Building Specialized Regression Models in scikit-learn

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Overview

Regression models and measuring fit of a model

The bias-variance trade-off and overfitted models

Lasso and Ridge regression to mitigate overfitting

Support vector regression models

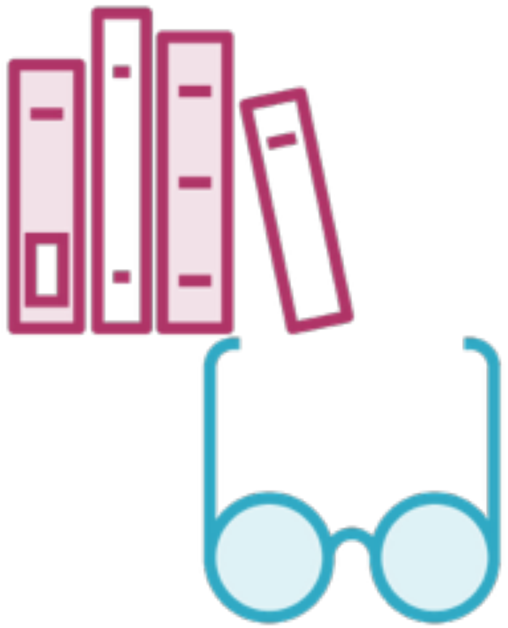
Setting Up The Regression Problem

Types of Machine Learning Problems

Classification

Regression

Clustering



Rule-extraction

Types of Machine Learning Problems

Classification

Regression

Clustering

Rule-extraction

X Causes Y

Cause

Independent variable

Effect

Dependent variable

X Causes Y

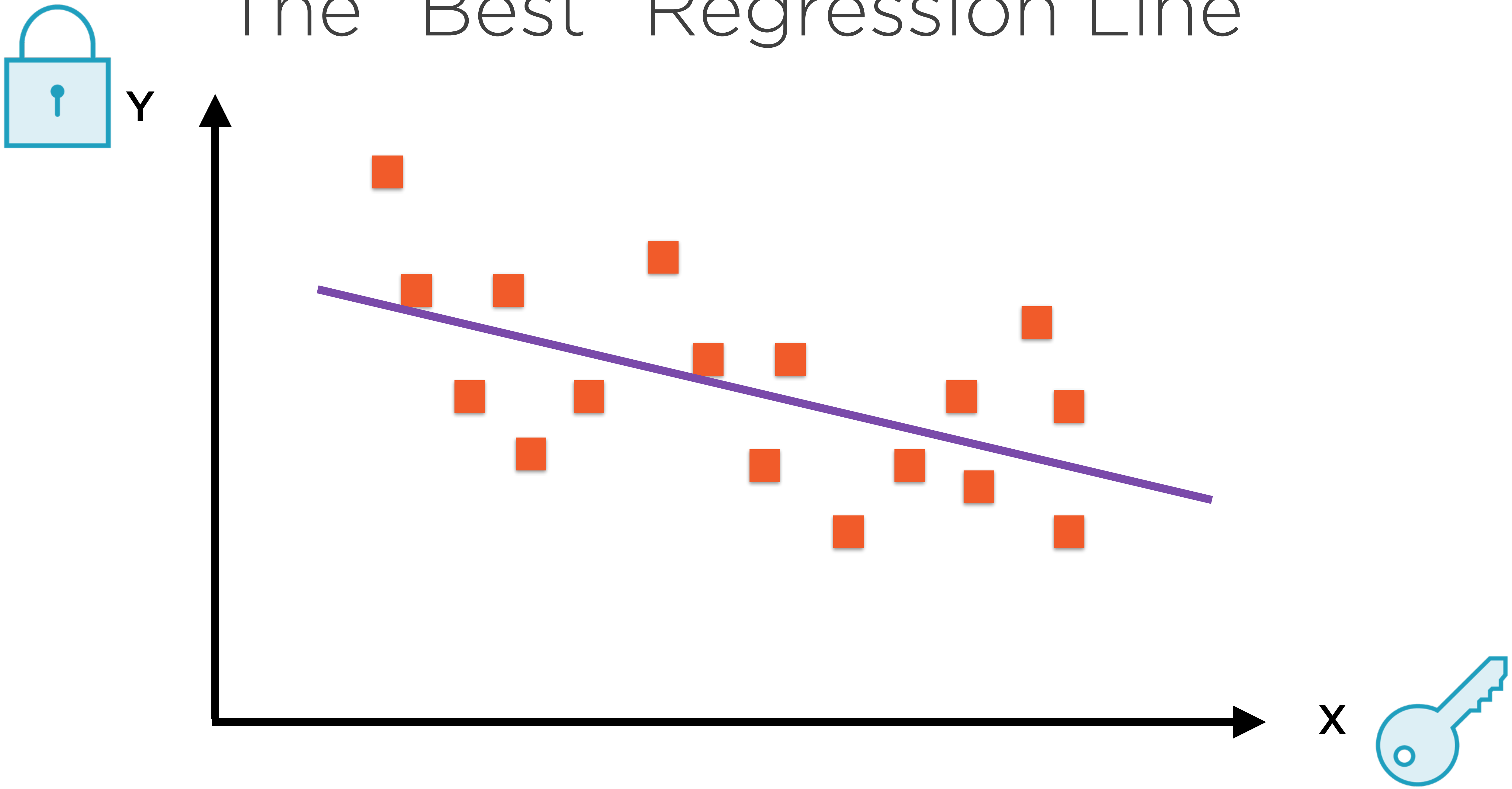
Cause

Explanatory variable

Effect

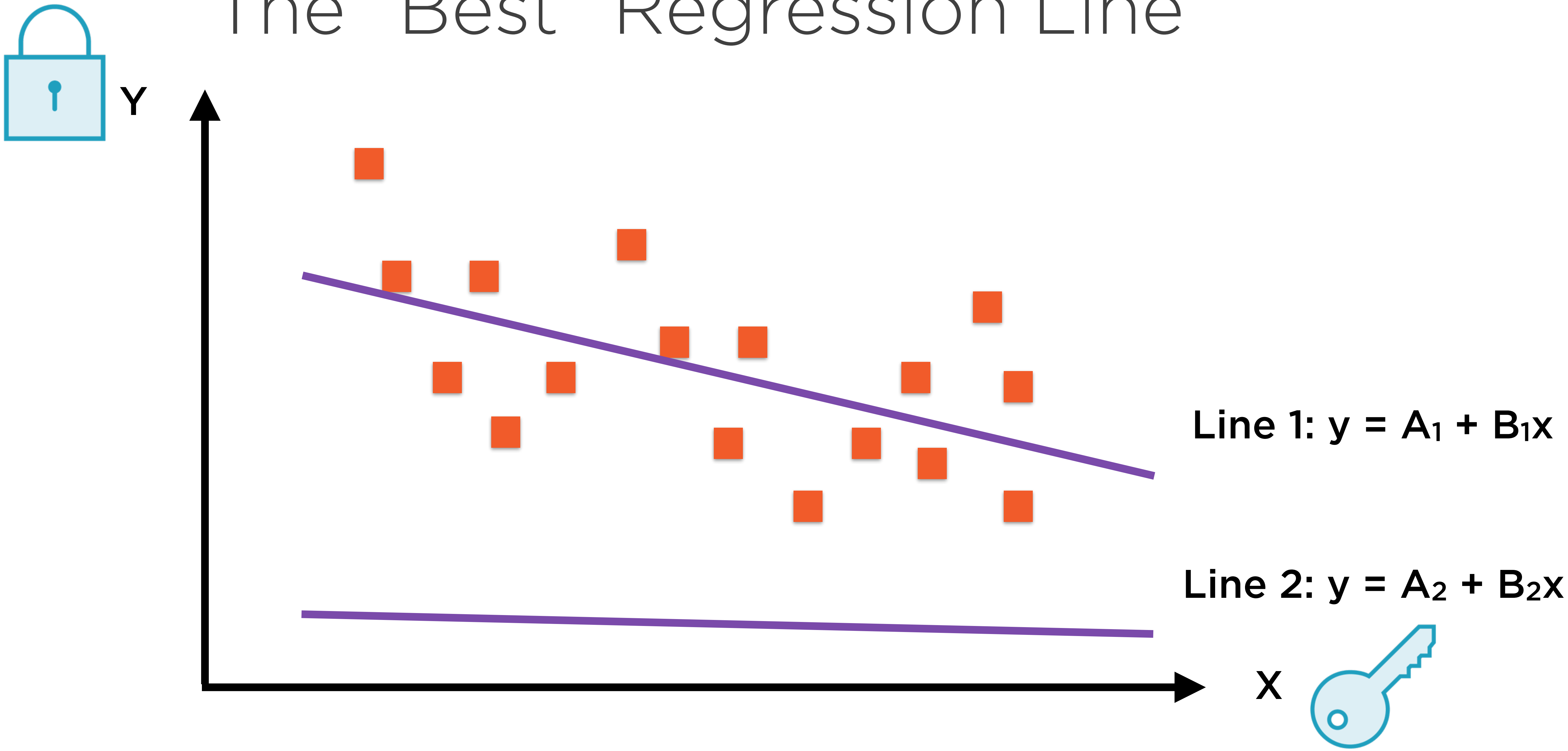
Dependent variable

The "Best" Regression Line



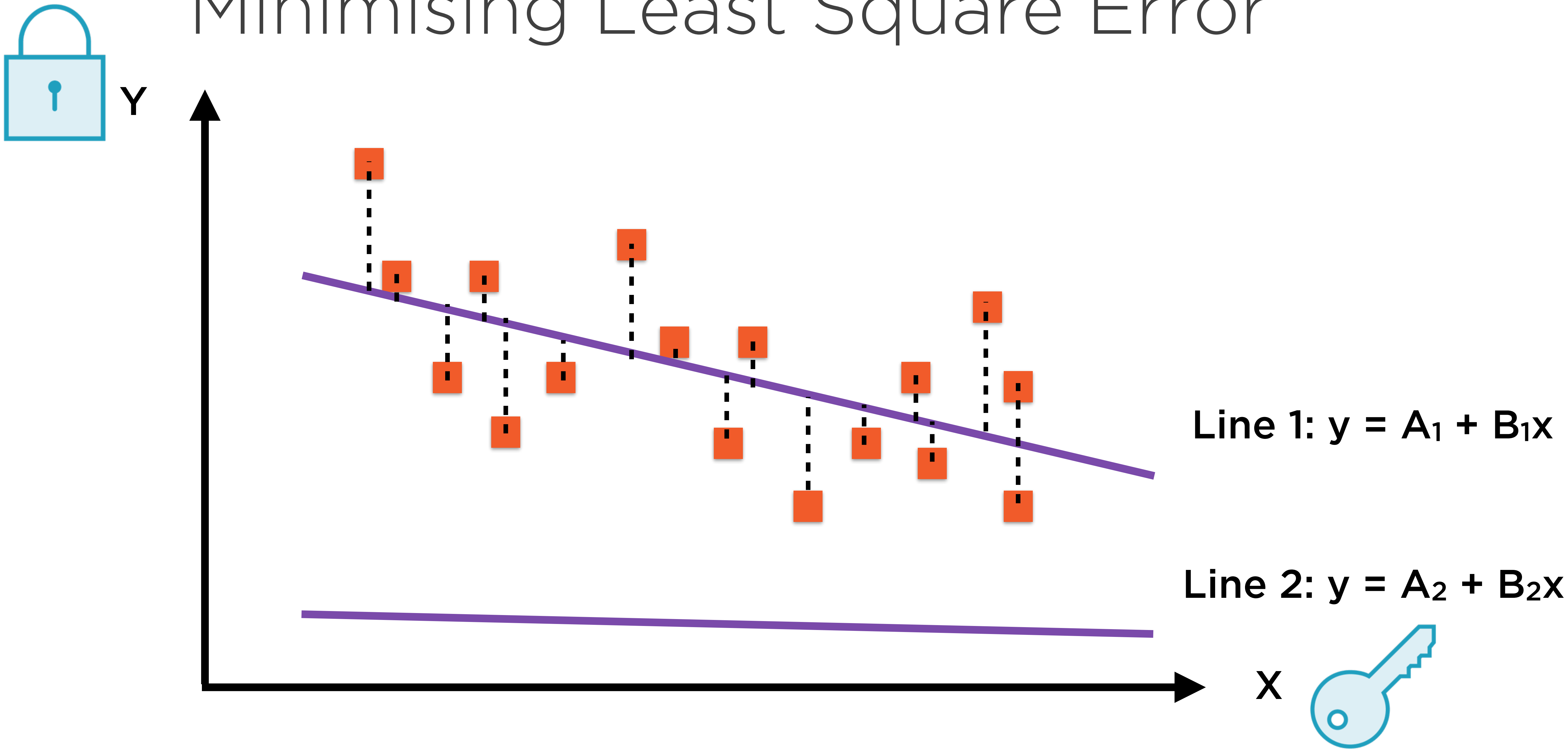
Linear Regression involves finding the "best fit" line

The “Best” Regression Line



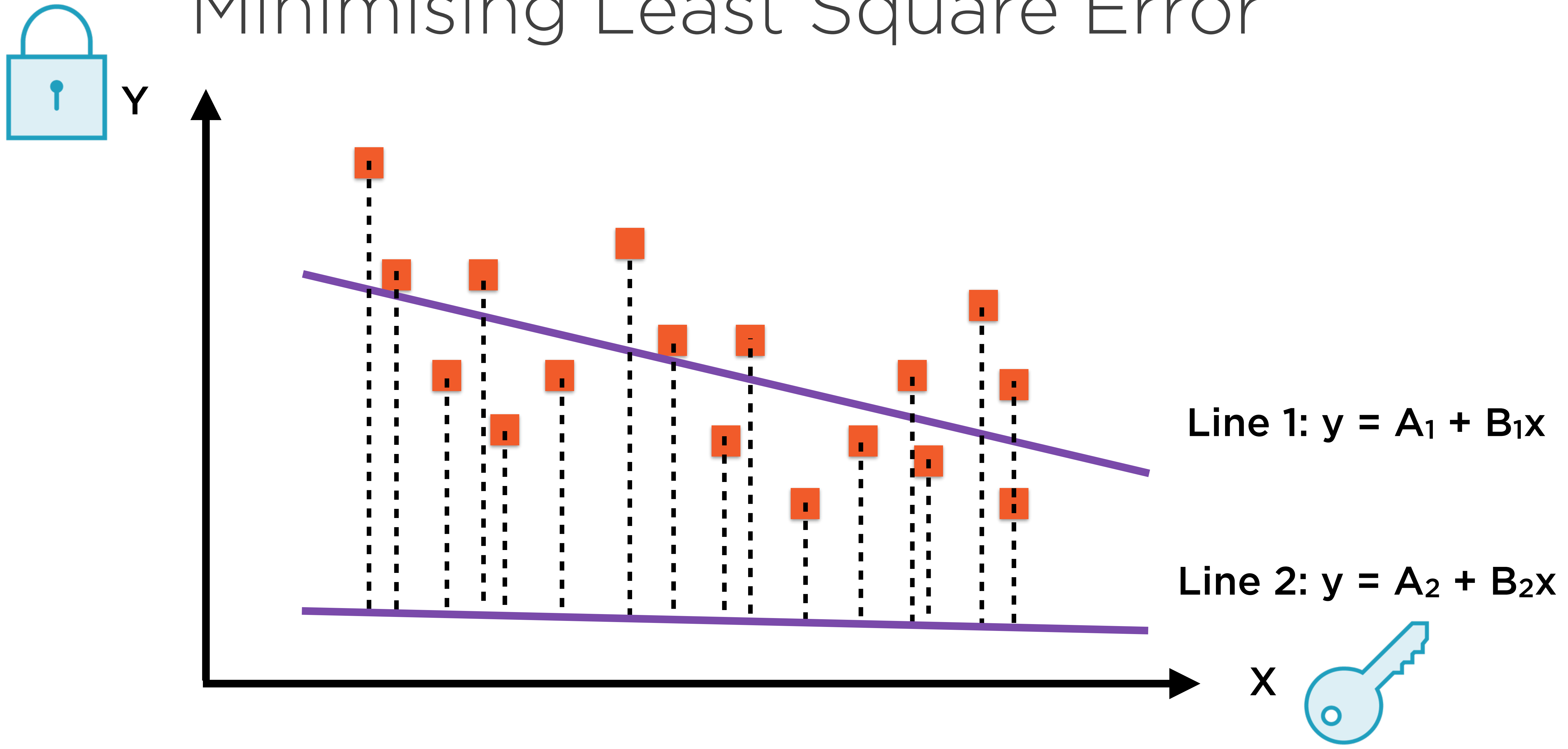
Let’s compare two lines, Line 1 and Line 2

Minimising Least Square Error



Drop vertical lines from each point to the lines 1 and 2

Minimising Least Square Error



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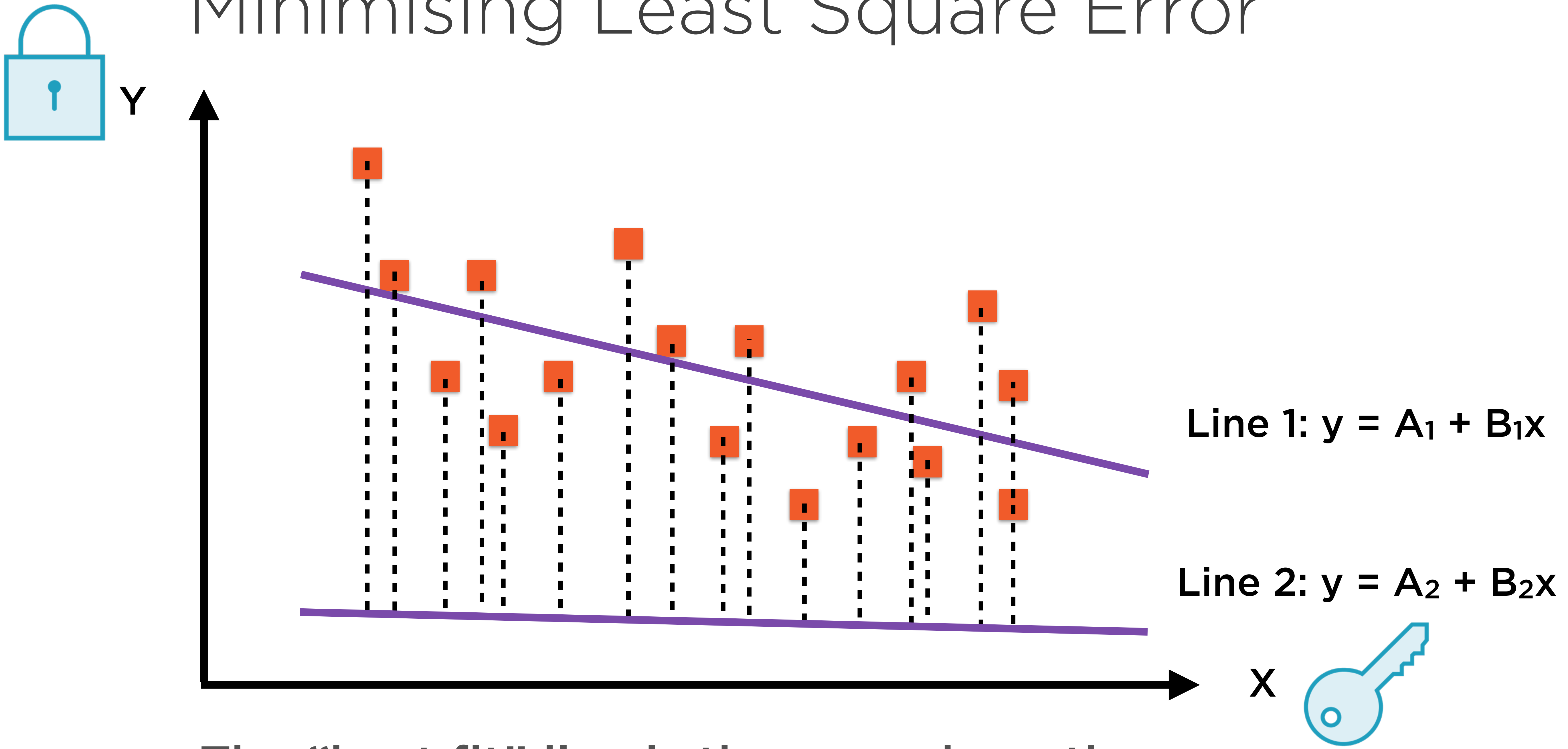
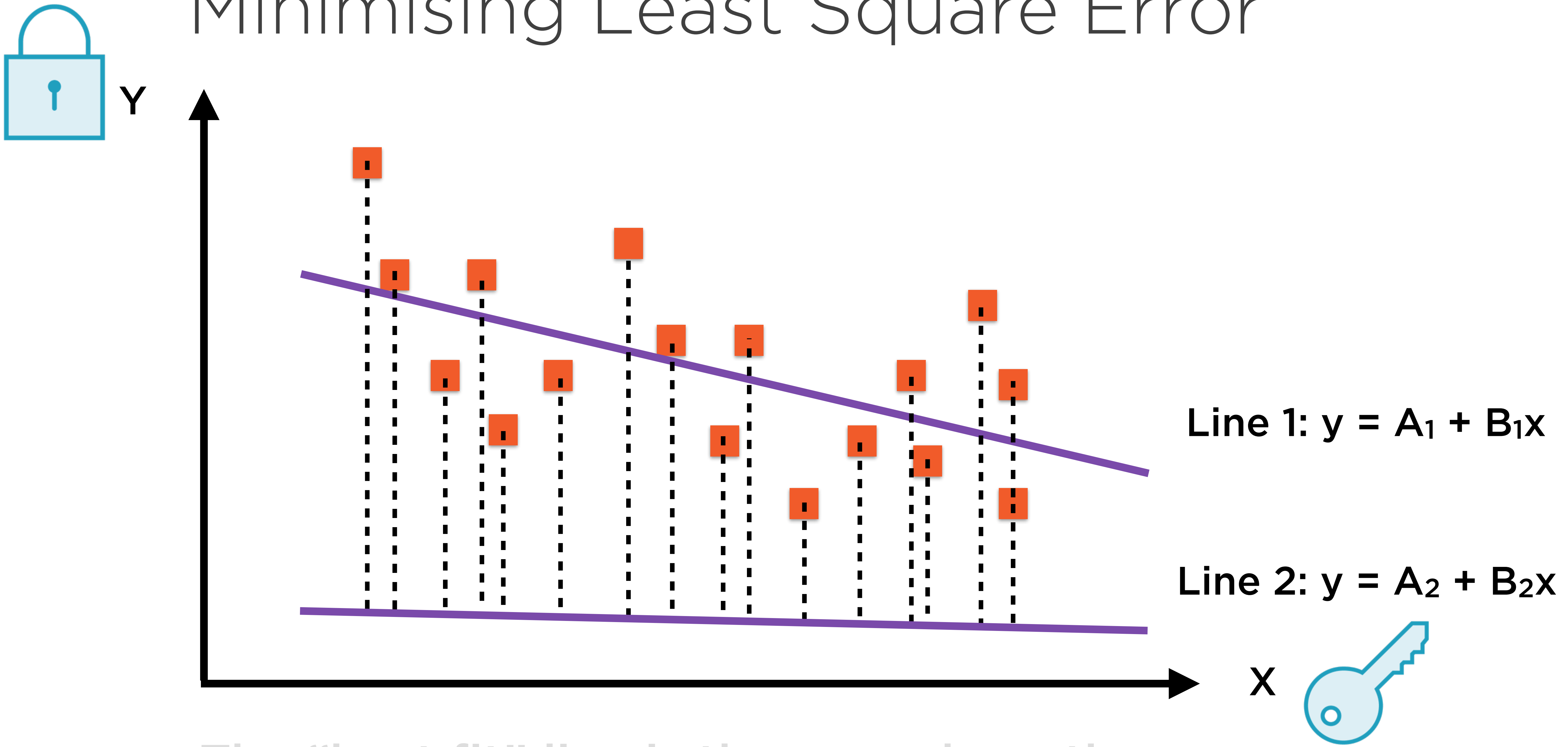


