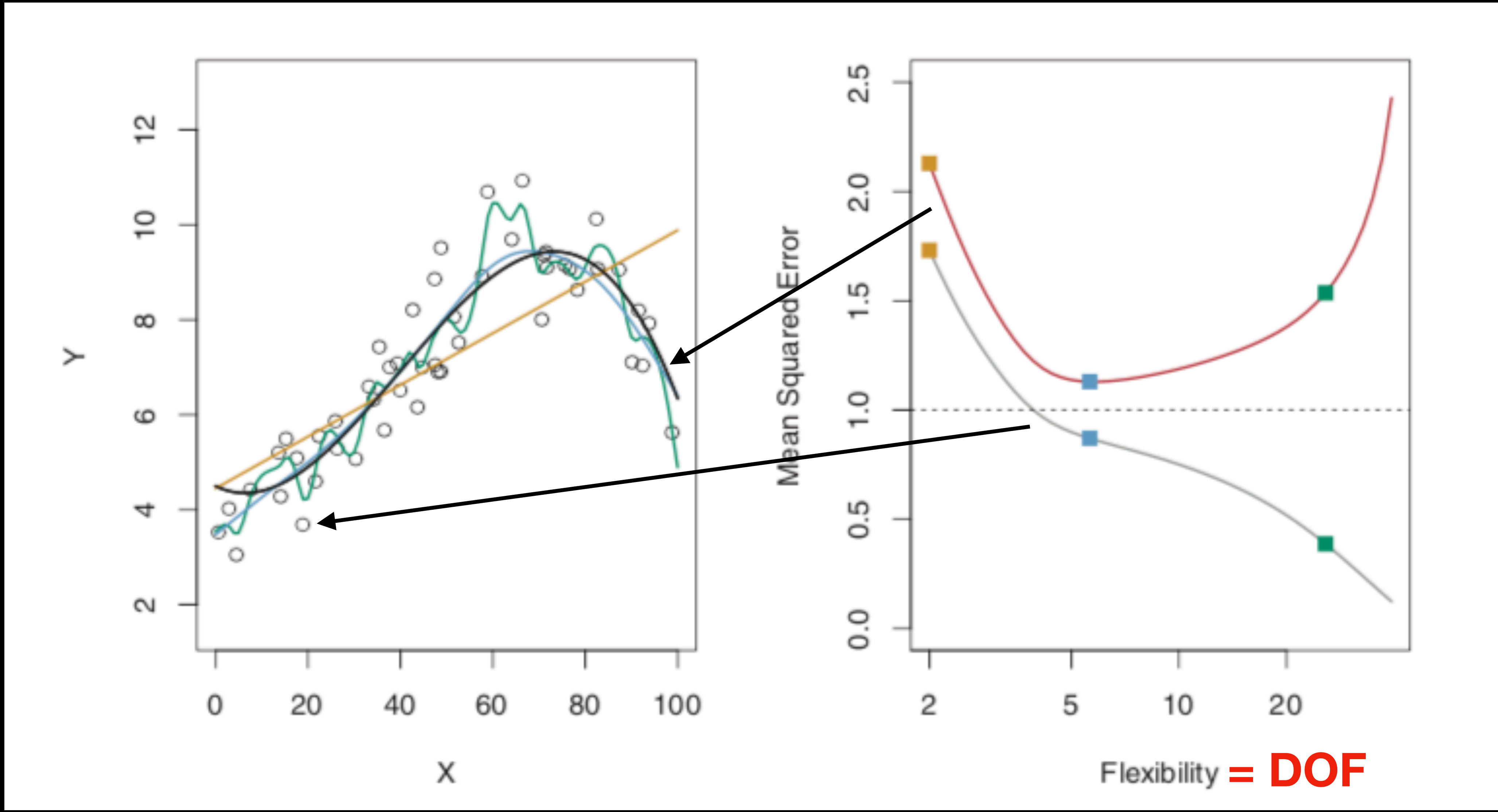


Underfit?