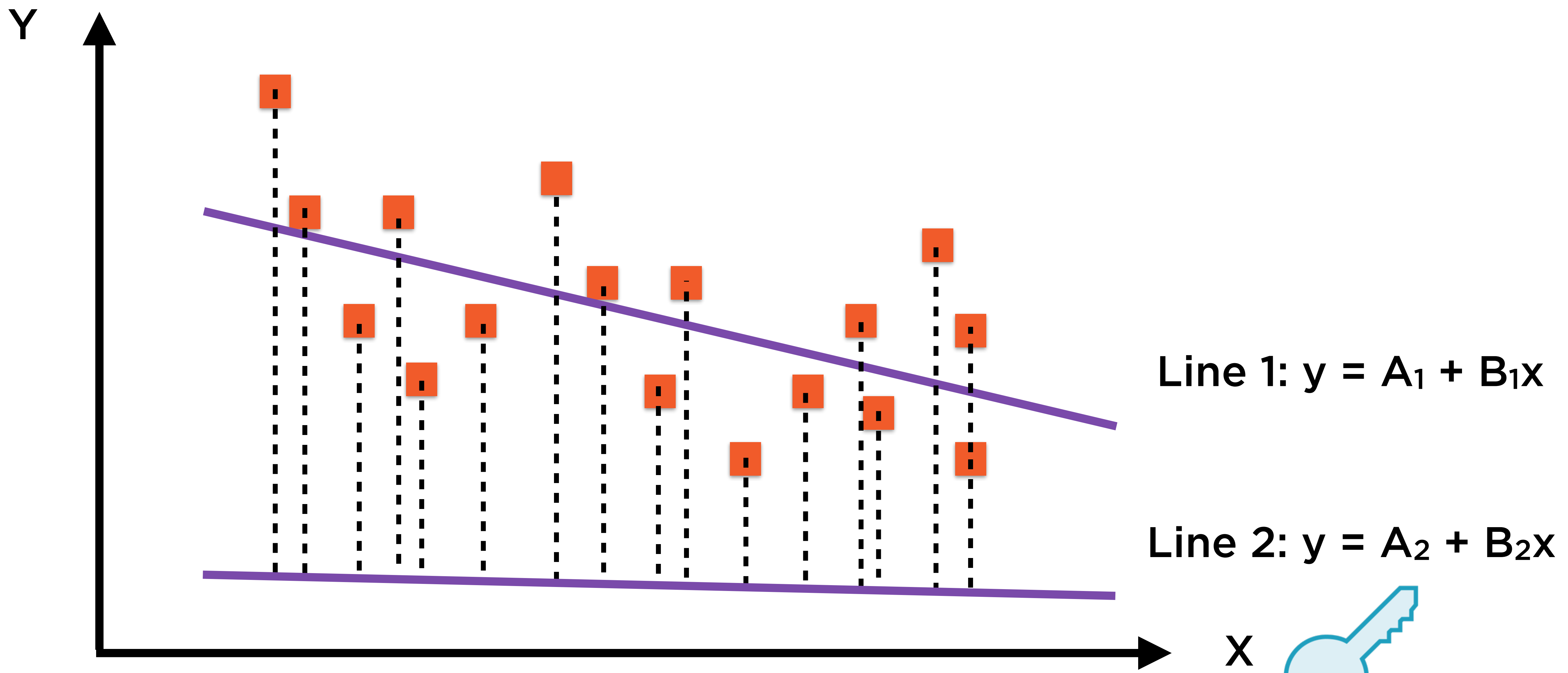
The "best fit" line is the one where the sum of the squares of the lengths of these dotted lines is minimum

Minimising Least Square Error



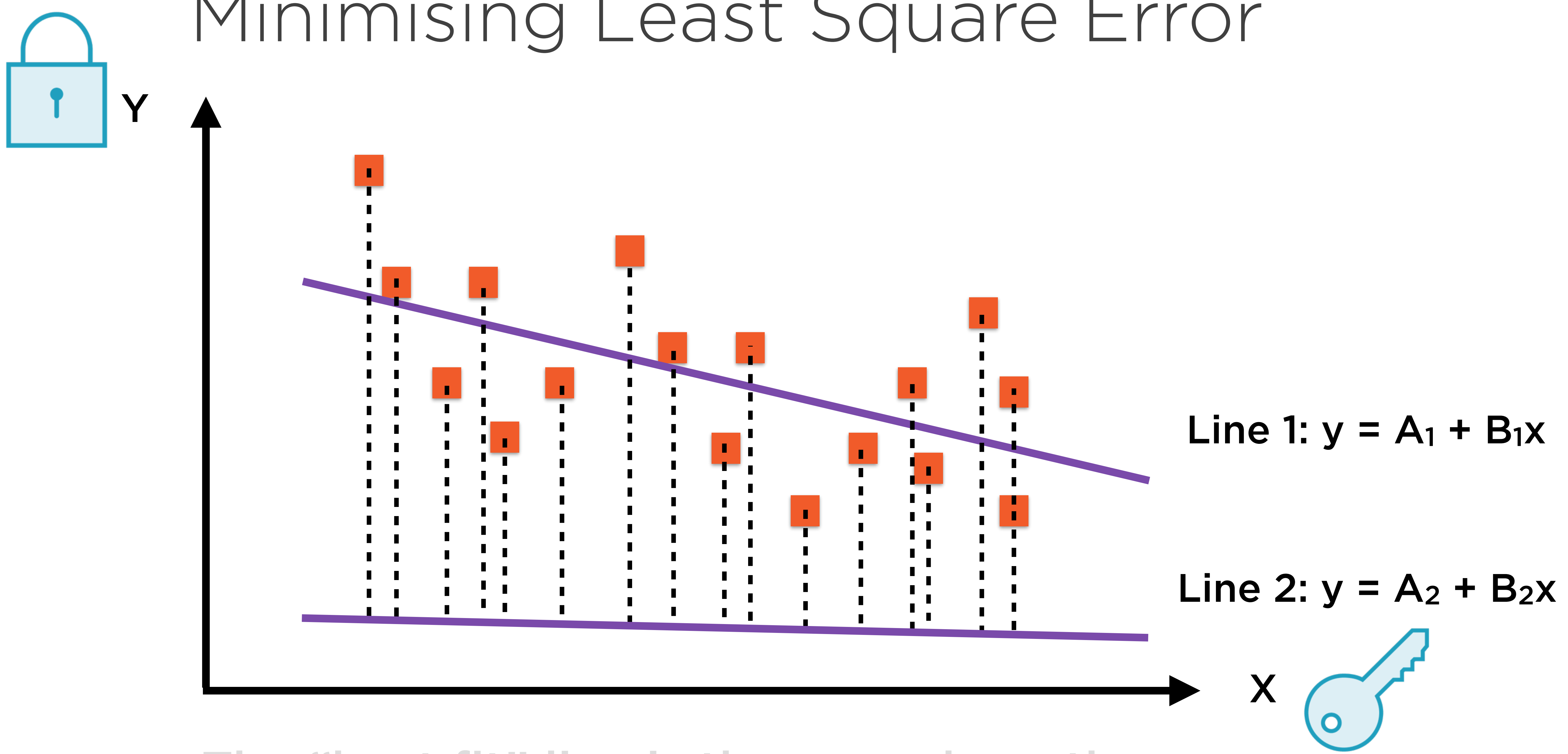
The "best fit" line is the one where the sum of the squares of the **lengths of these dotted lines** is minimum

Minimising Least Square Error



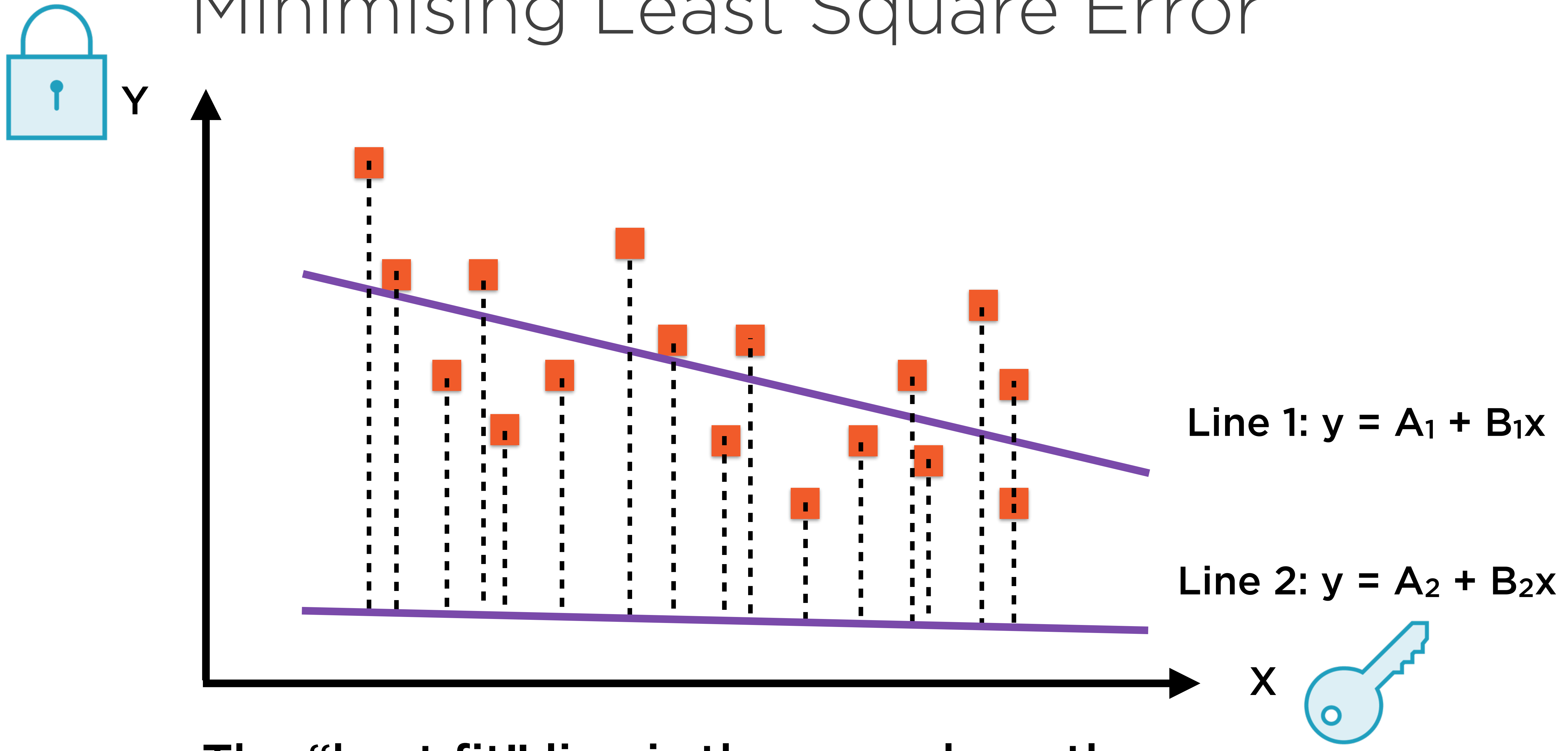
The "best fit" line is the one where the **sum of the squares** of the lengths of these dotted lines is minimum

Minimising Least Square Error



The "best fit" line is the one where the sum of the squares of the lengths of the errors is minimum

Minimising Least Square Error



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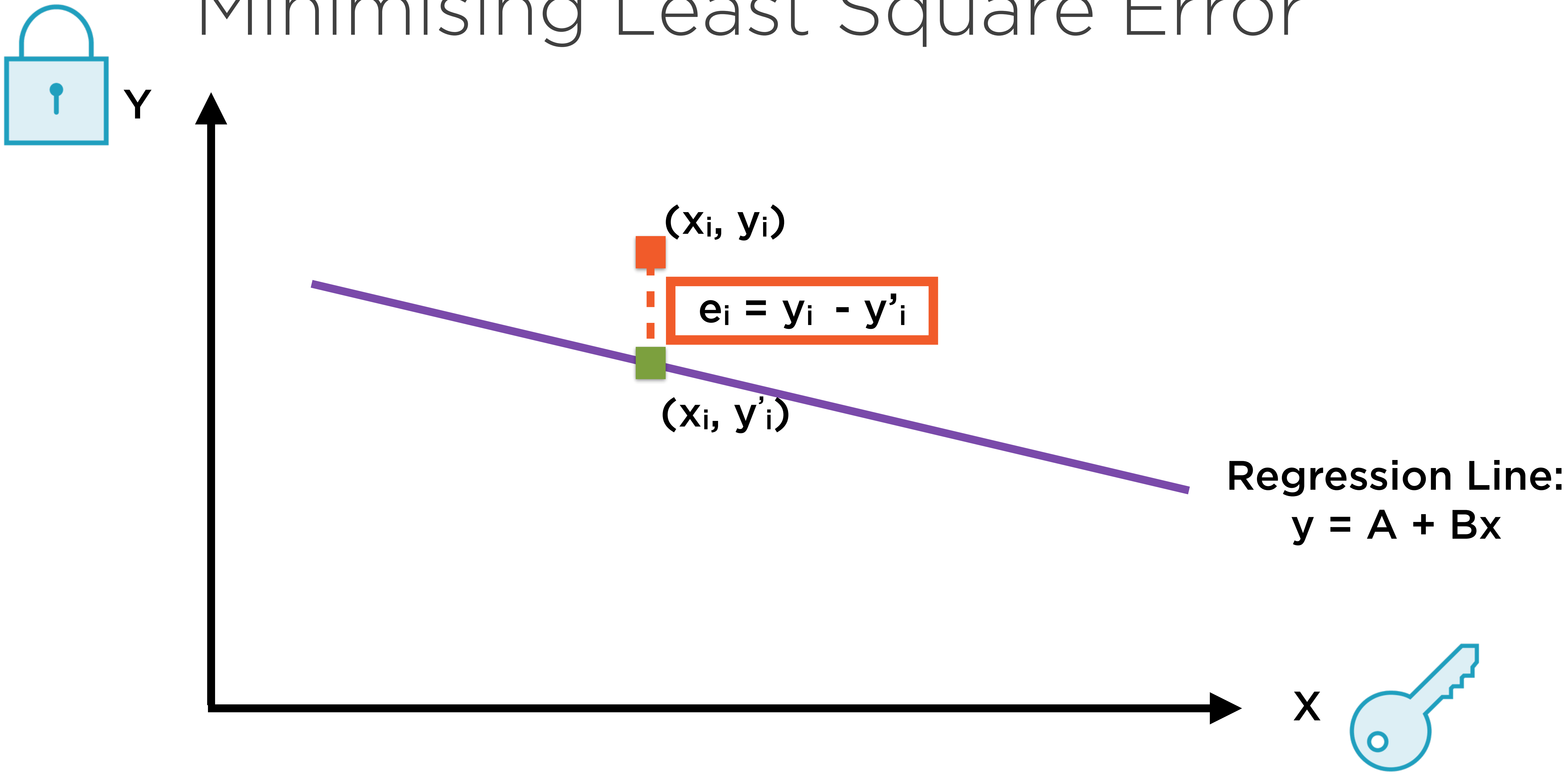
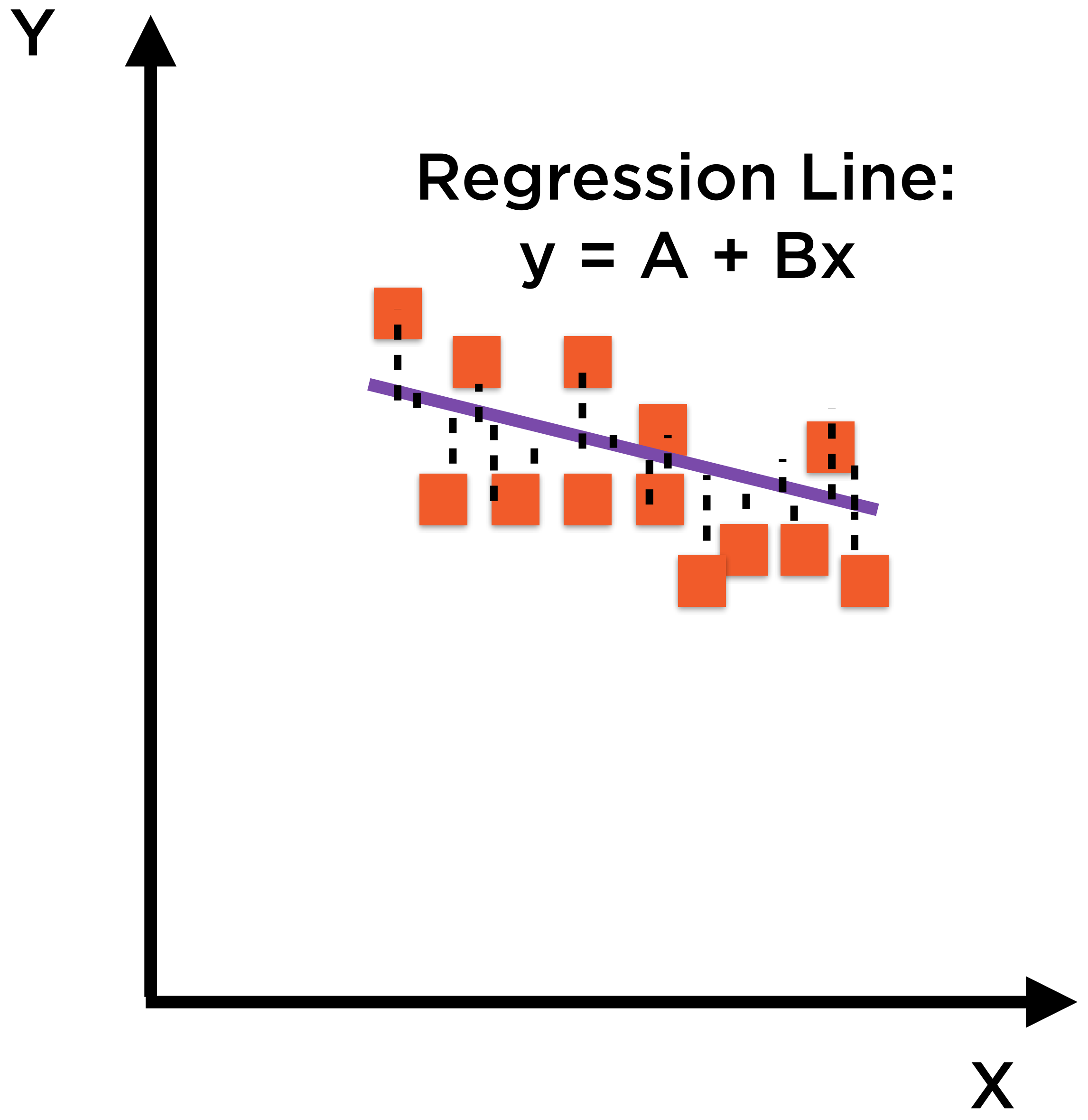
Minimising Least Square Error



Residuals of a regression are the difference between actual and fitted values of the dependent variable



Ideally, residuals should

- have zero mean
- common variance
- be independent of each other
- be independent of x
- be normally distributed

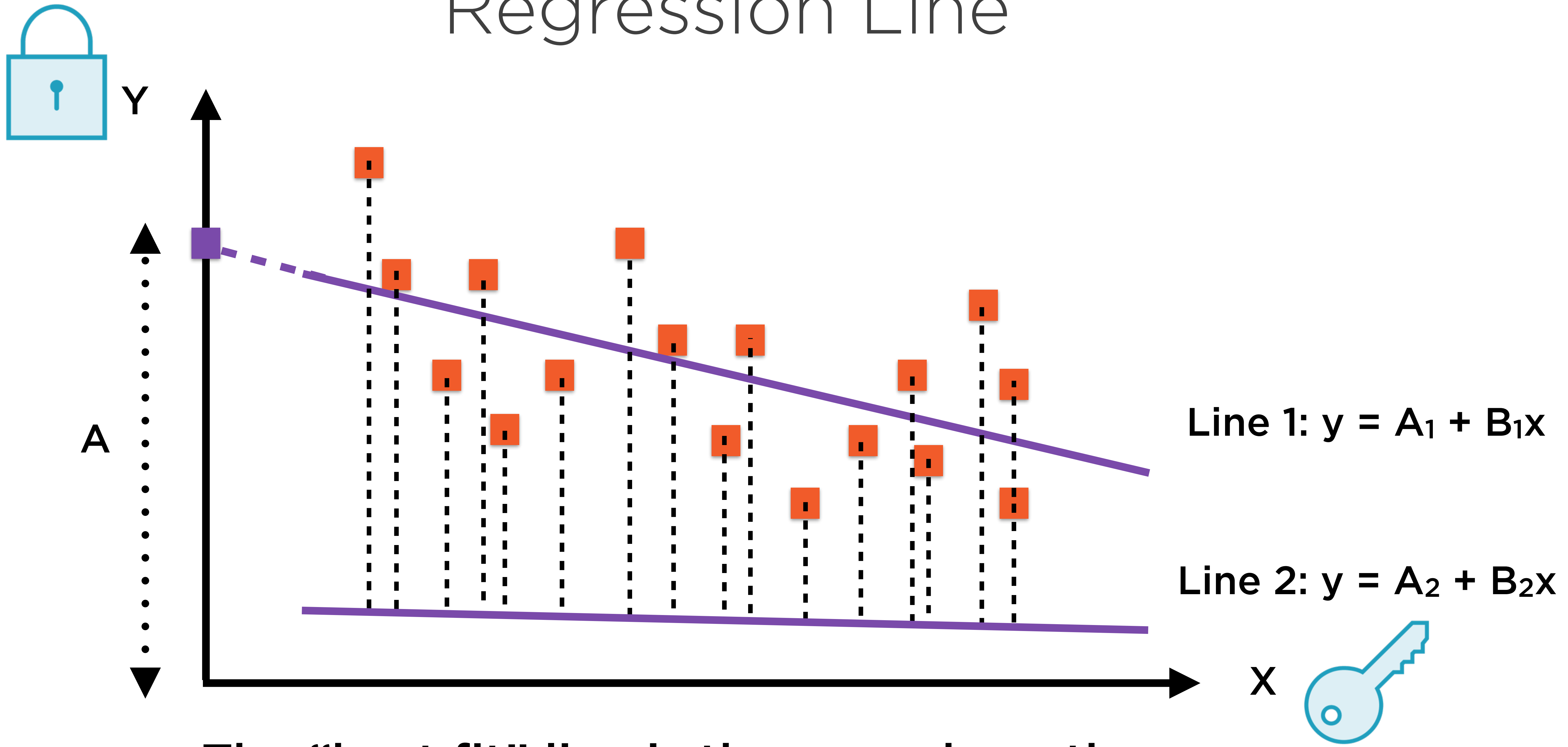
Linear Regression as an Optimization Problem

$y = A + Bx$

Regression Line

The “best fit” line which minimizes the sum of the squares of the errors

Regression Line



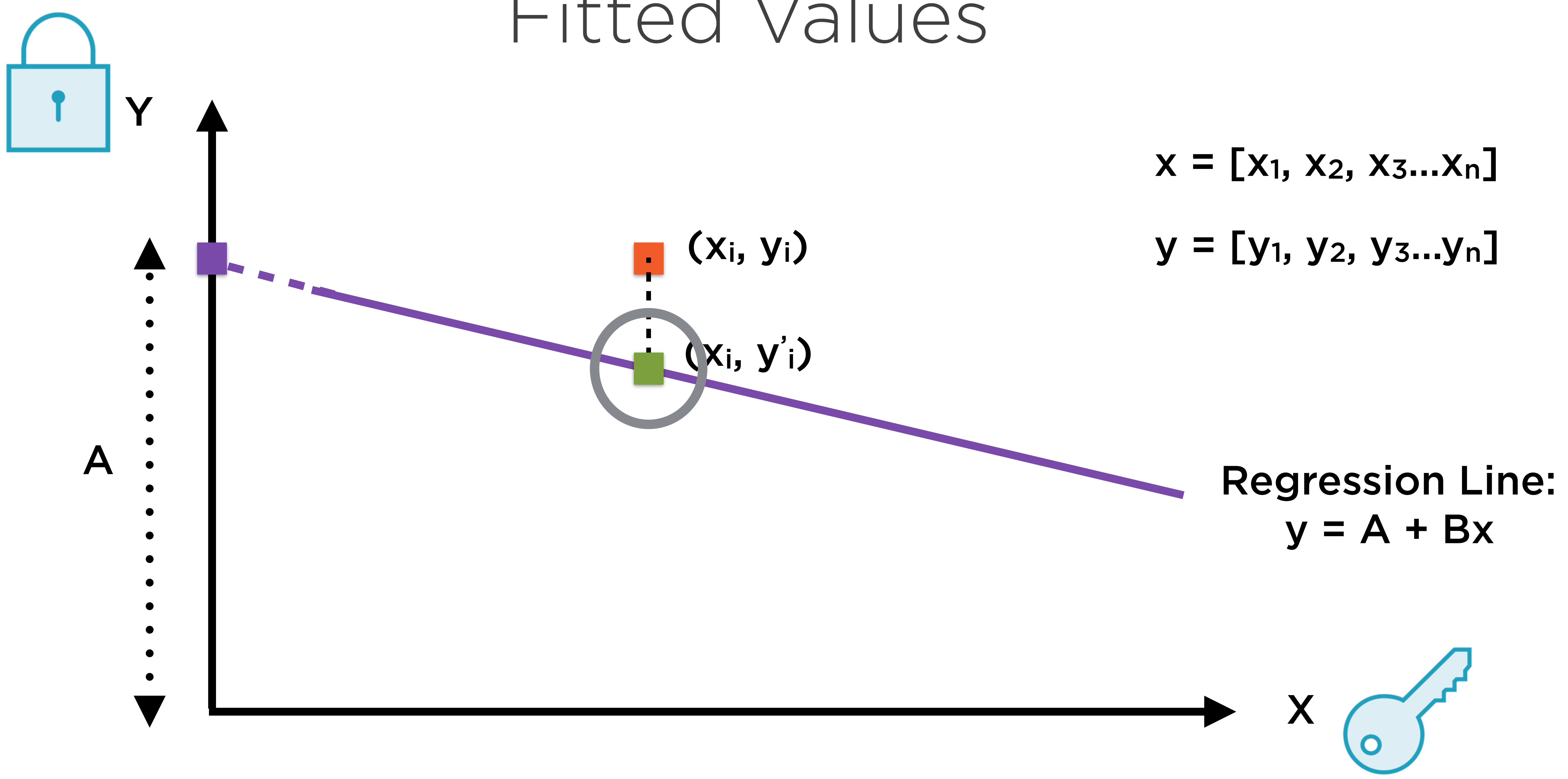
The "best fit" line is the one where the sum of the squares of the lengths of the errors is minimum

$y' = A + Bx$

Fitted Values of Dependent Variable

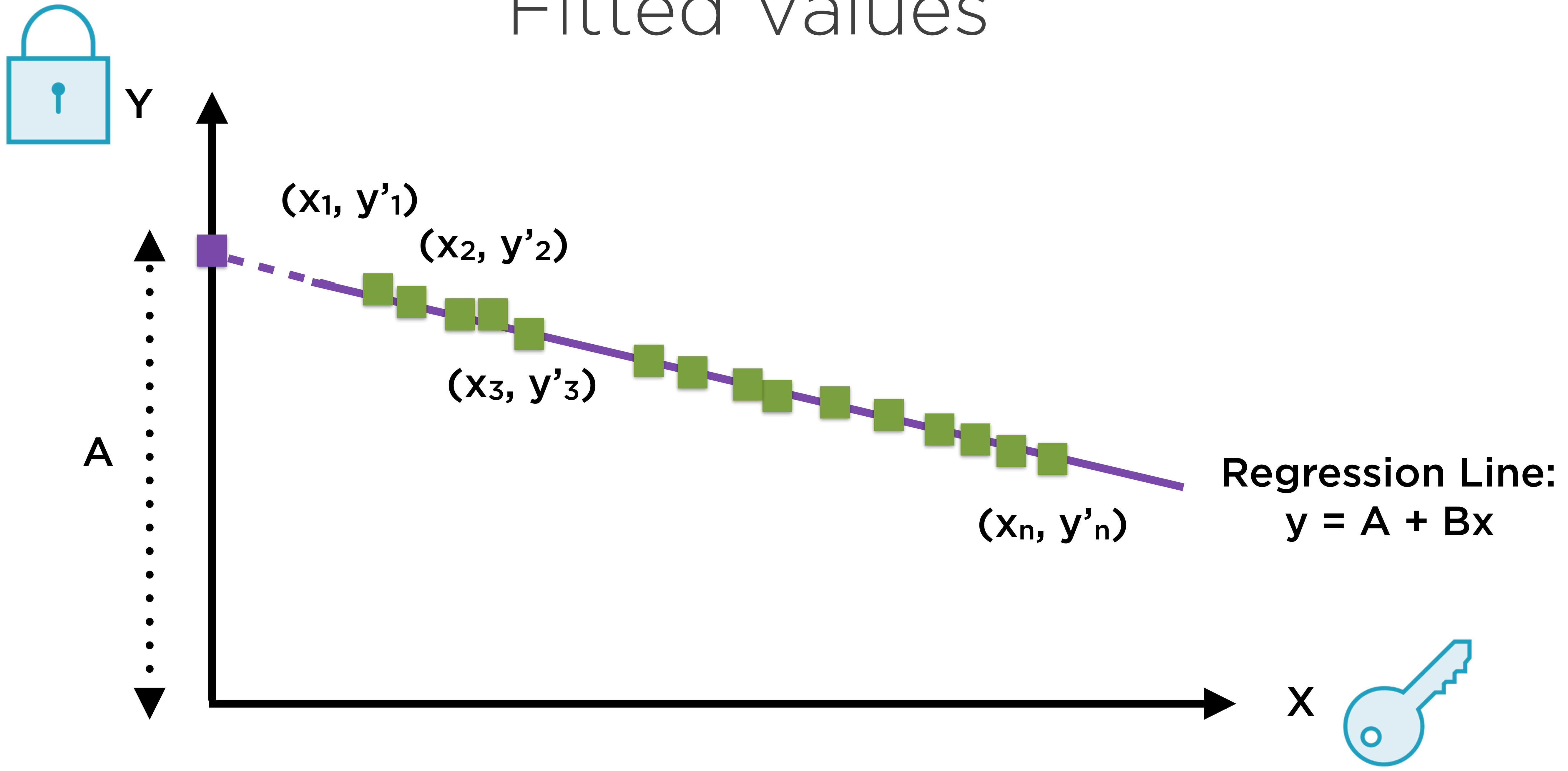
The fitted line $y = A + Bx$ will yield a different set of values, called the fitted values

Fitted Values



Each point (x_i,y_i) has a corresponding point (x_i,y'_i) on the regression line

Fitted Values



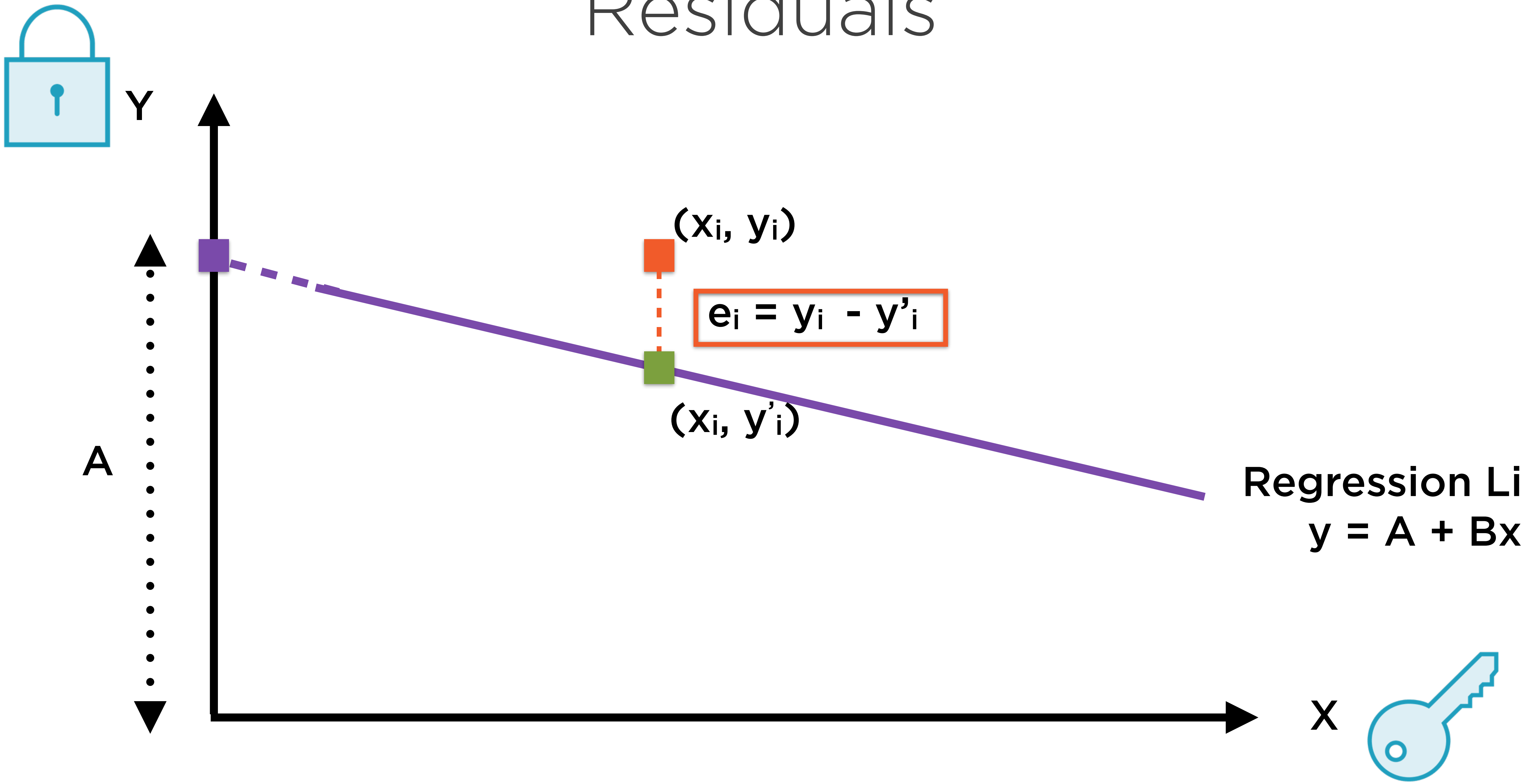
The corresponding values of y'_i are called the fitted values

$e = y - y'$

Residuals

The residuals, or errors, are the differences between the actual and fitted values of the dependent variable

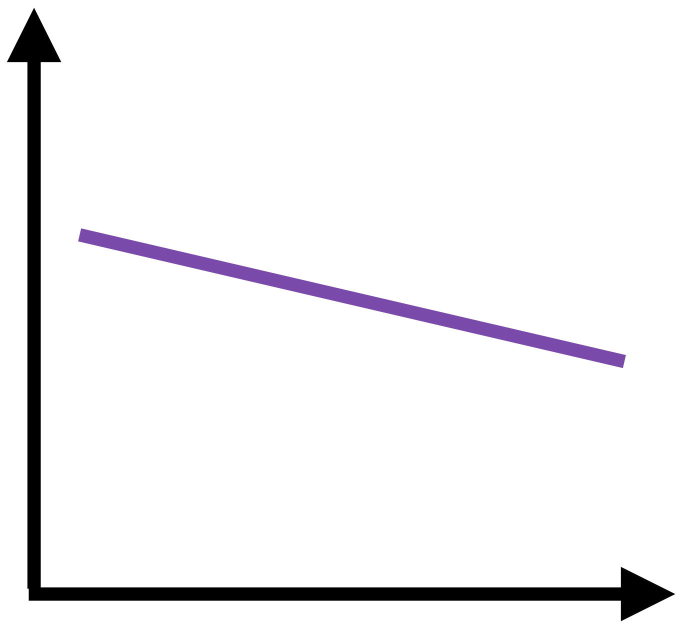
Residuals



Residuals of a regression are the difference between actual and fitted values of the dependent variable

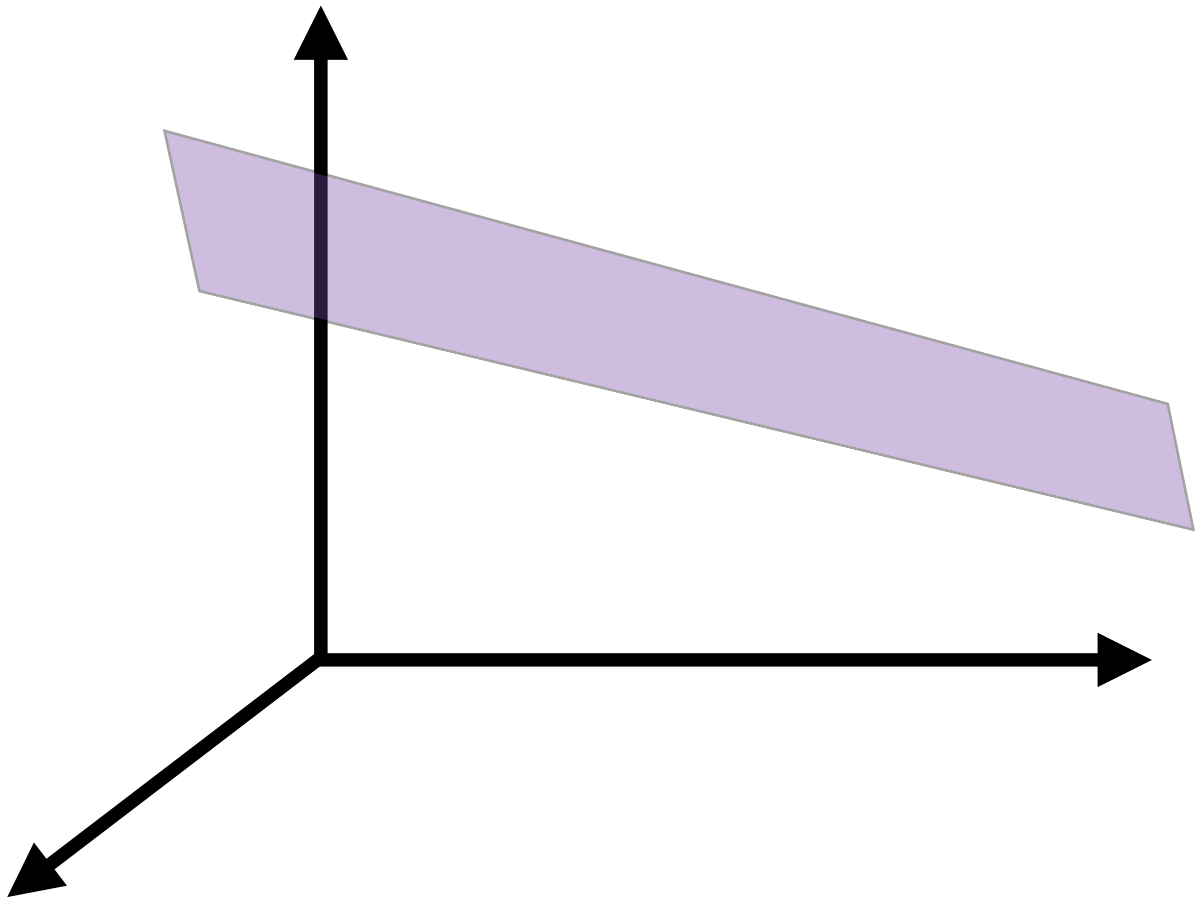
The regression line is that line which minimizes the variance of the residuals (MSE)

MSE Minimization Extends To Multiple Regression



Simple Regression

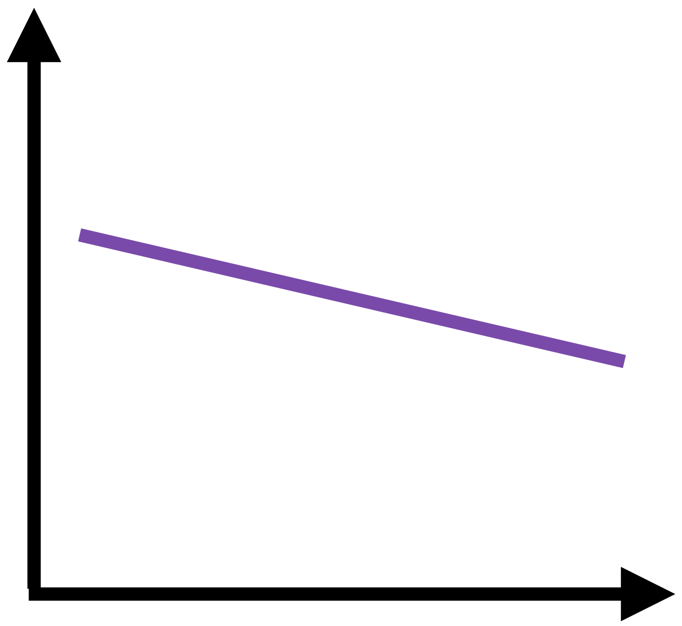
Data in 2 dimensions



Multiple Regression

Data in > 2 dimensions

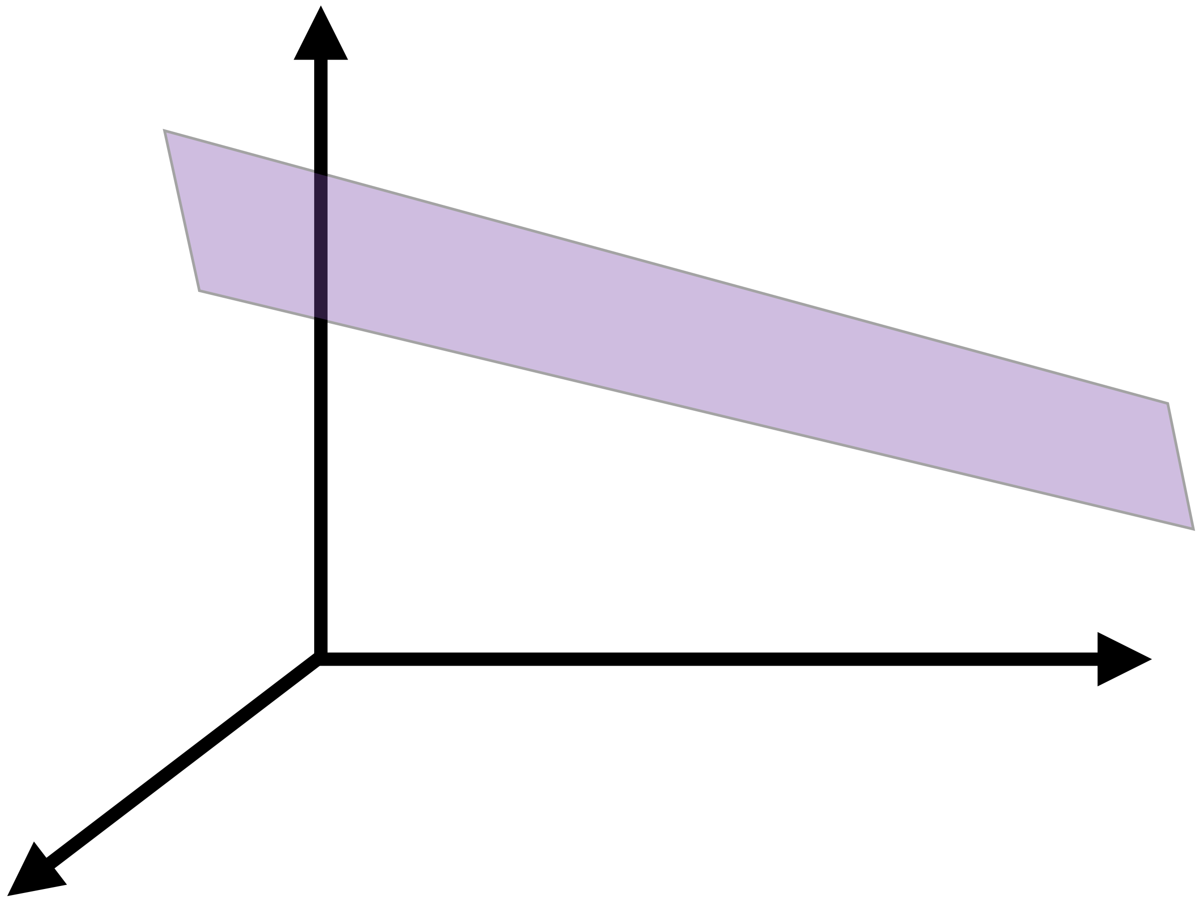
Simple and Multiple Regression



Simple Regression

One independent variable

$y = A + Bx$



Multiple Regression

Multiple independent variables

$y = A + B_1x_1 + B_2x_2 + B_3x_3$

“Best Linear Unbiased Estimator” (BLUE)

“Best”

Coefficients have minimum variance, i.e. are estimated with relatively high certainty

“Unbiased”

Residuals have zero mean, are uncorrelated to each other and have equal variance

Solving the regression problem with the method of least squares gives a BLUE solution