Is overfitting or underfitting worse?

Bias-Variance Trade-Off (Second Glance)

$$E\left(y_0 - \hat{f}(x_0)\right)^2 = \mathrm{Var}(\hat{f}(x_0)) + [\mathrm{Bias}(\hat{f}(x_0))]^2 + \mathrm{Var}(\epsilon).$$



Actual underlying function - y
o Simulated data with added error (ϵ)
Linear fit
Low “flexibility” smooth spline
High “flexibility” smooth spline

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mean square error if we kept estimating response variable y by our fitted function of our explanatory variables, f(x) with different sample datasets at point x_0

Inherent error in our measurements

Inherent error (bias) in the fact that any model is only an approximation to reality

how much our function, f, changes if we use a different random sample (variance)

Bias-Variance Trade-Off (Second Glance)

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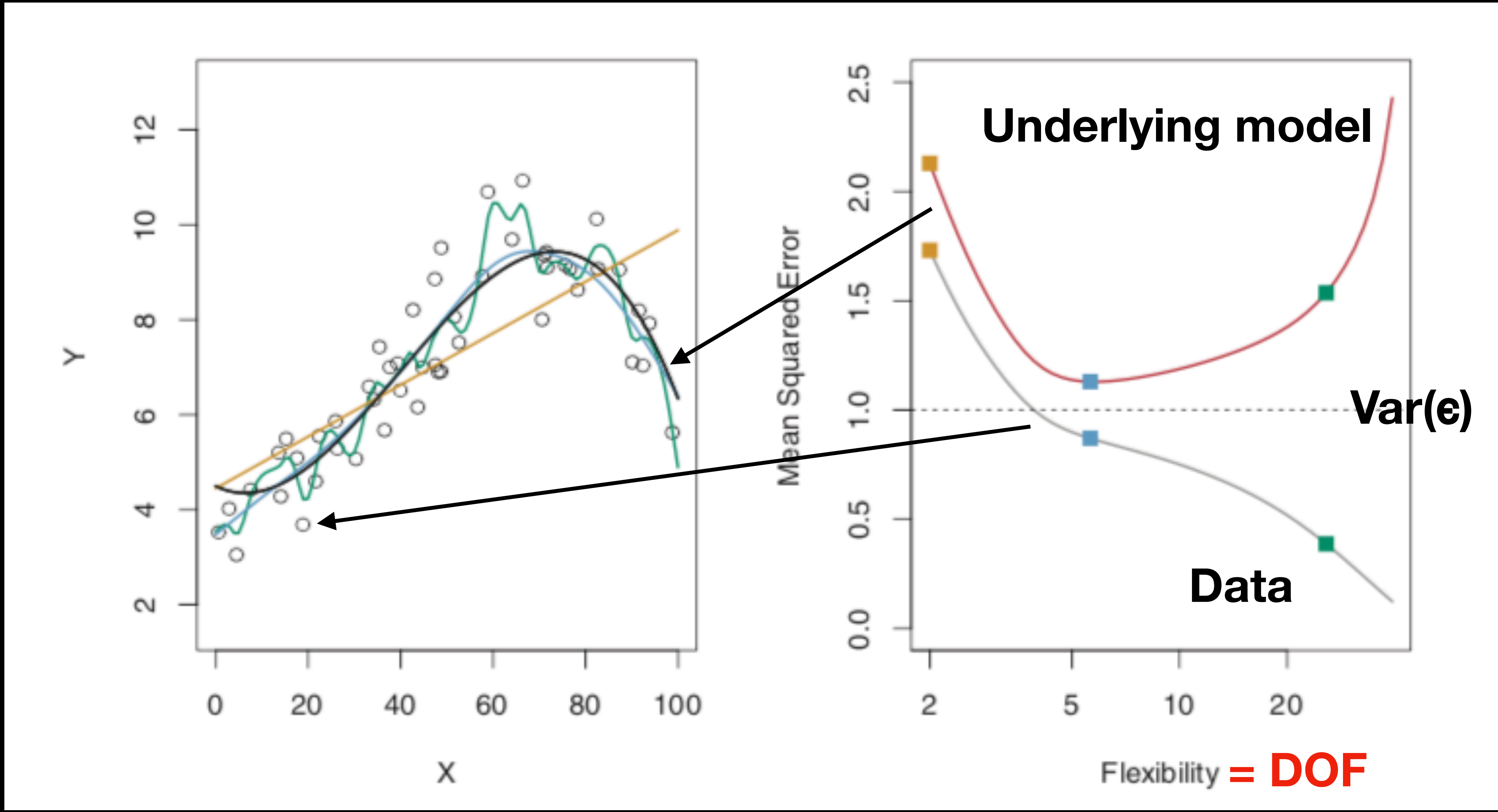

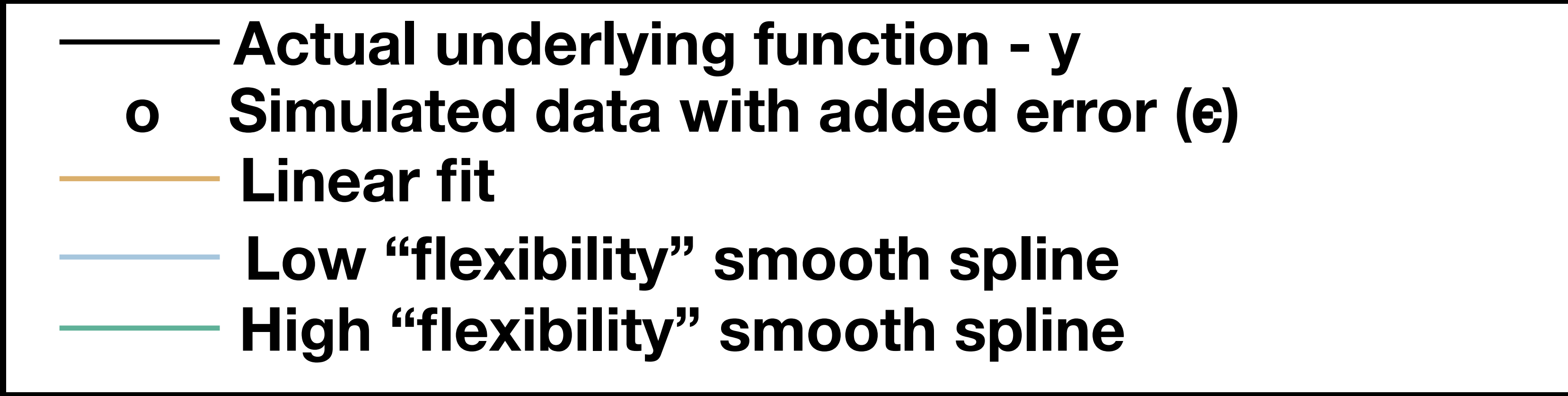

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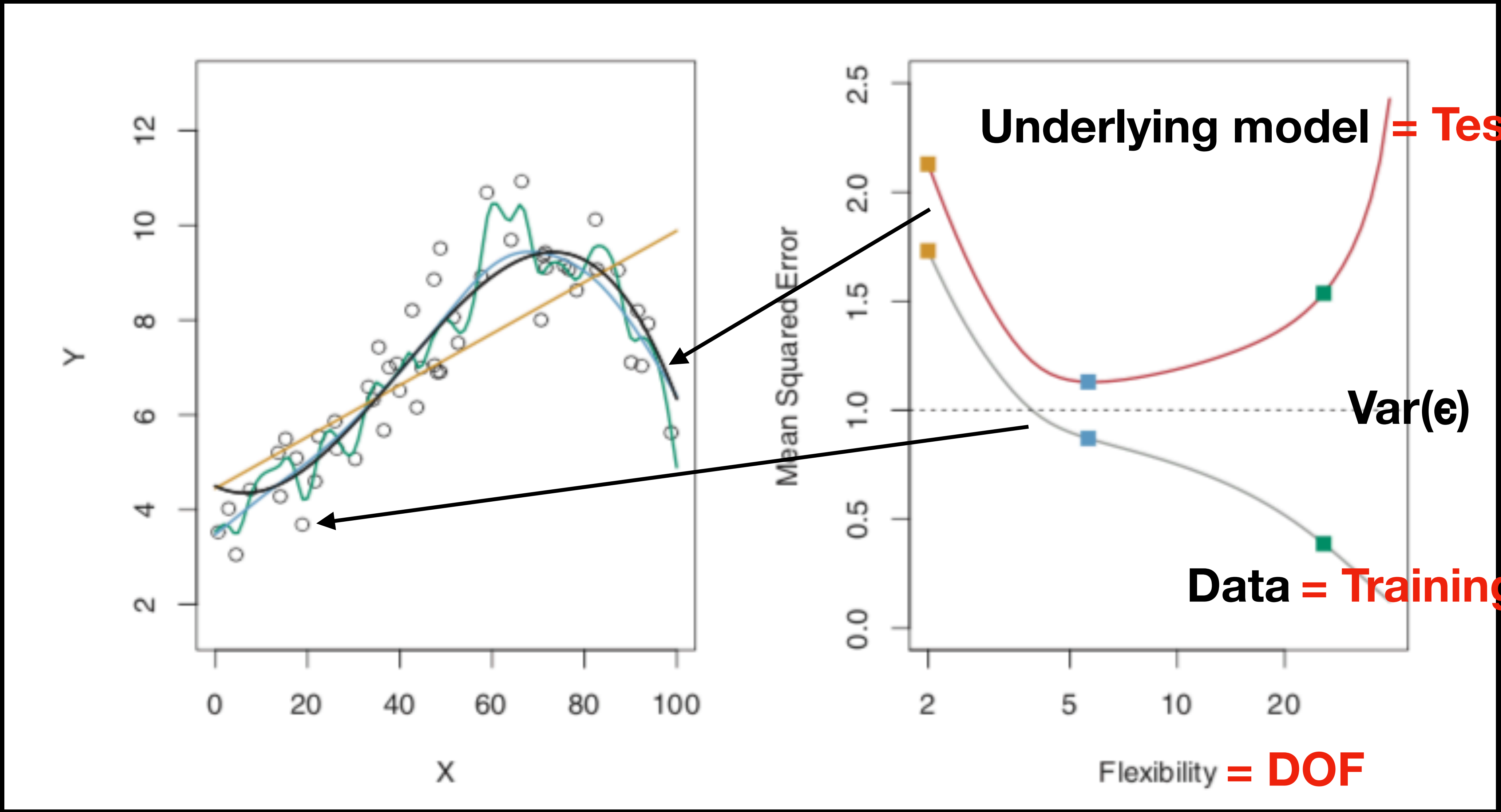

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- In contrast, the training error can be easily calculated by applying the statistical learning method to the observations used in its training.