$R^2 = ESS / TSS$

R^2

R^2 = Explained Sum of Squares / Total Sum of Squares

R^2

ESS - Variance of fitted values

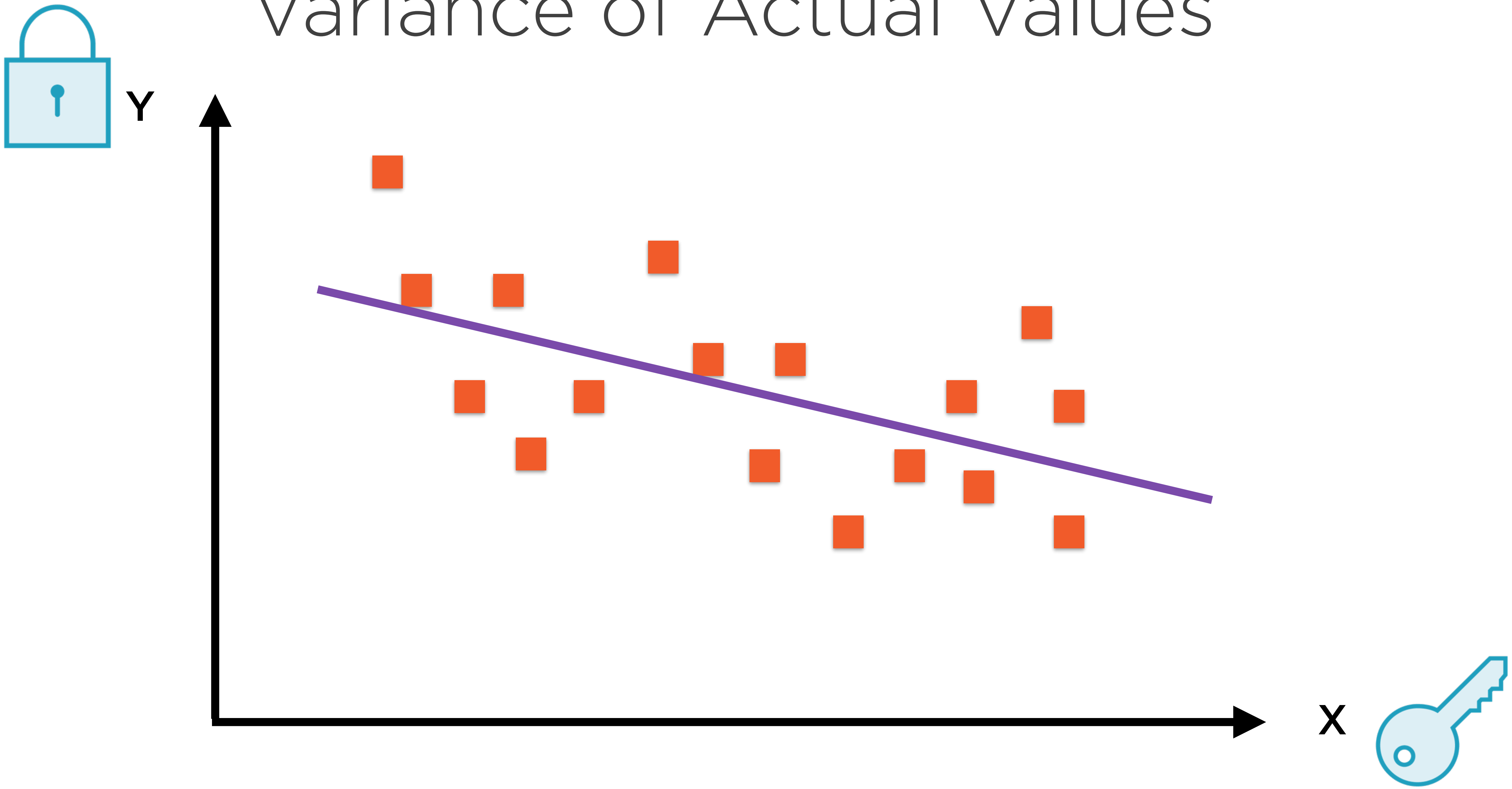
TSS - Variance of actual values

R^2 = Explained Sum of Squares / Total Sum of Squares

R^2

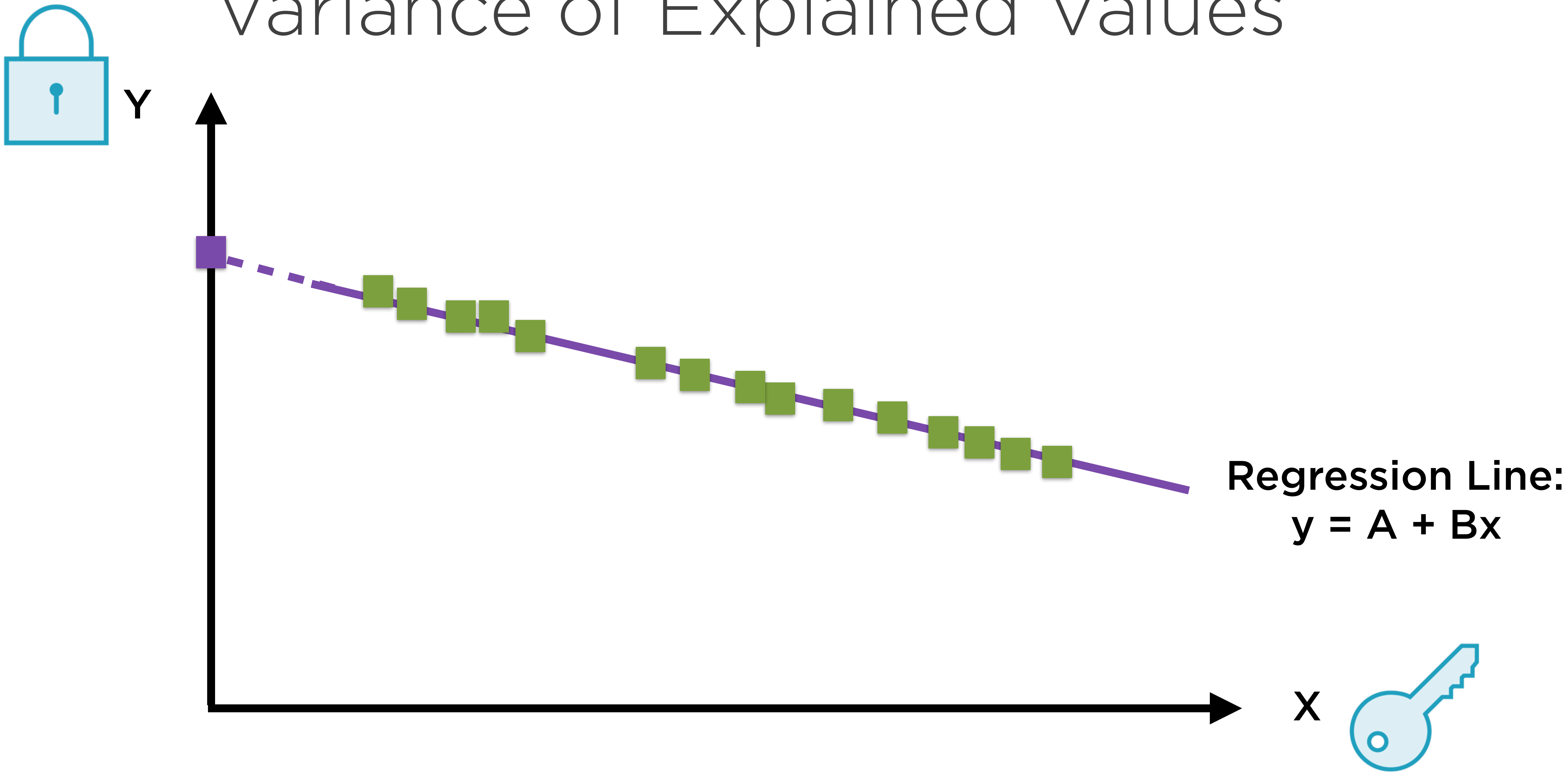
The percentage of total variance explained by the regression. Usually, the higher the R^2, the better the quality of the regression (upper bound is 100%)

Variance of Actual Values



The original data points have some variance (TSS)

Variance of Explained Values



The fitted data points have their own variance (ESS)

$$R^2 = ESS \;/\; TSS$$

R^2

How much of the original variance is captured in the fitted values?

Generally, higher this number the better the regression

The regression line found by minimizing variance of residuals (MSE) is the line with the **best R^2**

Other Types of Regression

Other forms of regression alter the objective function of the optimization

Ridge	Lasso
Elastic Net	SVR

Demo

Implementing linear regression in scikit-learn

Distance Measures

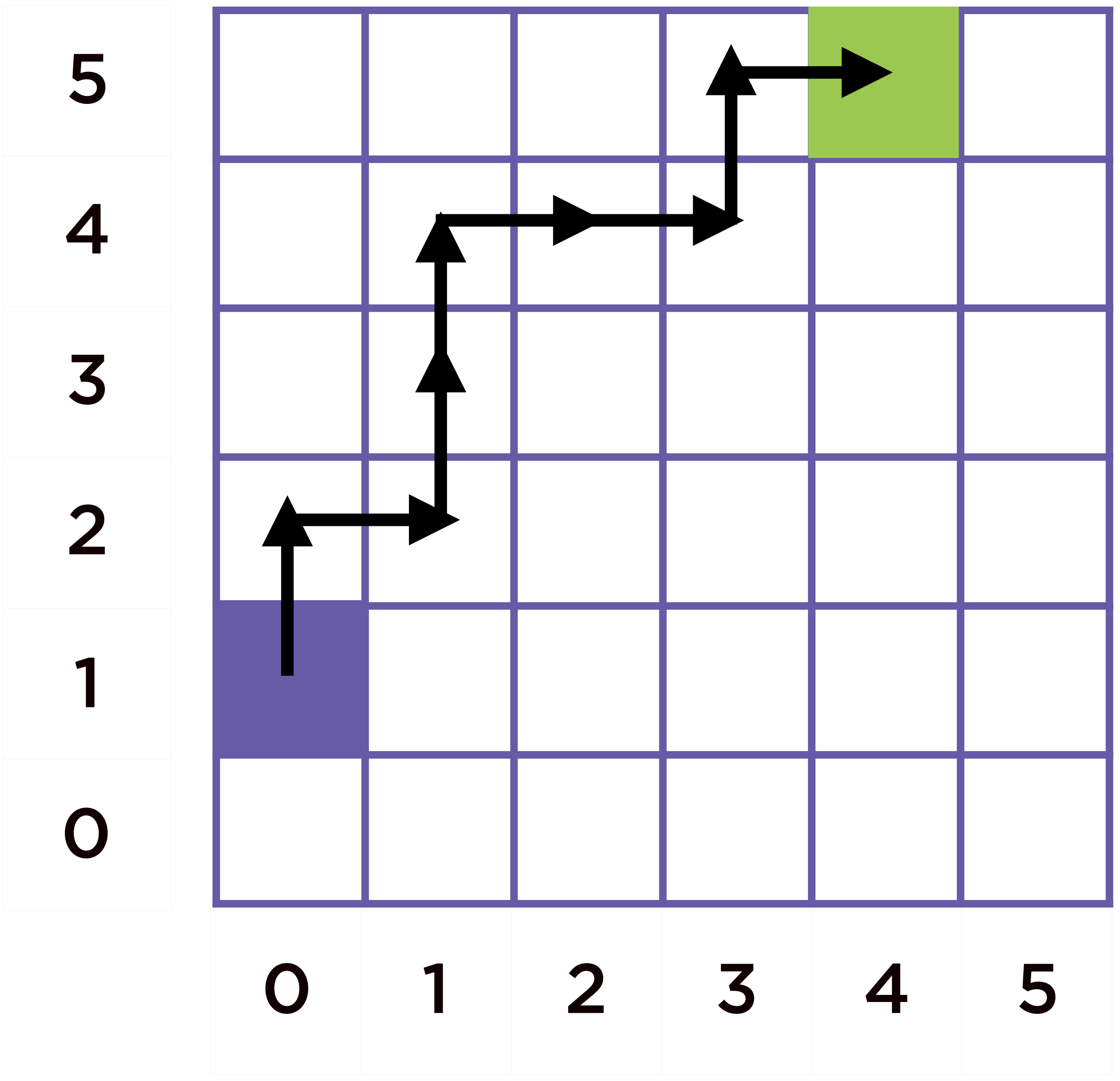
L1 distance

Snake distance

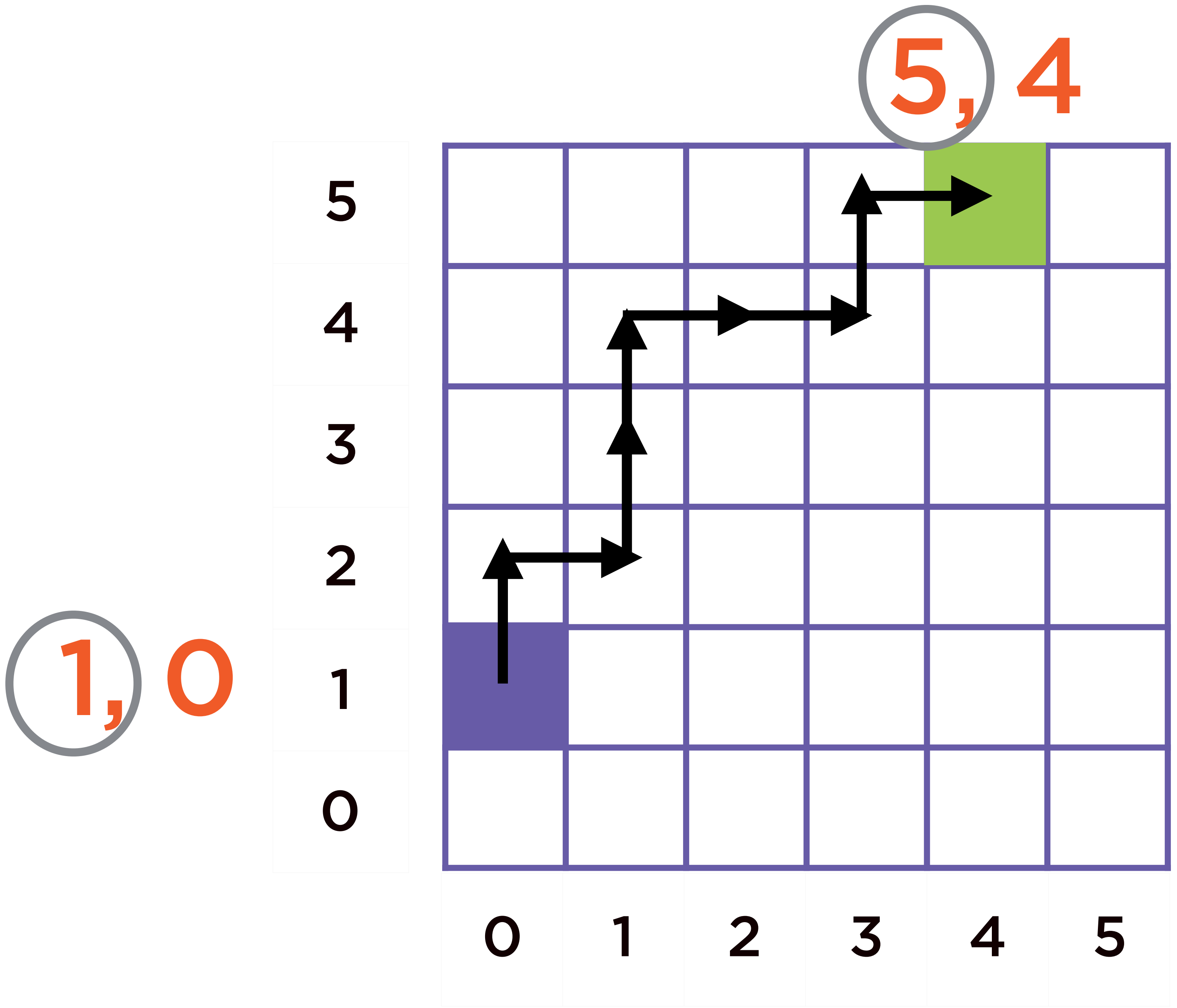
City block distance

Manhattan distance

Distance Measure

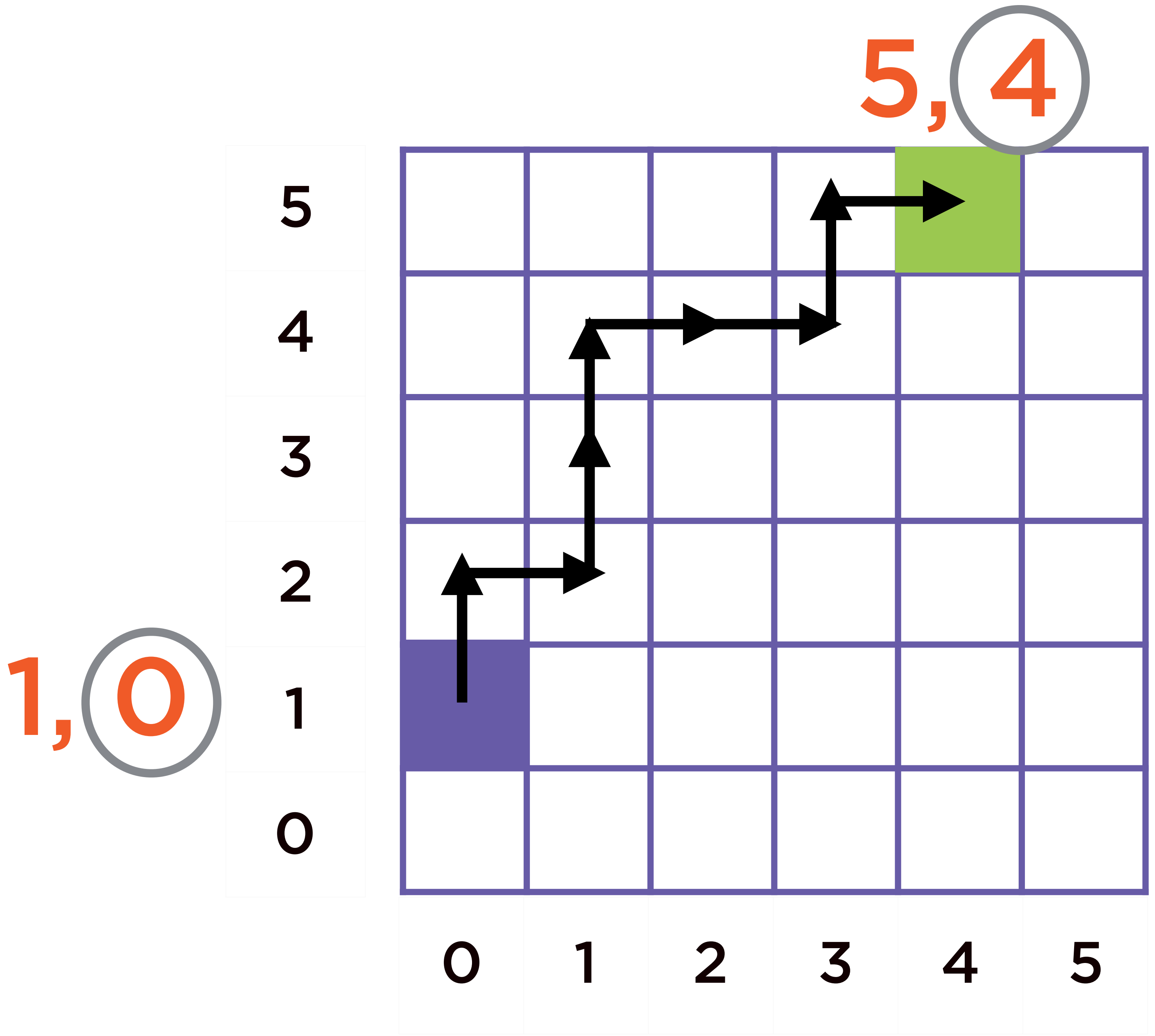


L1 Distance



5-1 = 4

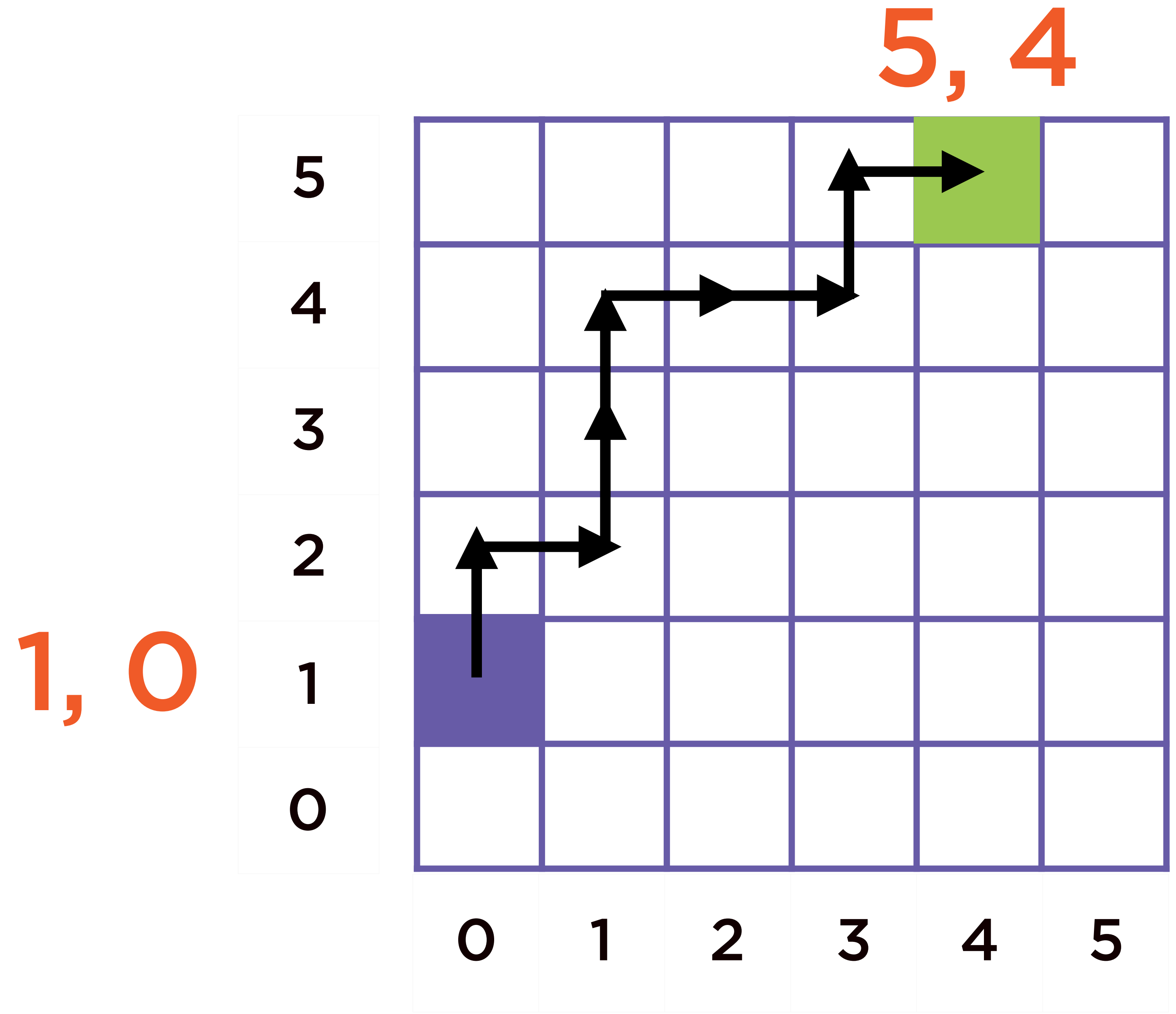
L1 Distance



5-1 = 4

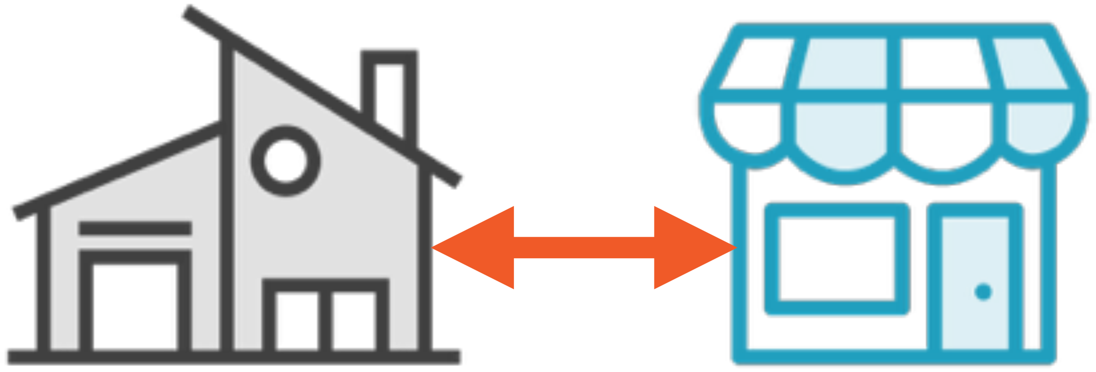
4-0 = 4

L1 Distance



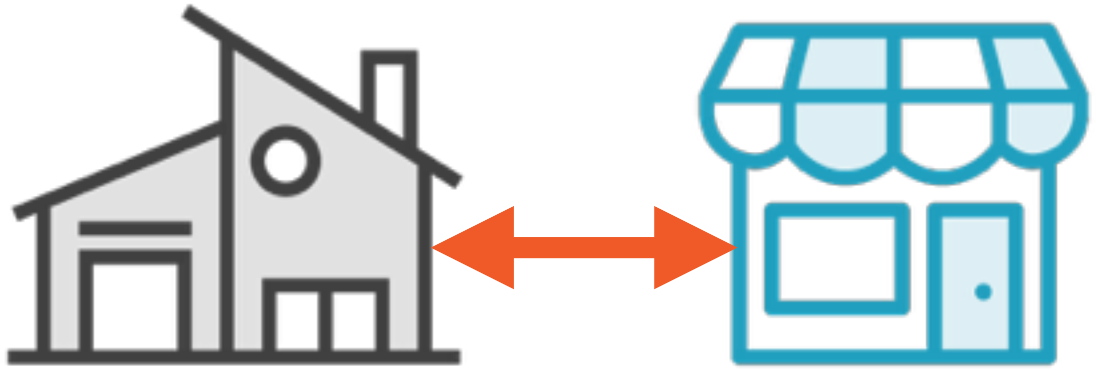
$$5-1 = 4$$
$$4-0 = 4$$
$$= 8$$

Distance Measures



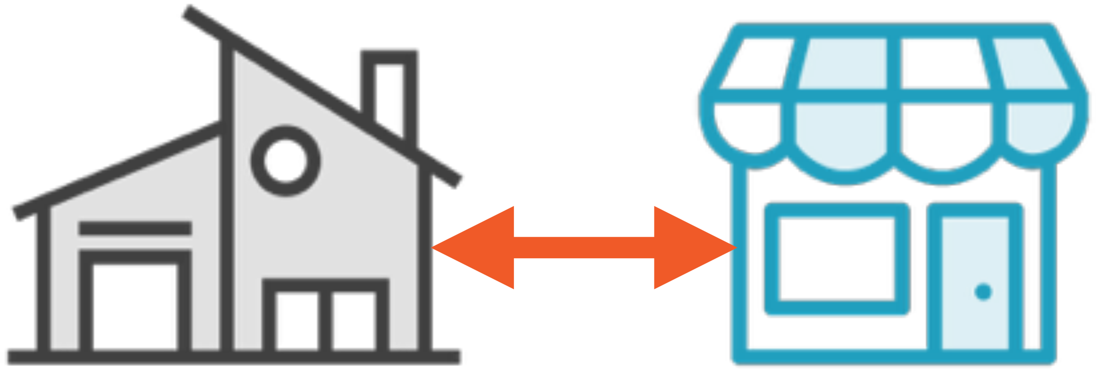
$$\text{L1 Distance}(t1,\ t2) = \text{sum}(\text{abs}(t1_i - t2_i))$$

Distance Measures



L1 Distance(t1, t2) = sum(abs($t1_i$ − $t2_i$))

Distance Measures



L1 Distance(t1, t2) = sum(abs($t1_i$ - $t2_i$))

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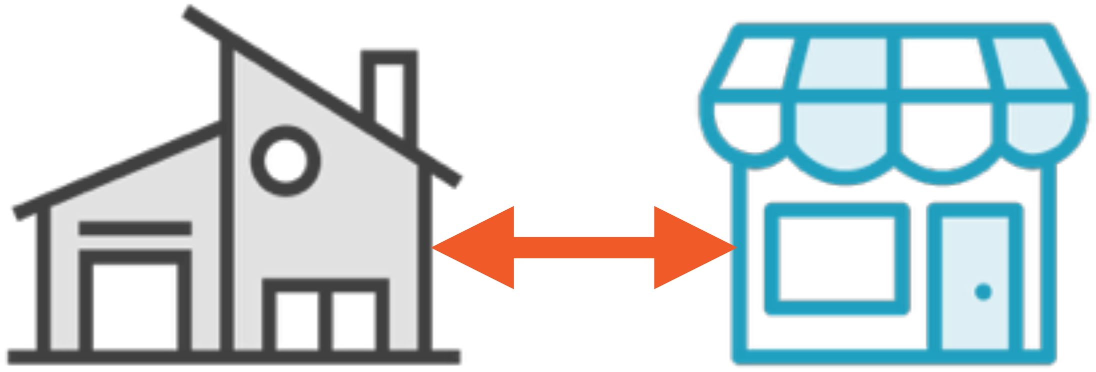
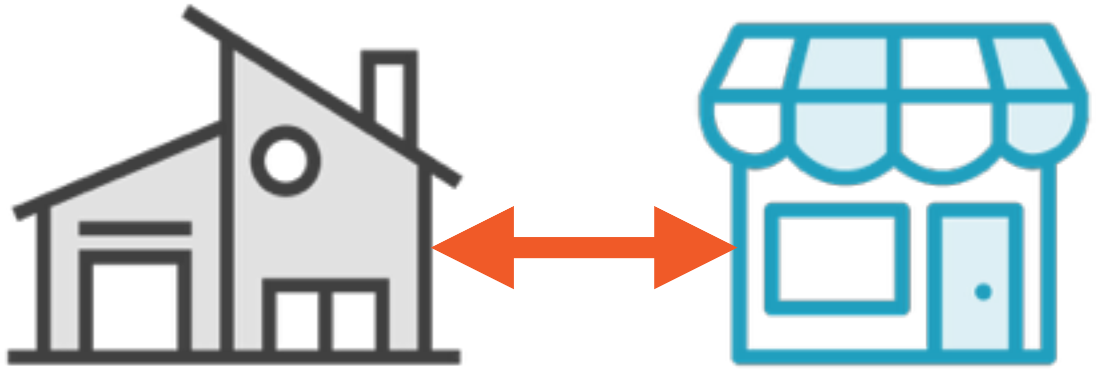


`L1 Distance(t1, t2) = sum(abs(t1_i - t2_i))`

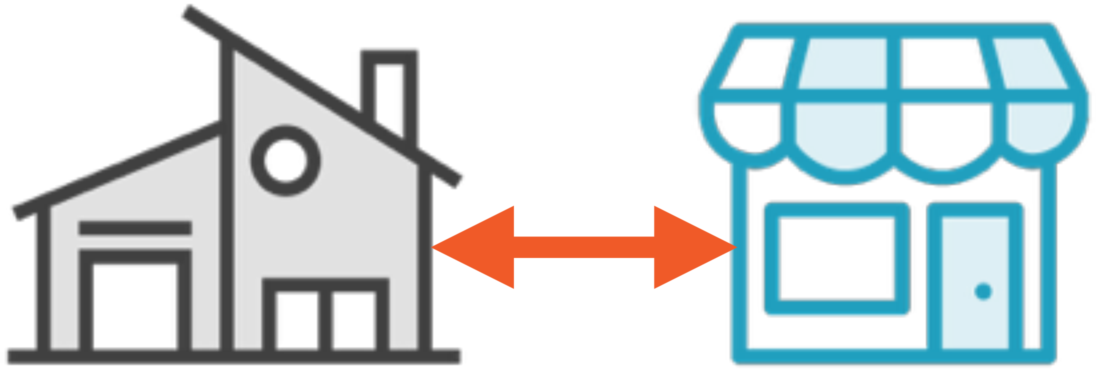
$$\text{L1 Distance}(t1, t2) = \text{sum}(\text{abs}(t1_i - t2_i))$$

Distance Measures



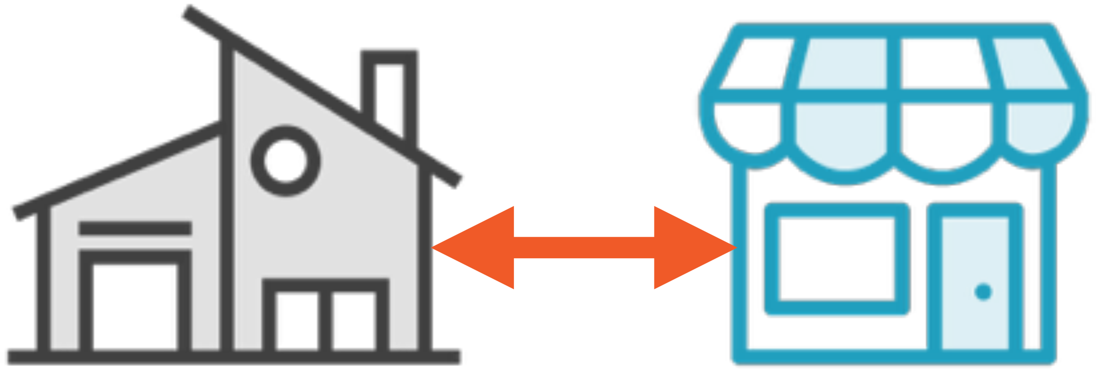
$$L1\ Distance(t1,\ t2) = sum(abs(t1_i - t2_i))$$

L-1 Norm



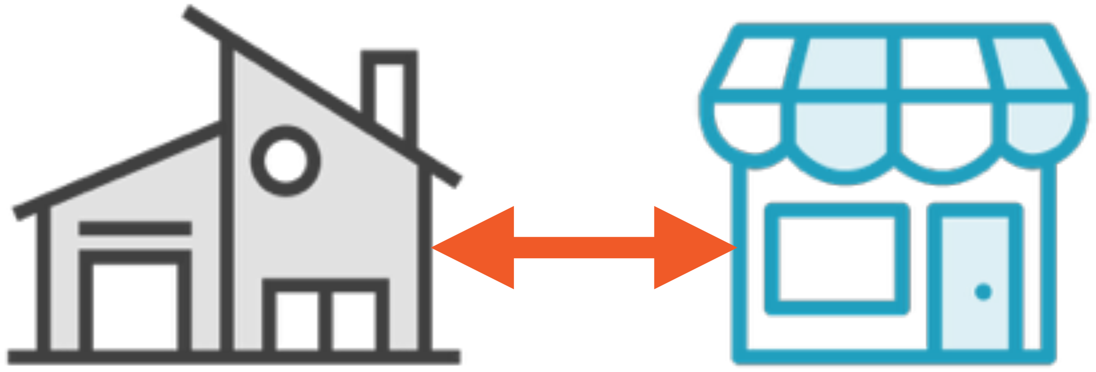
$$\text{L1-Norm}(A, B_1, B_2 \ldots B_n) = |A| + |B_1| + |B_2| \ldots + |B_n|$$

L-1 Norm



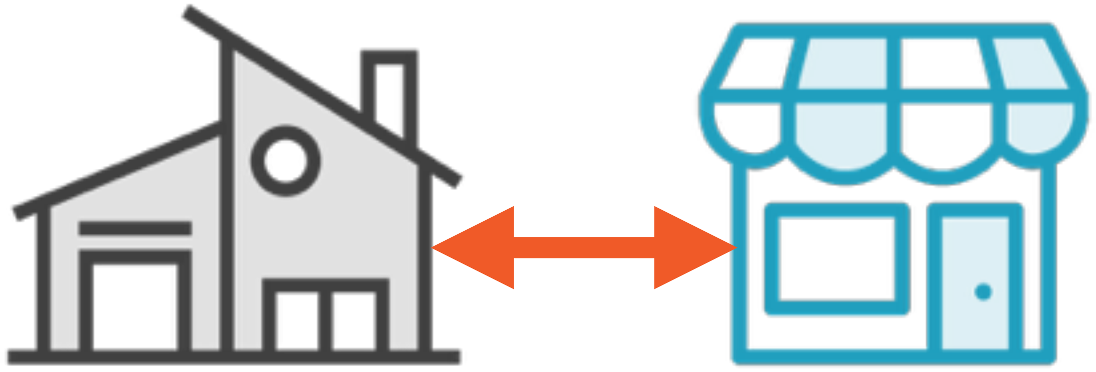
$$L1\text{-}Norm(A, B_1, B_2 \ldots B_n) = |A|^1 + |B_1|^1 + |B_2|^1 \ldots + |B_n|^1$$

L-2 Norm



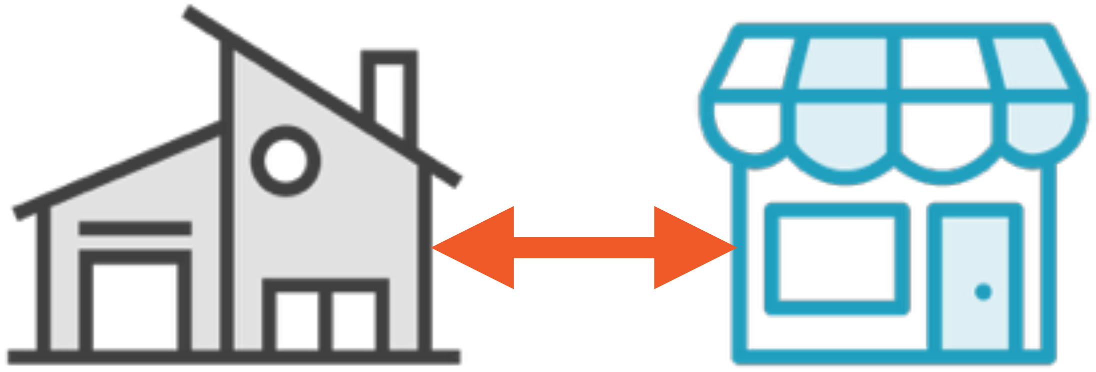
$$L2\text{-}Norm(A, B_1, B_2 \ldots B_n) = |A|^2 + |B_1|^2 + |B_2|^2 \ldots + |B_n|^2$$

L-2 Norm



$$\text{L2-Norm}(A, B_1, B_2 \ldots B_n) = |A|^2 + |B_1|^2 + |B_2|^2 \ldots + |B_n|^2$$