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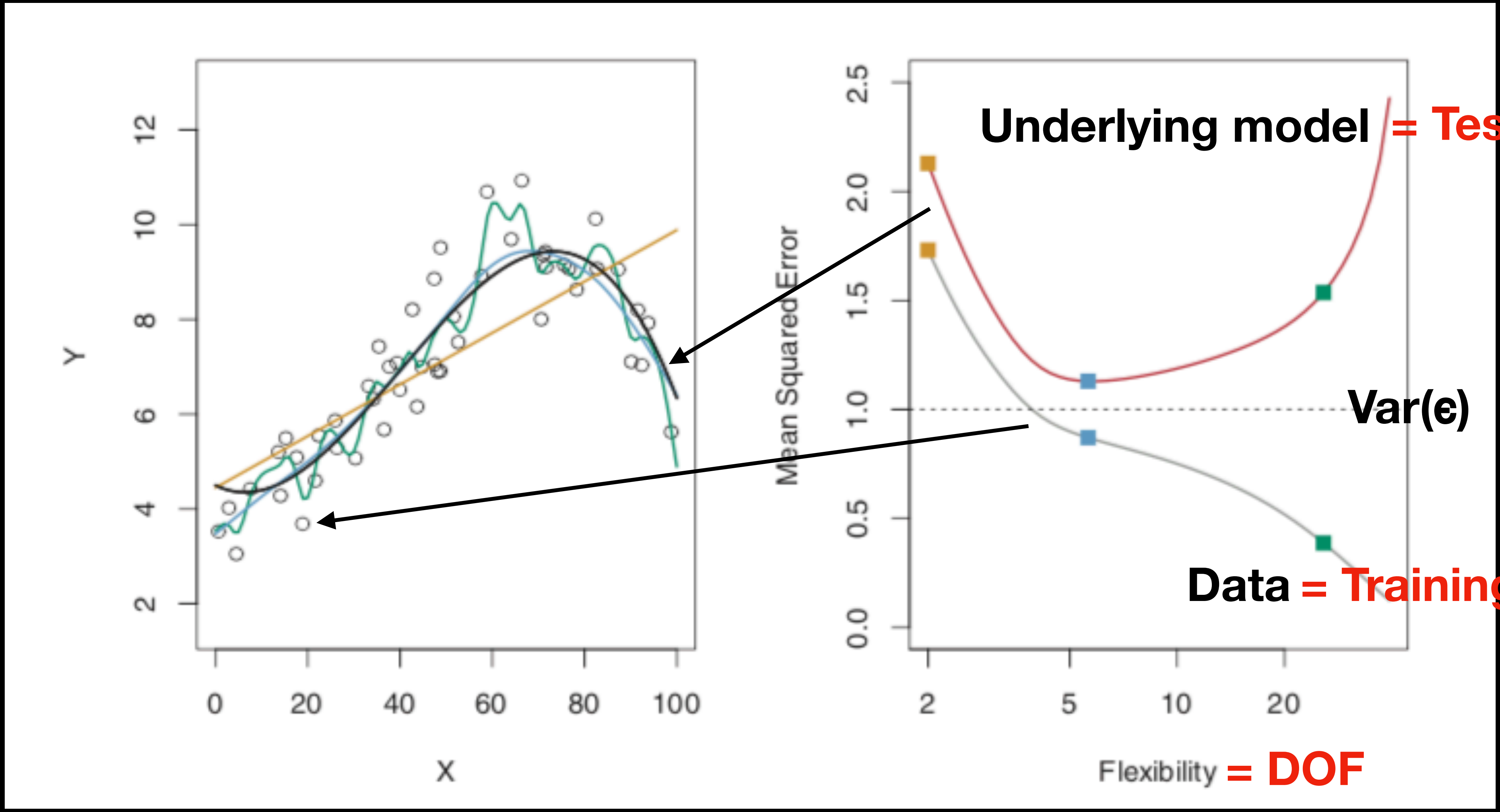