L-2 Norm

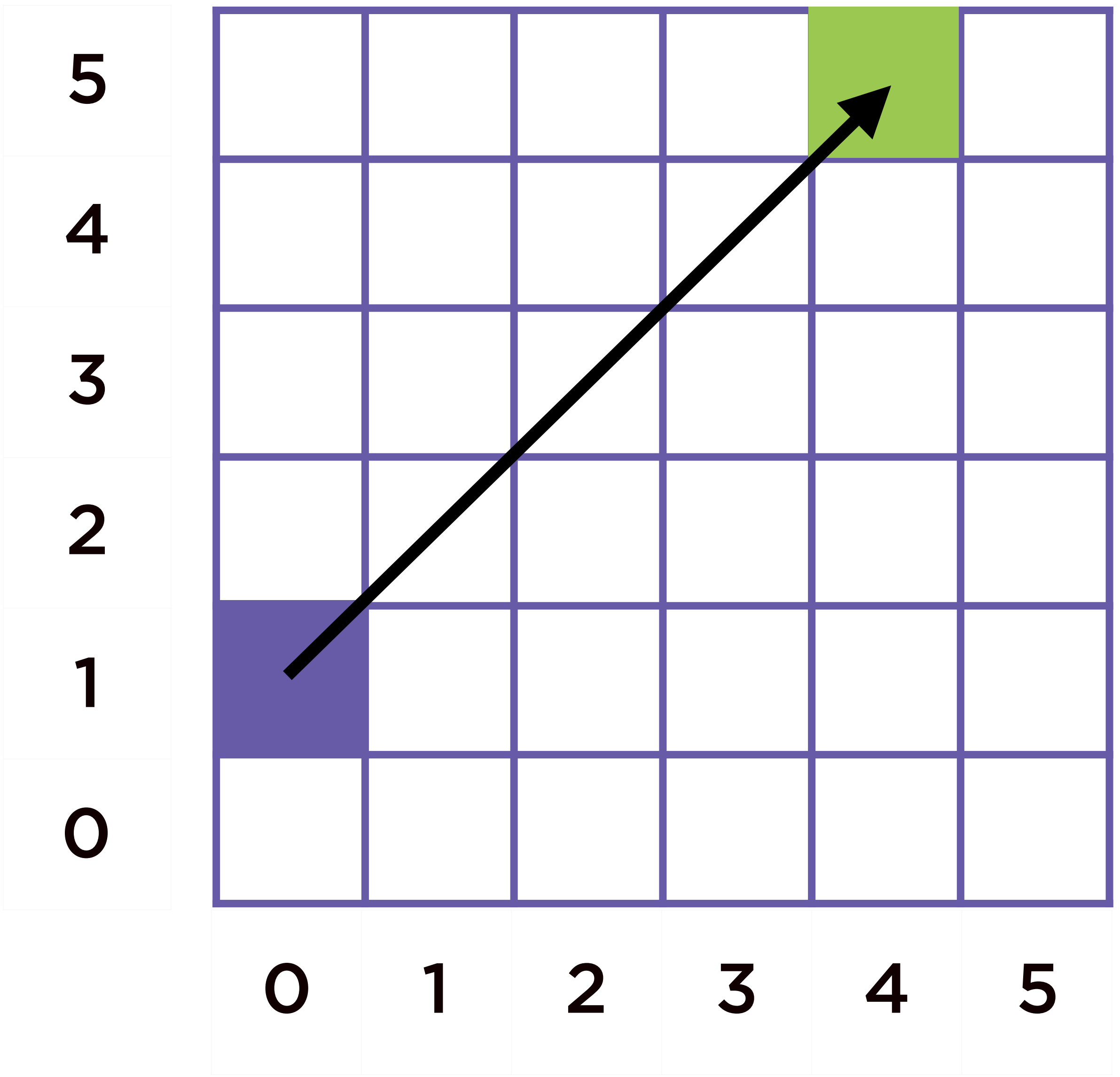


$$L2\text{-}Norm(A, B_1, B_2 \ldots B_n) = A^2 + B_1^2 + B_2^2 \ldots + B_n^2$$

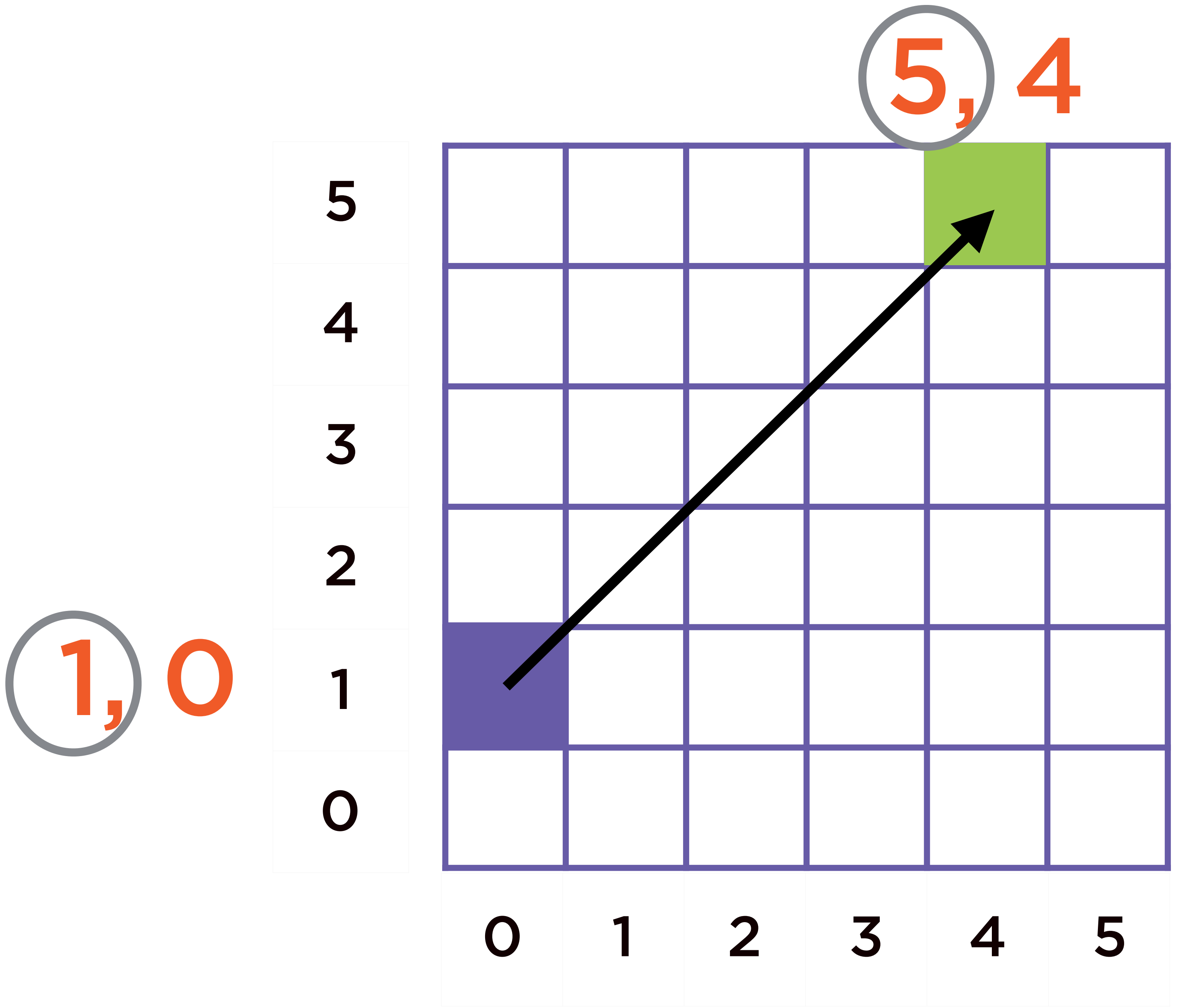
Euclidean Distance

As the crow flies

Distance Measure

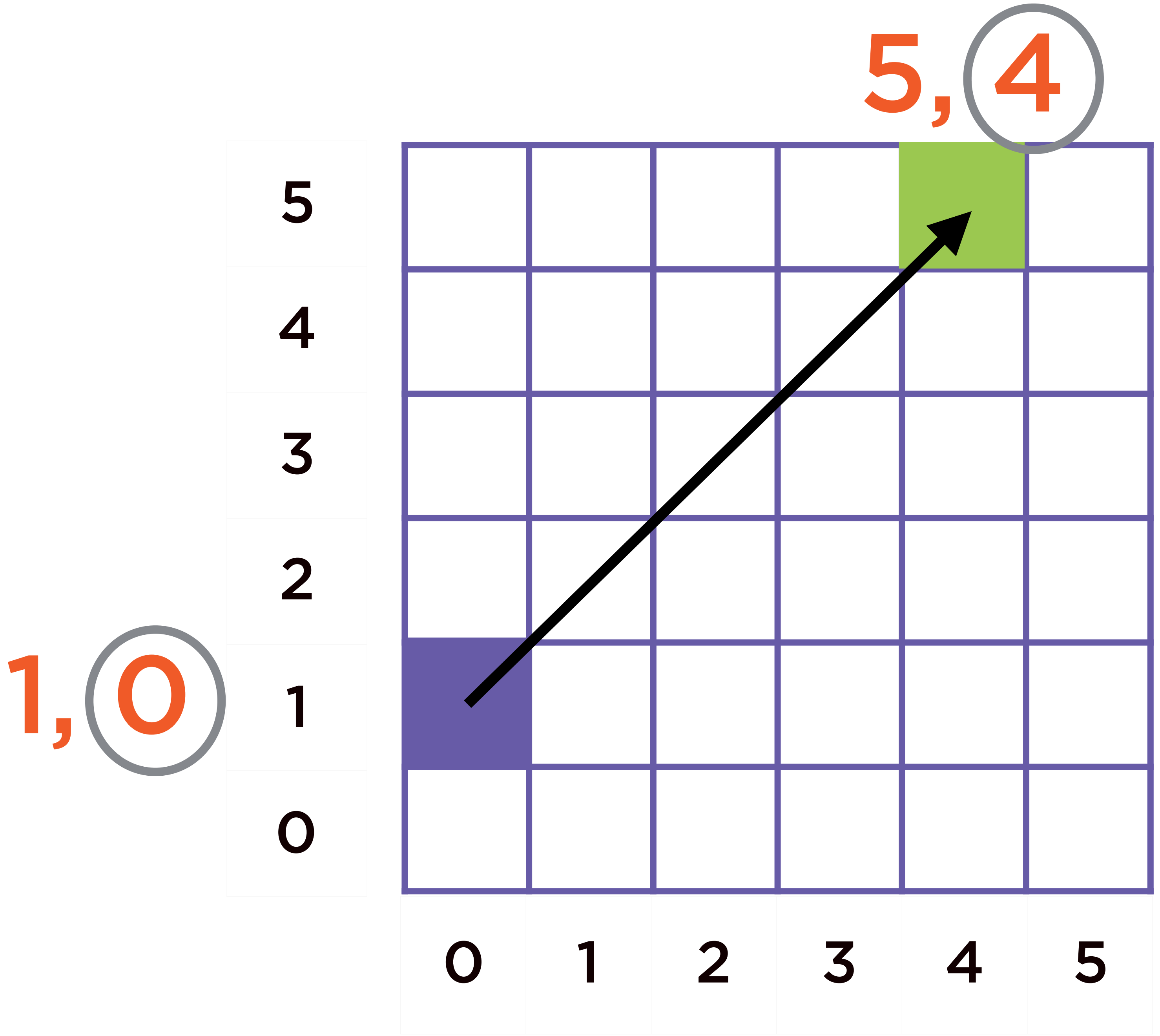


L2 Distance



$(5-1)^2 = 16$

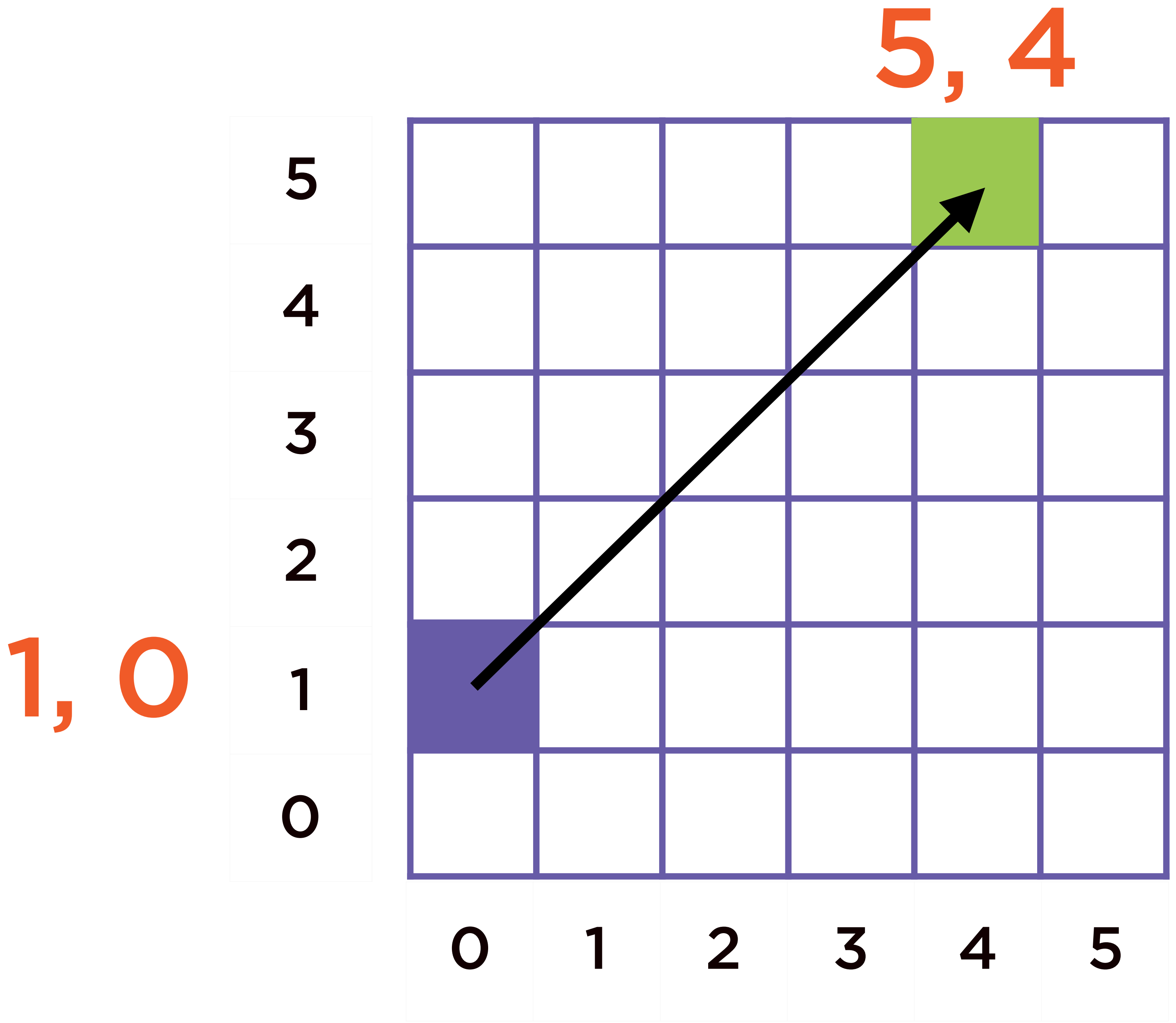
L2 Distance



$$(5-1)^2 = 16$$

$$(4-0)^2 = 16$$

L2 Distance

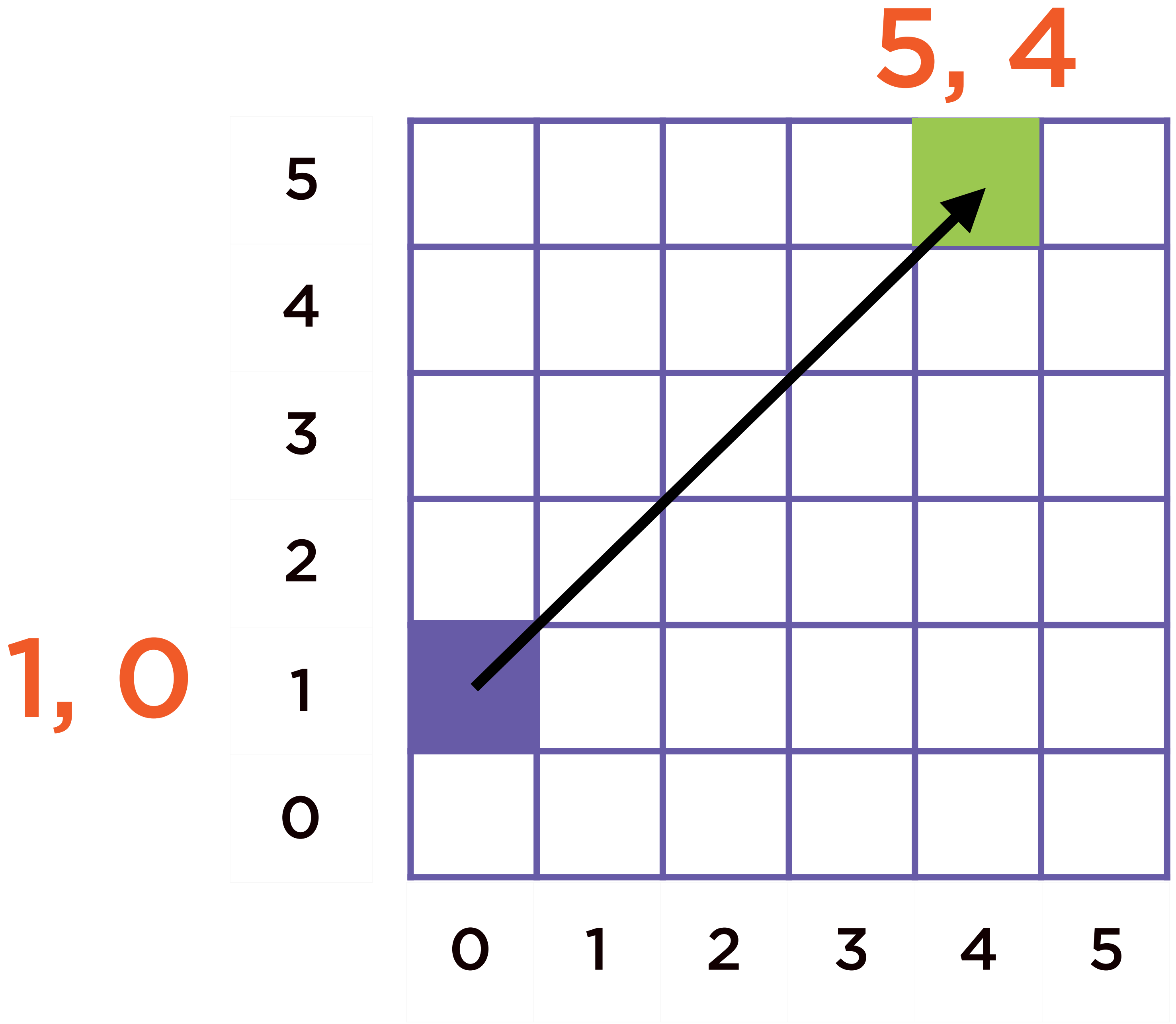


$$(5-1)^2 = 16$$

$$(4-0)^2 = 16$$

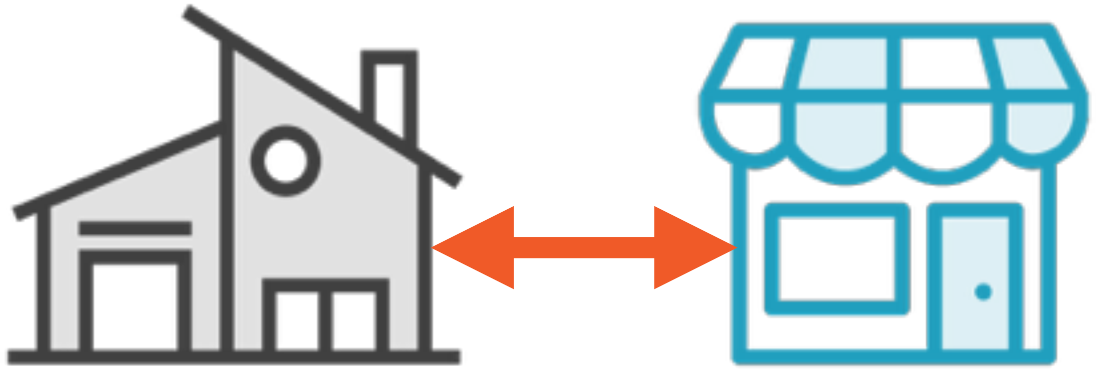
$$= 32$$

L2 Distance



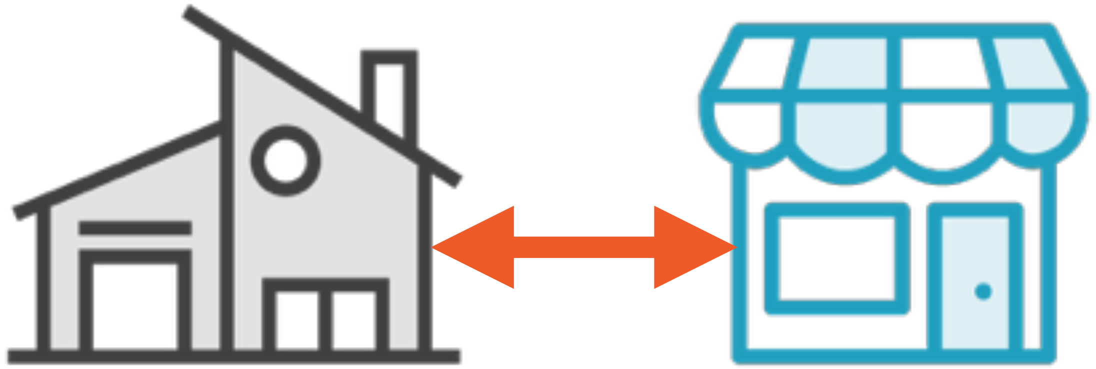
$$(5-1)^2 = 16$$
$$(4-0)^2 = 16$$
$$= 32$$
$$\text{sqrt}(32) = 5.65$$

Distance Measures



$$\text{L2 Distance}(t1, t2) = \text{sqrt}(\text{sum}((t1_i - t2_i)^2))$$

Distance Measures



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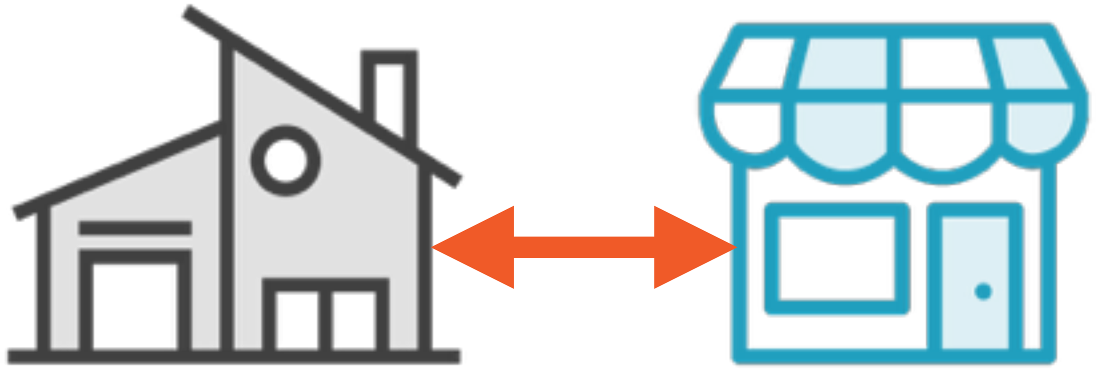

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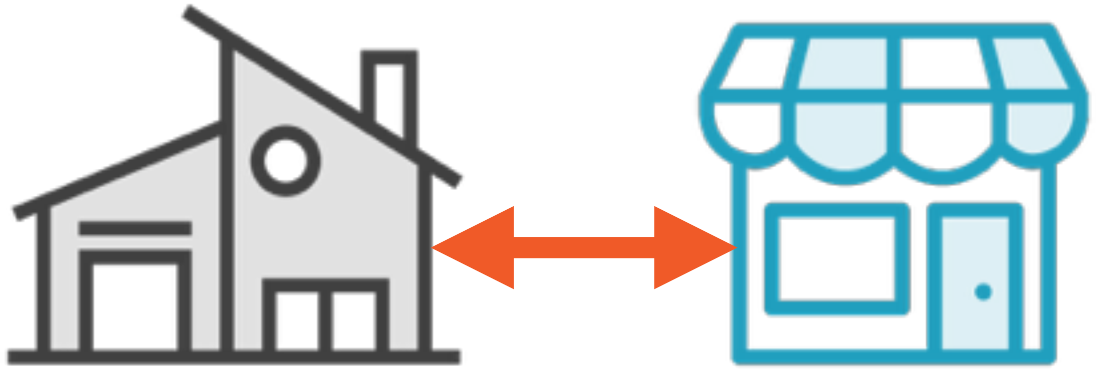

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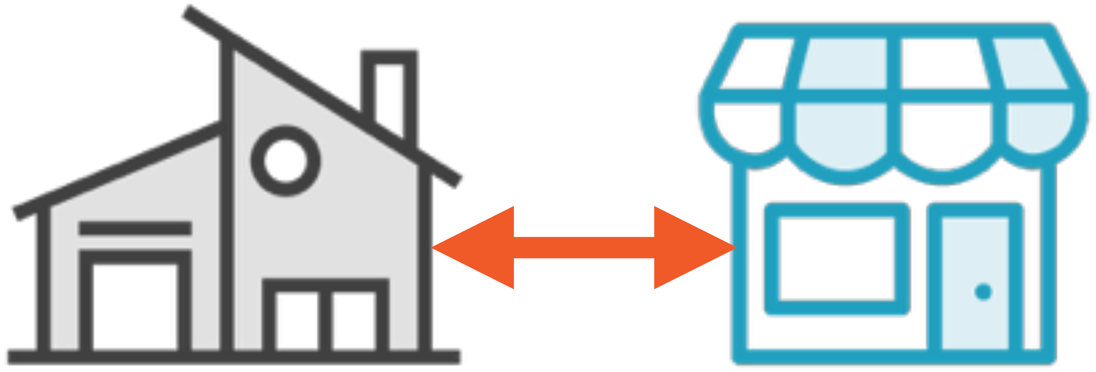

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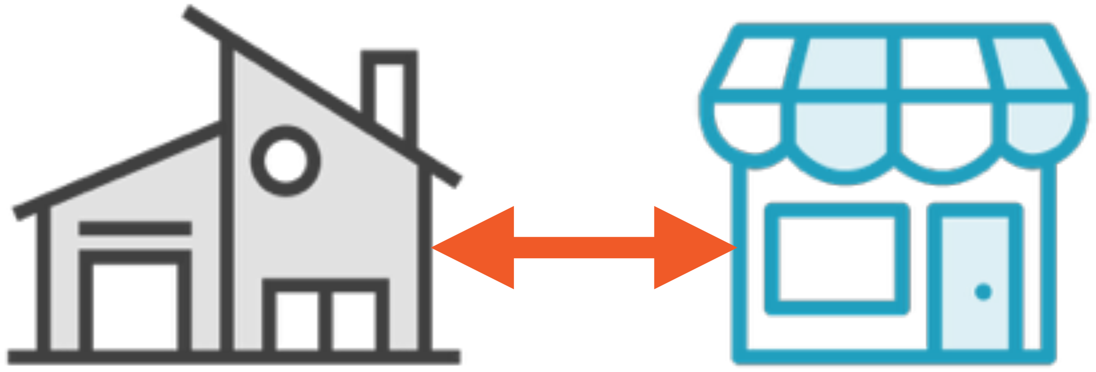
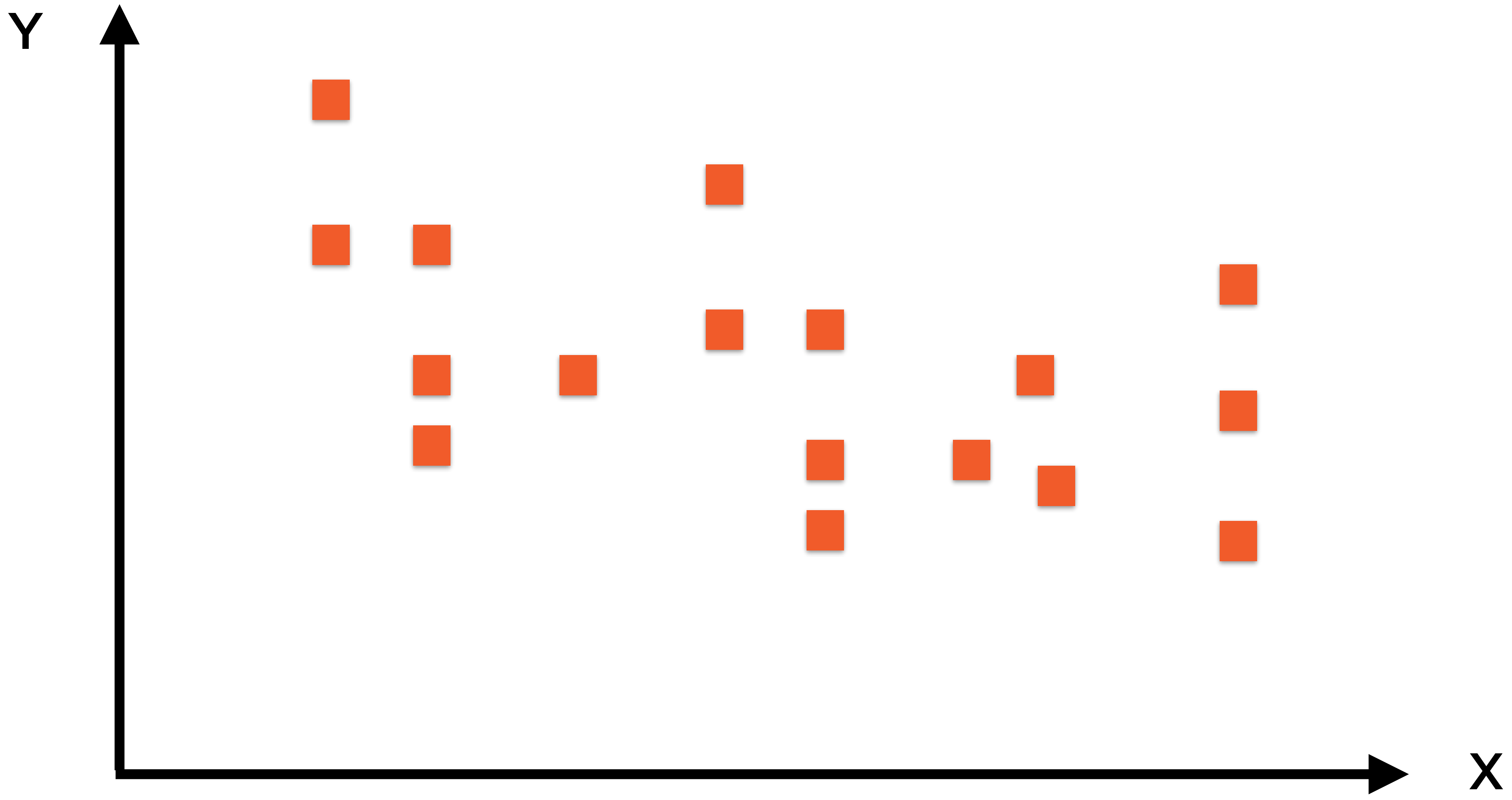
Distance Measures



$$\text{L2 Distance}(t1,\ t2) = \text{sqrt}(\text{sum}((t1_i - t2_i)^2))$$

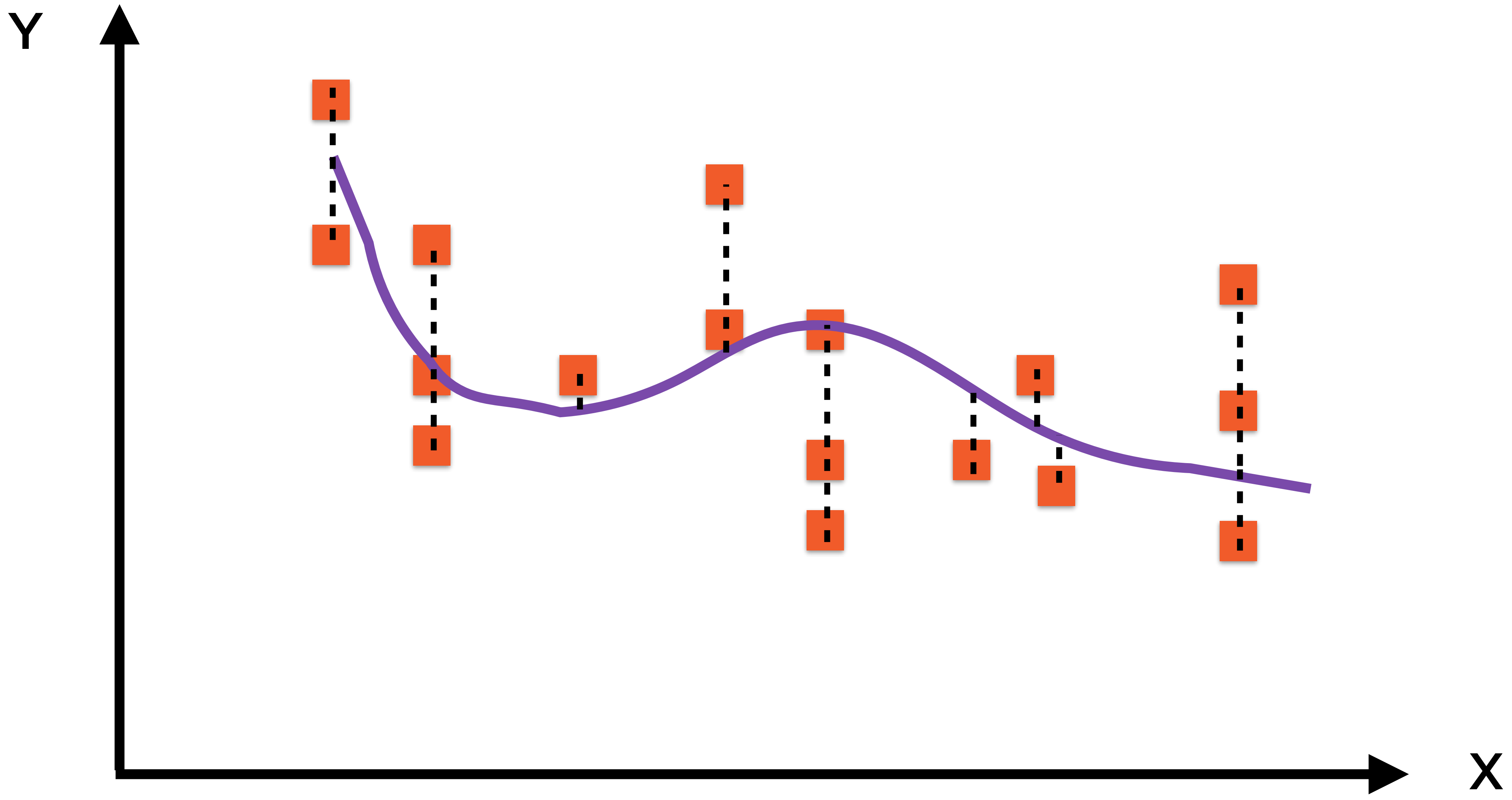
Bias-variance Trade-off

Connecting the Dots



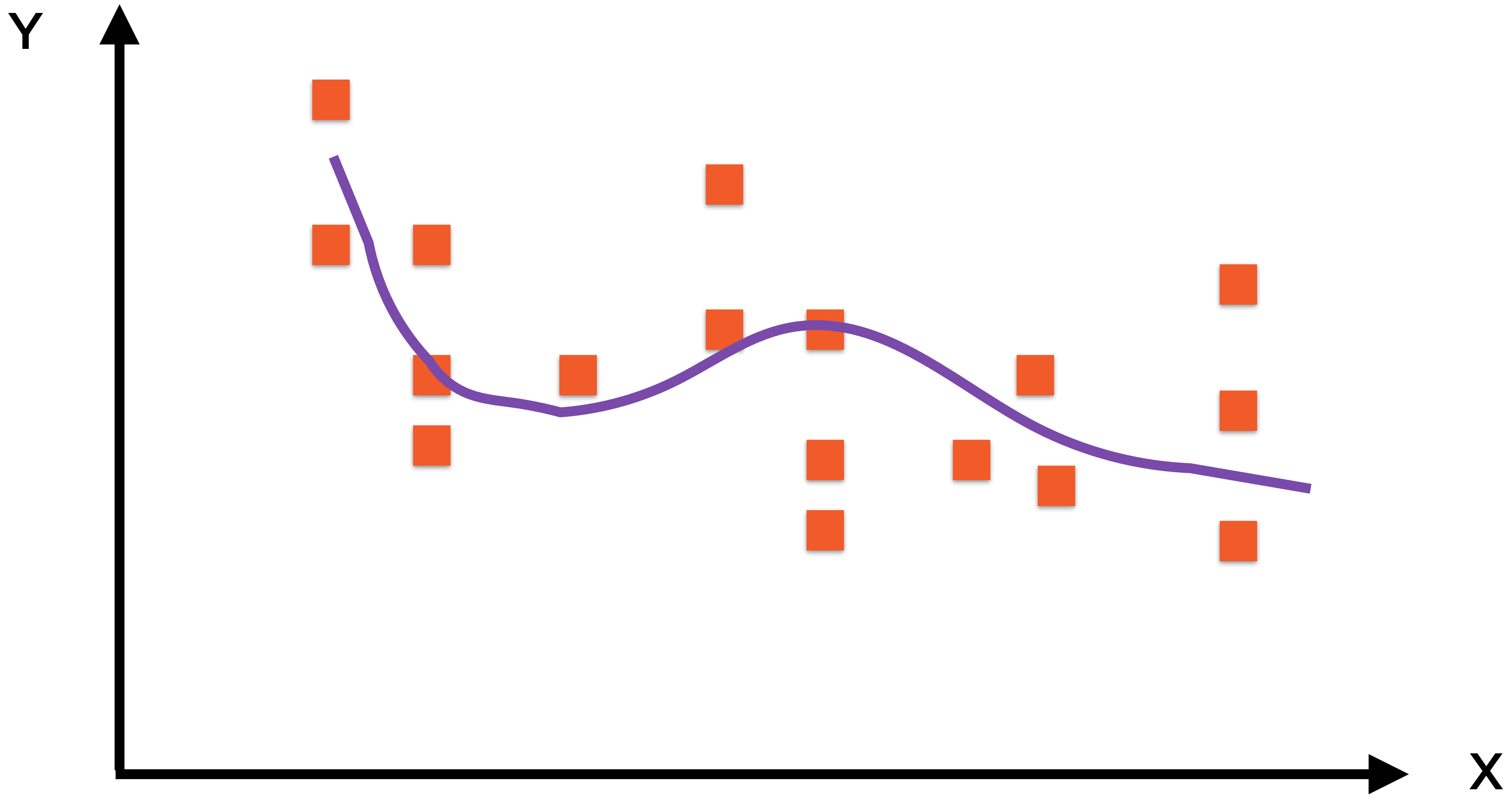
Challenge: Fit the "best" curve through these points

Good Fit?



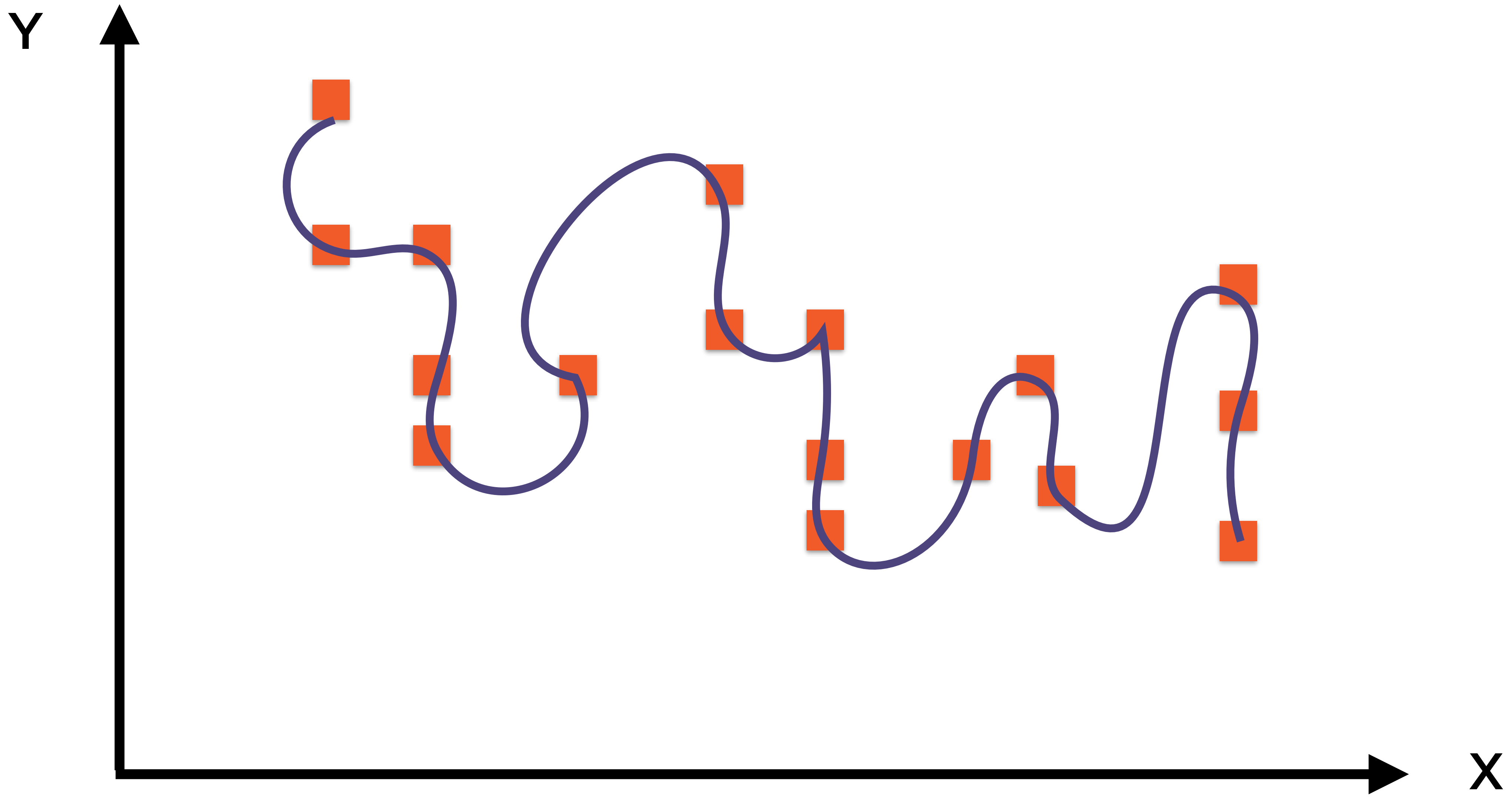
A curve has a "good fit" if the distances of points from the curve are small

Connecting the Dots



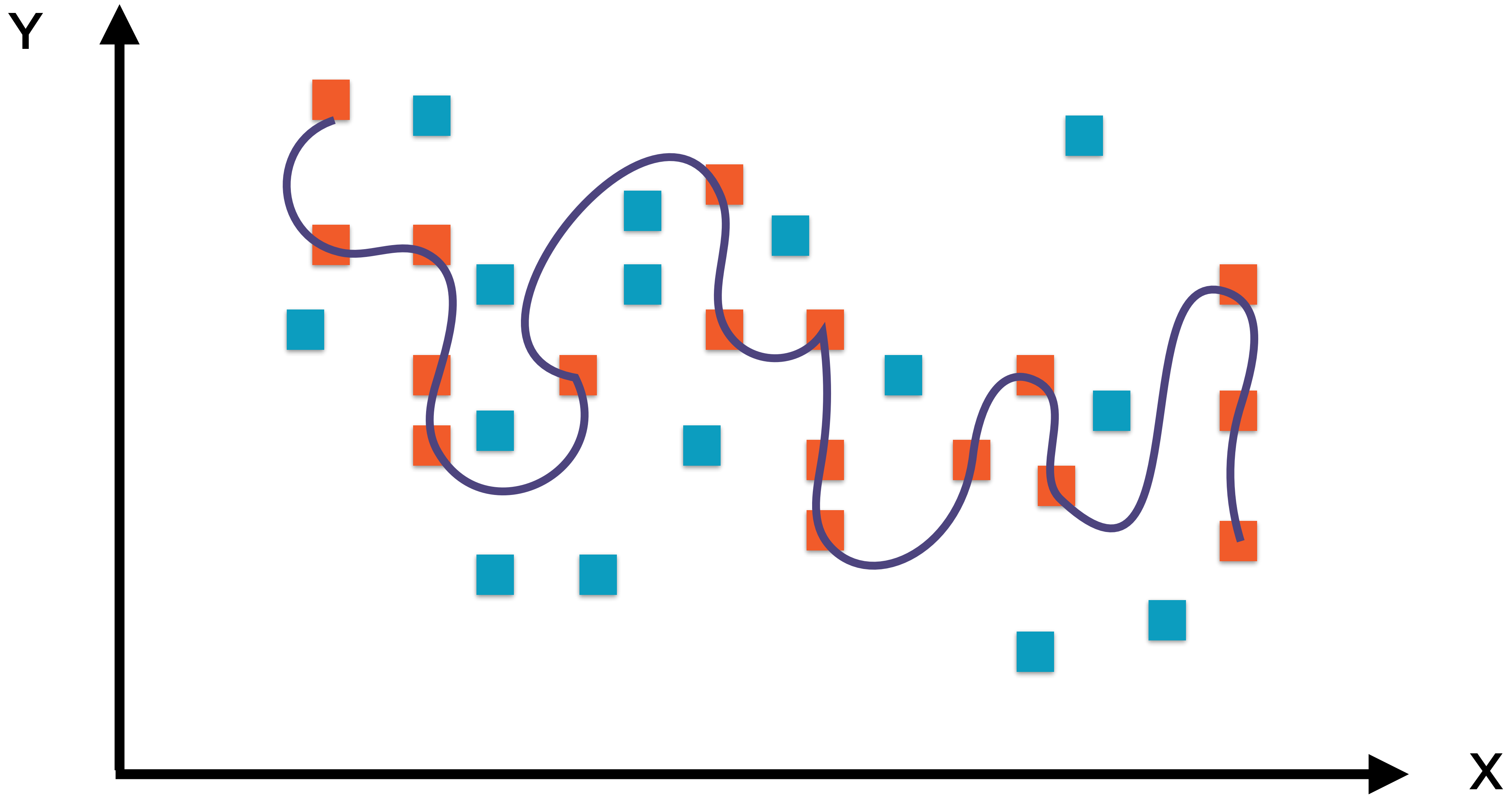
We could draw a pretty complex curve

Connecting the Dots



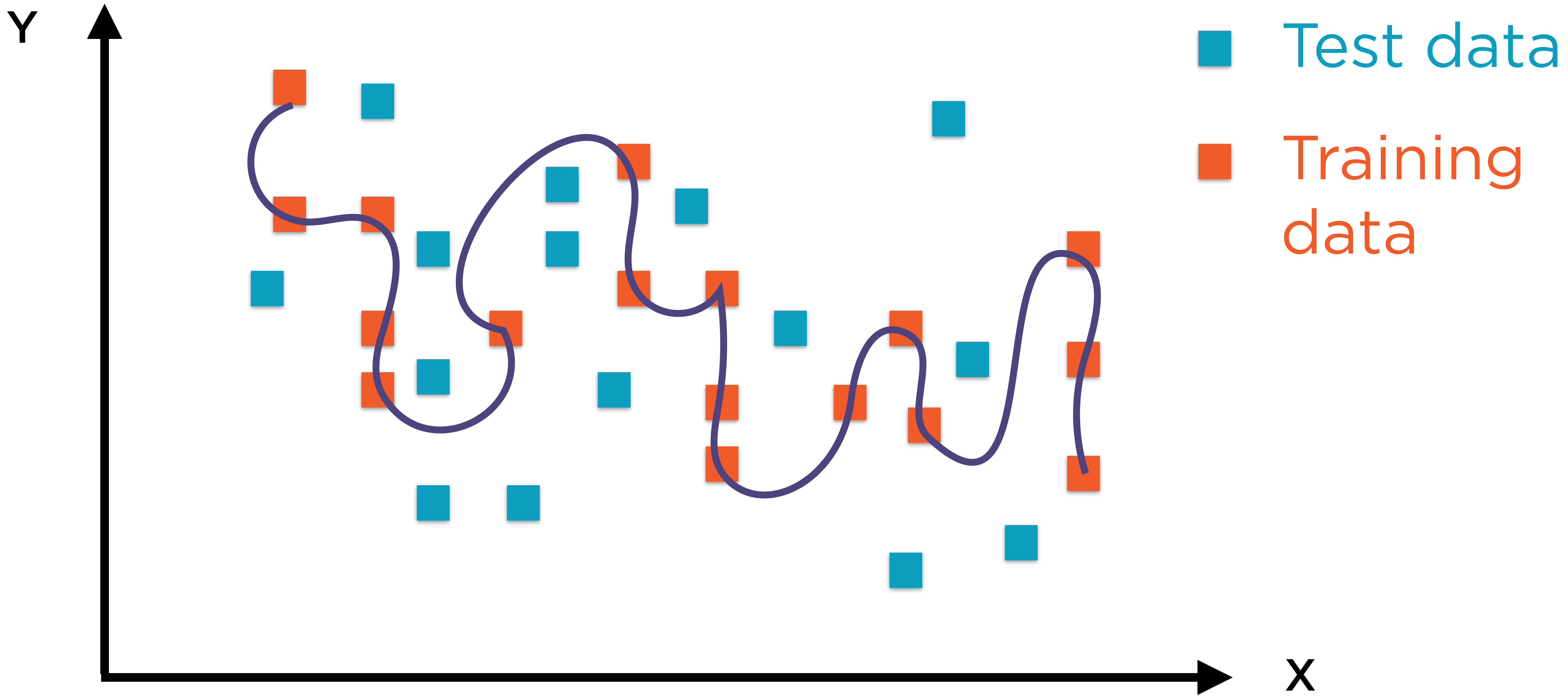
We can even make it pass through every single point

Connecting the Dots



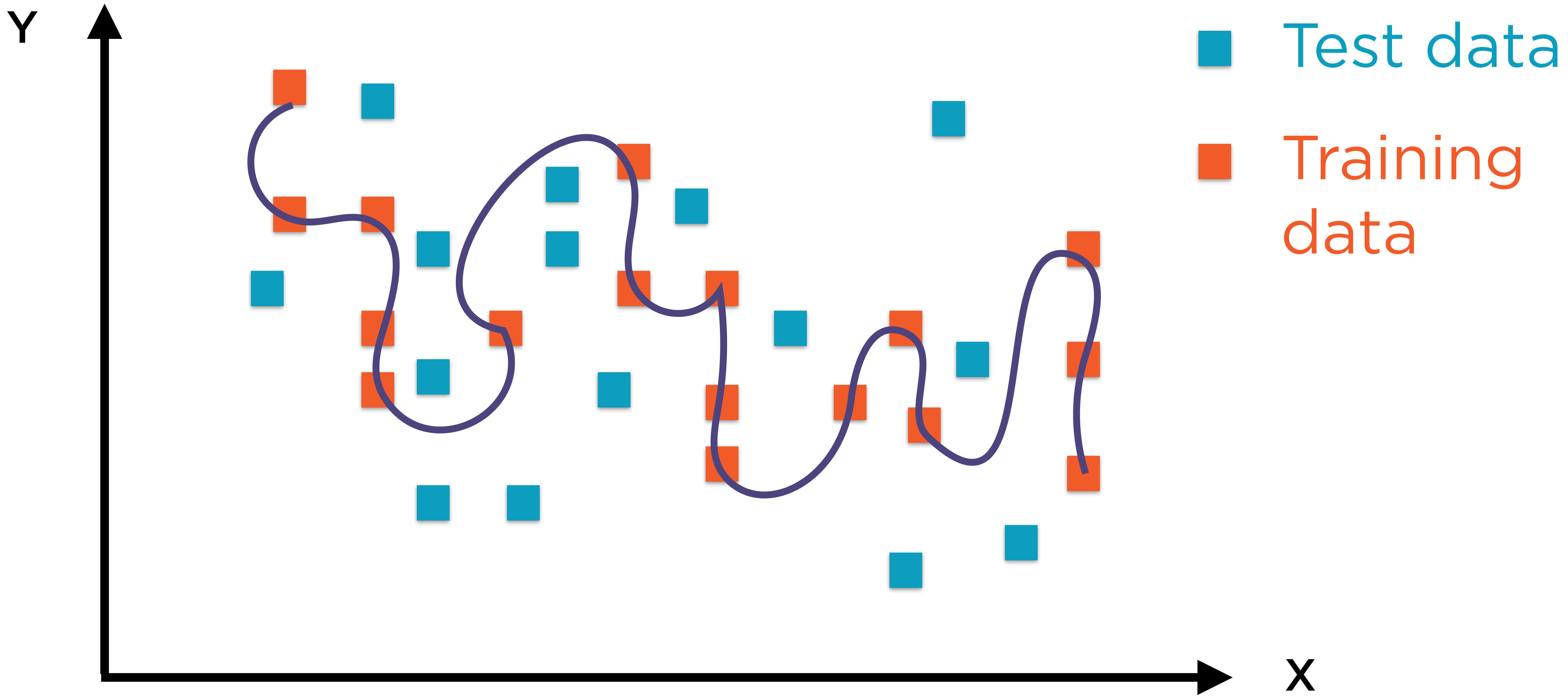
But given a new set of points, this curve might perform quite poorly

Connecting the Dots



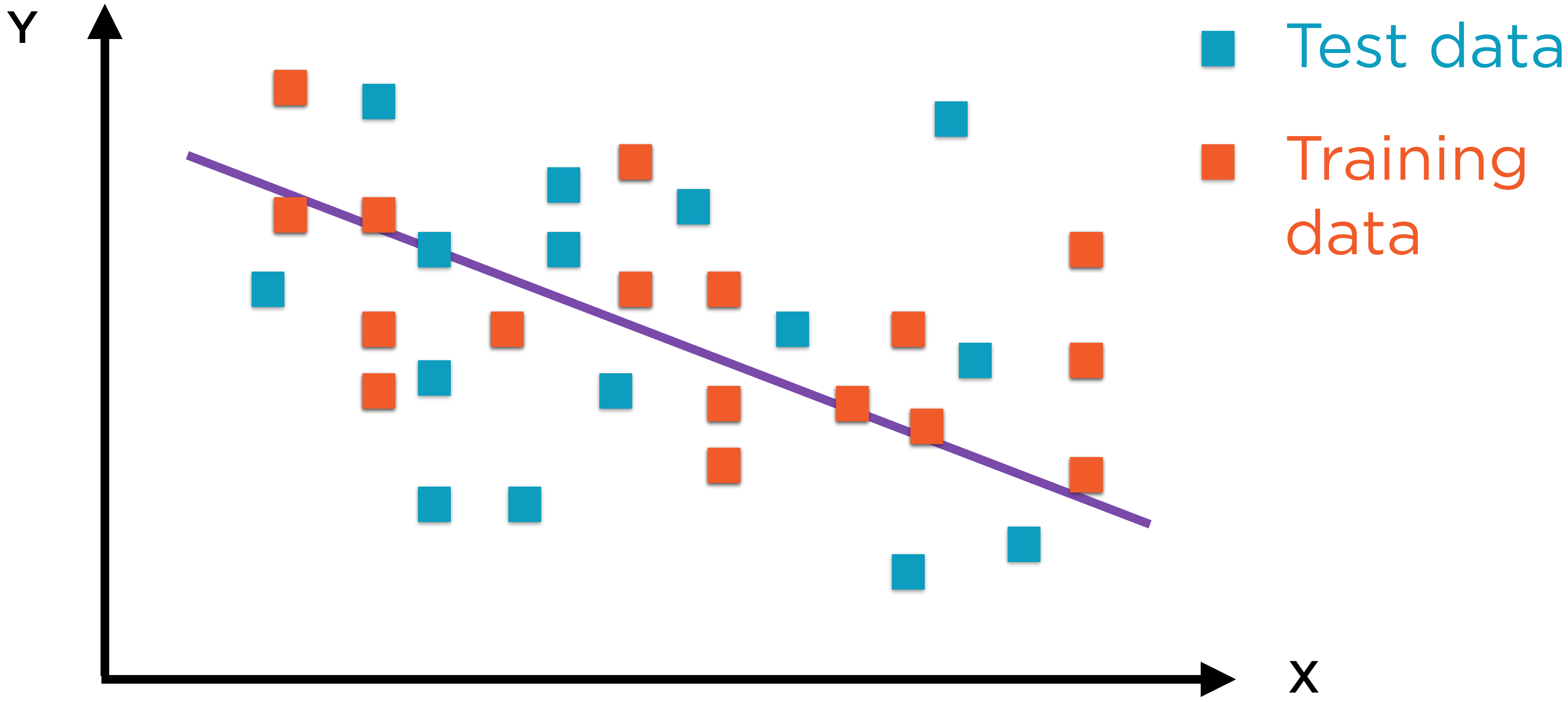
The original points were "training data", the new points are "test data"