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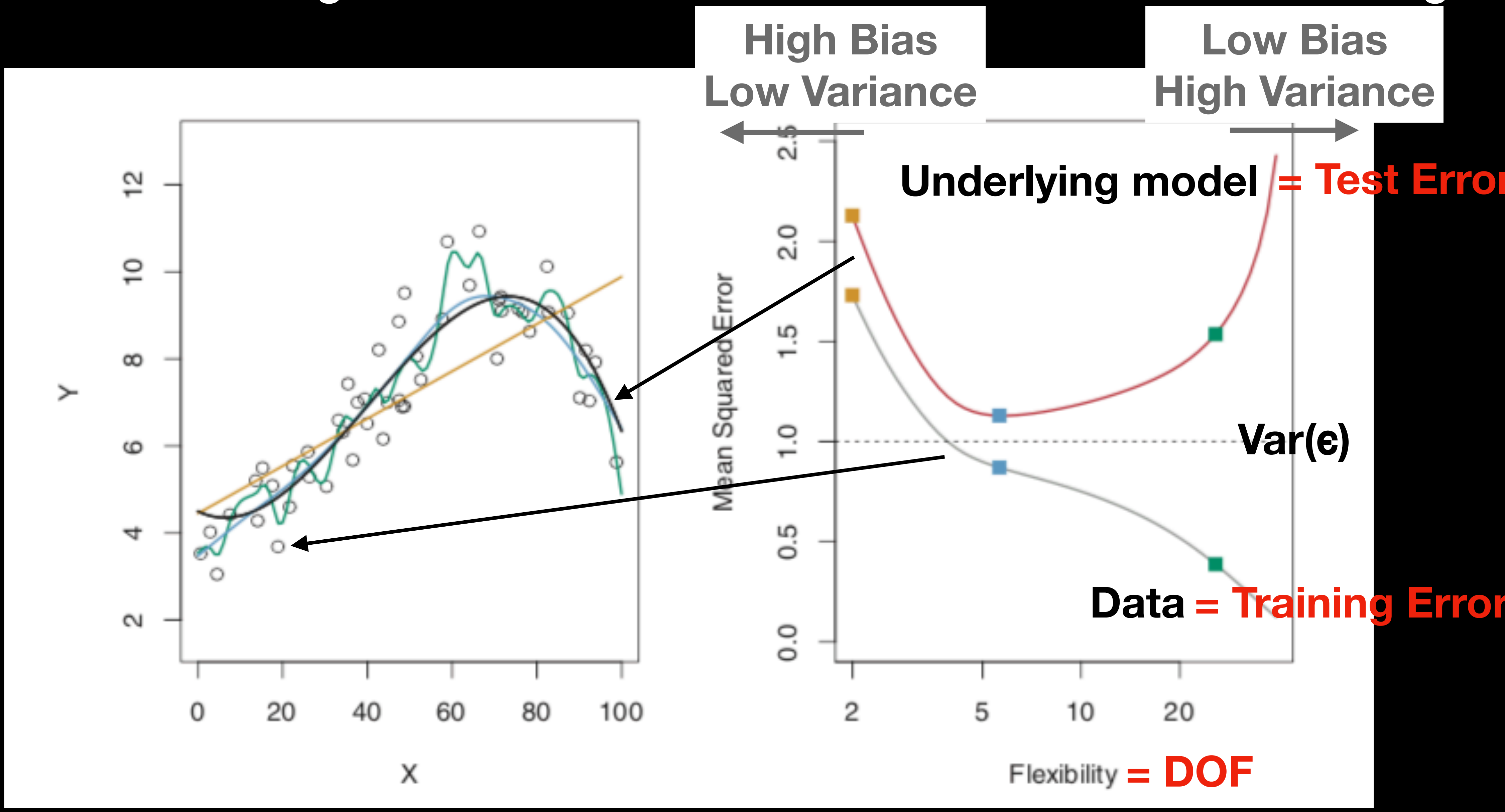

Test & Training Error in KNN: With Math!

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$$\text{Ave}\left(I(y_0 \neq \hat{y}_0)\right)$$

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new observation, requires we know what that would be from an underlying model (or more observations)

What our calculated fit/ model would predict

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$$\frac{1}{n}\sum_{i=1}^{n} I(y_i \neq \hat{y}_i)$$

an observation in our current dataset

What our fit/model would predict

Here I = 1 if y_i != $\hat{y}_i$ and I = 0 if y_i = $\hat{y}_i$, so larger I means worse model

K Nearest Neighbors (and MLR) → Cross-Validation & Bootstrap

p-values quantify the fit of individual parameters

quantify how good the *model* is

But first: some definitions!

Using our KNN example in R with an underlying model!