Overfitting



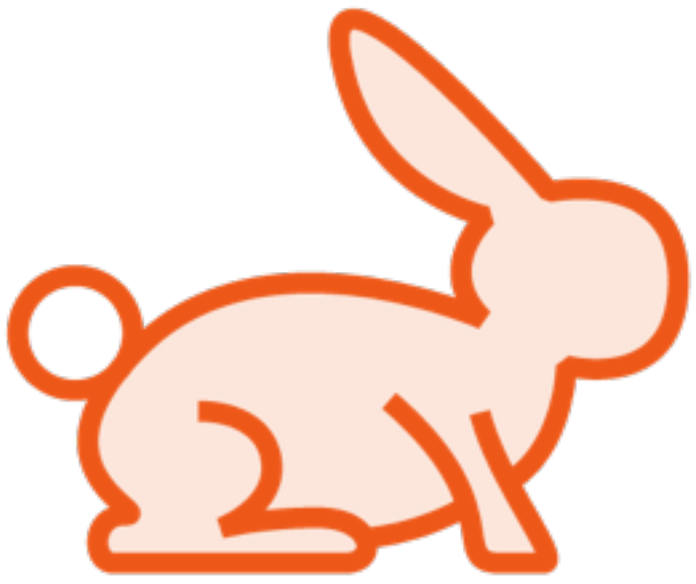
Great performance in training, poor performance in real usage

Connecting the Dots



A simple straight line performs worse in training, but better with test data

Overfitting

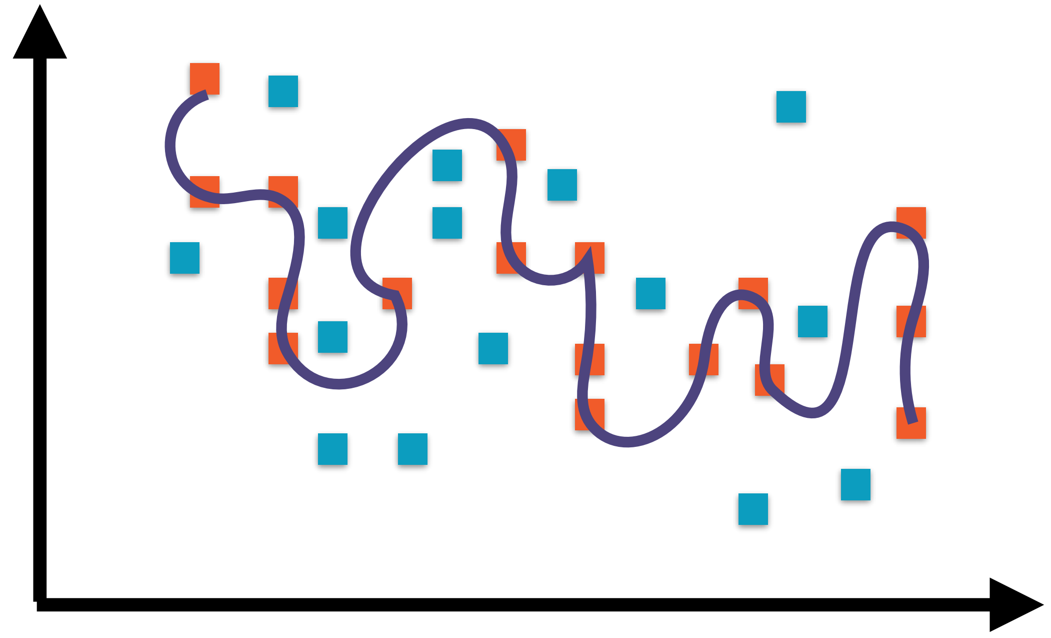


Low Training Error

Model does very well in training...

High Test Error

...but poorly with real data



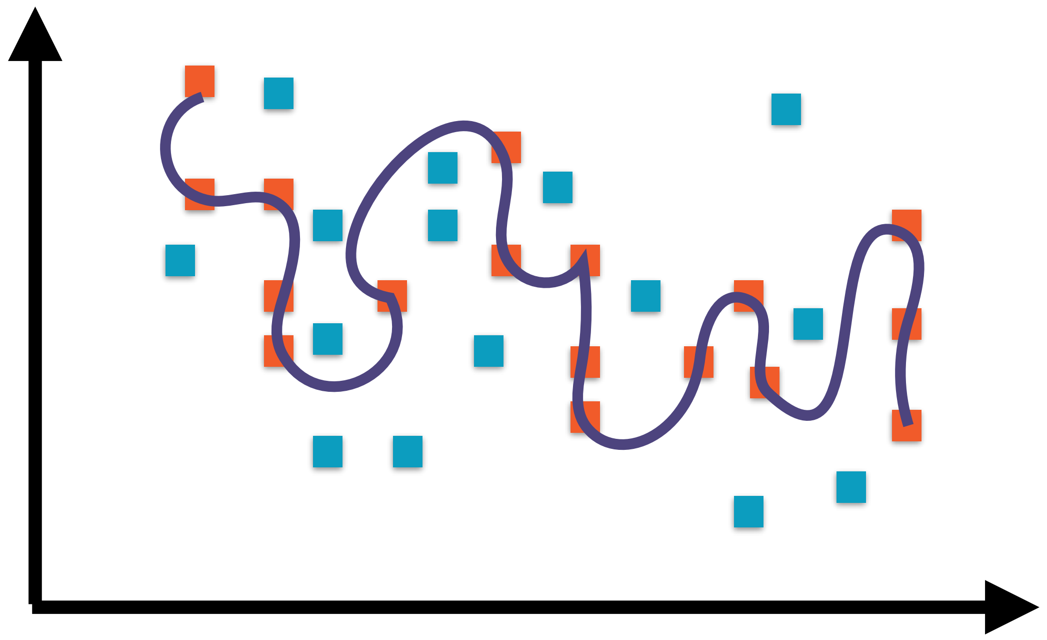
Cause of Overfitting

Sub-optimal choice in the bias-variance trade-off

An overfitted model has:

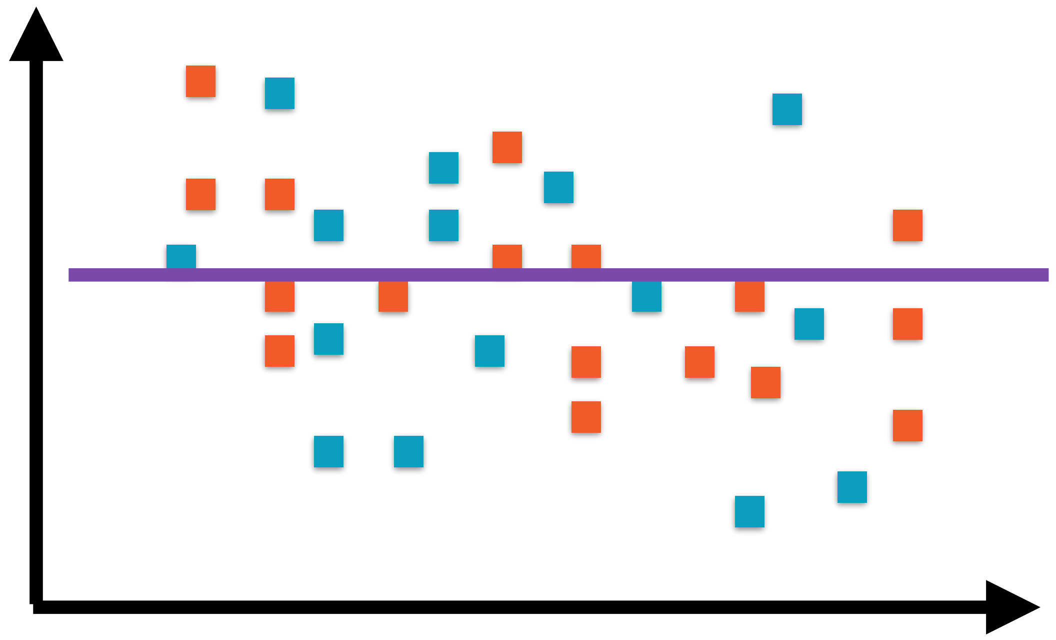
- high variance error
- low bias error

Bias



Low bias

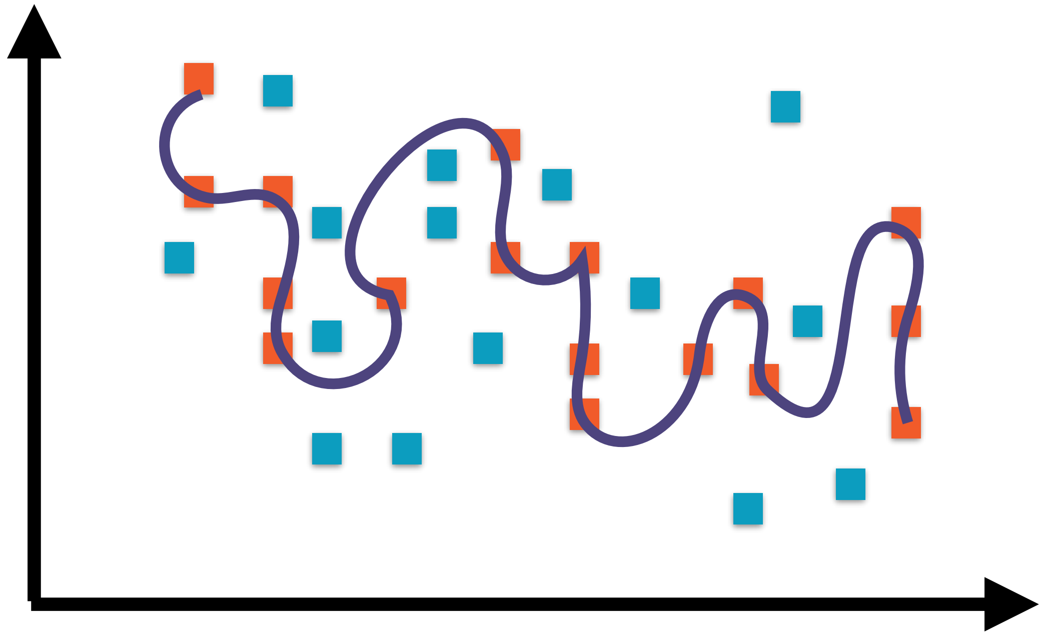
Few assumptions about the underlying data



High bias

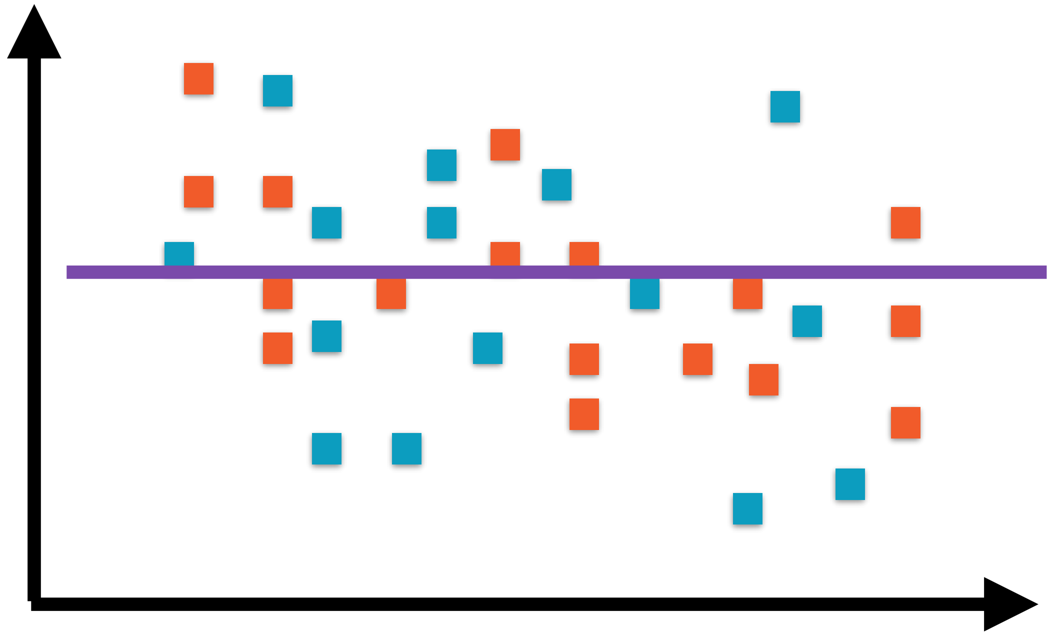
More assumptions about the underlying data

Bias



Model too complex

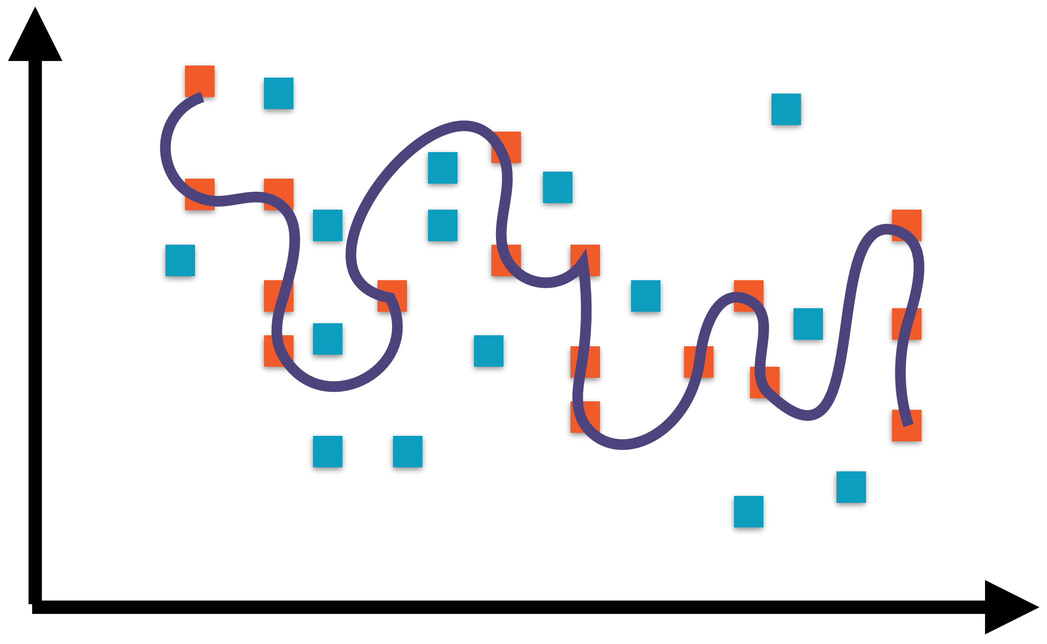
Training data all-important, model parameter counts for little



Model too simple

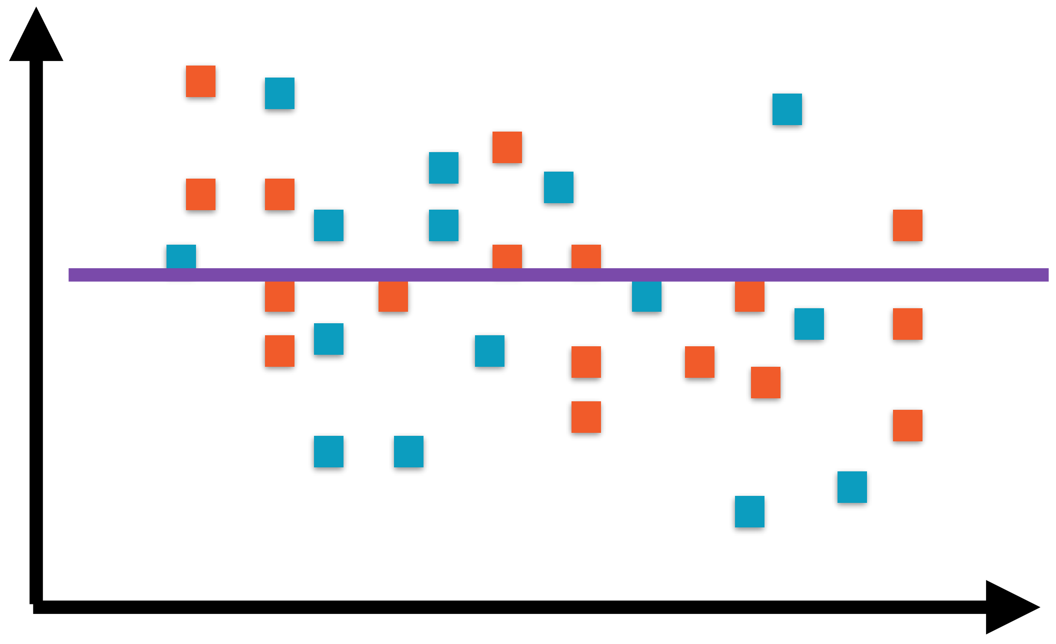
Model parameter all-important, training data counts for little

Variance



High variance

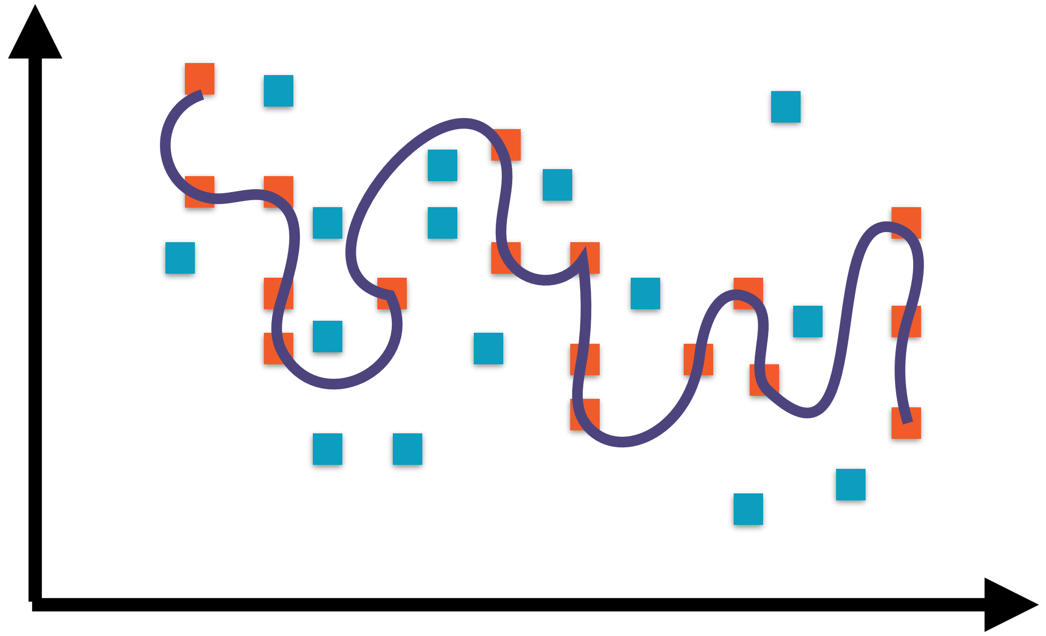
The model changes significantly when training data changes

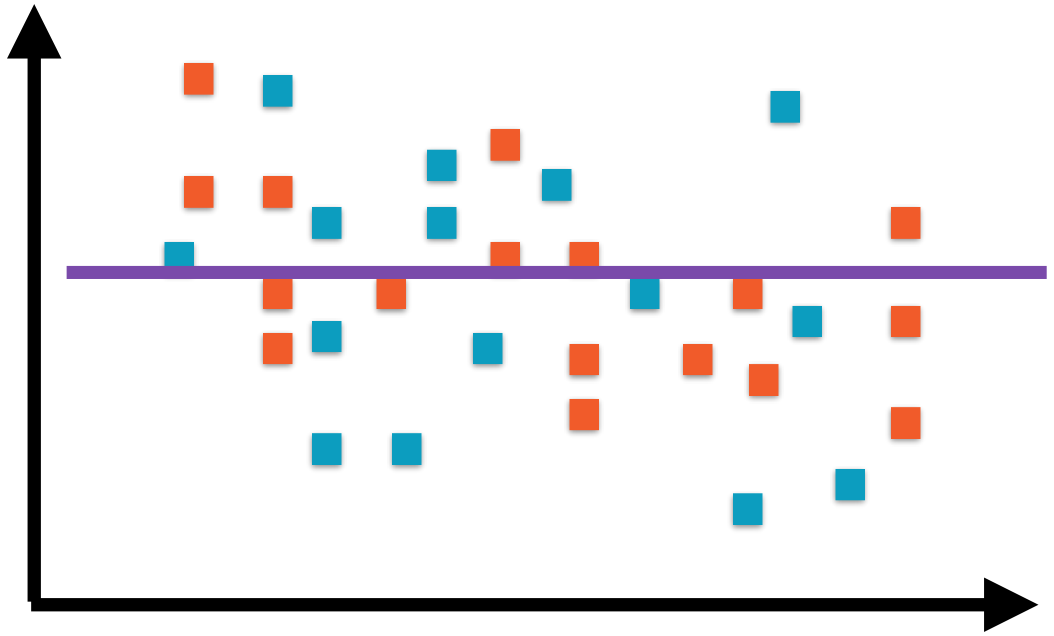


Low variance

The model doesn't change much when the training data changes

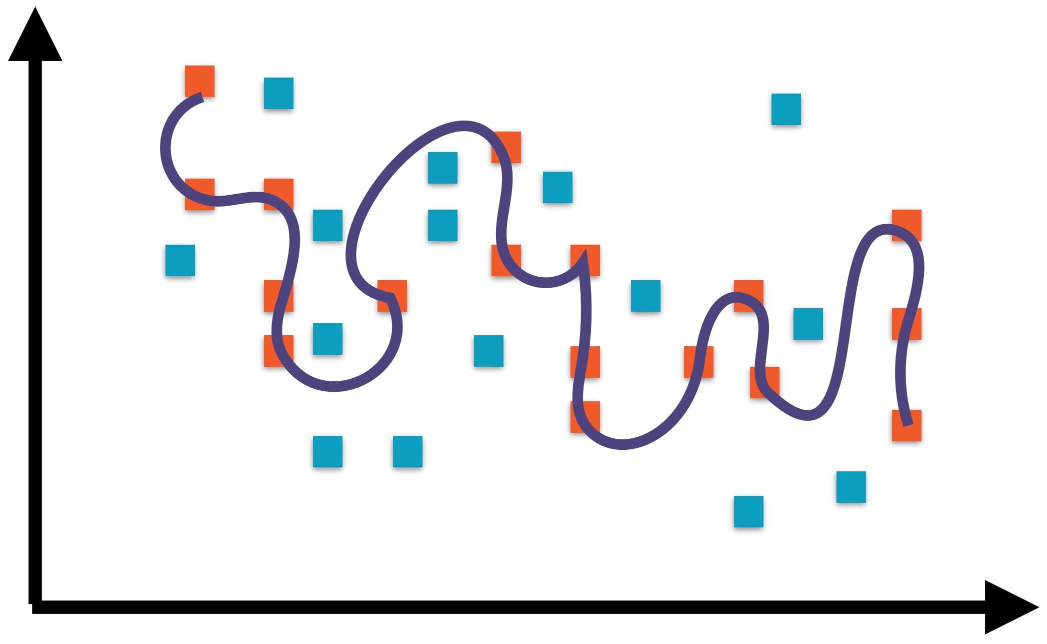
Variance





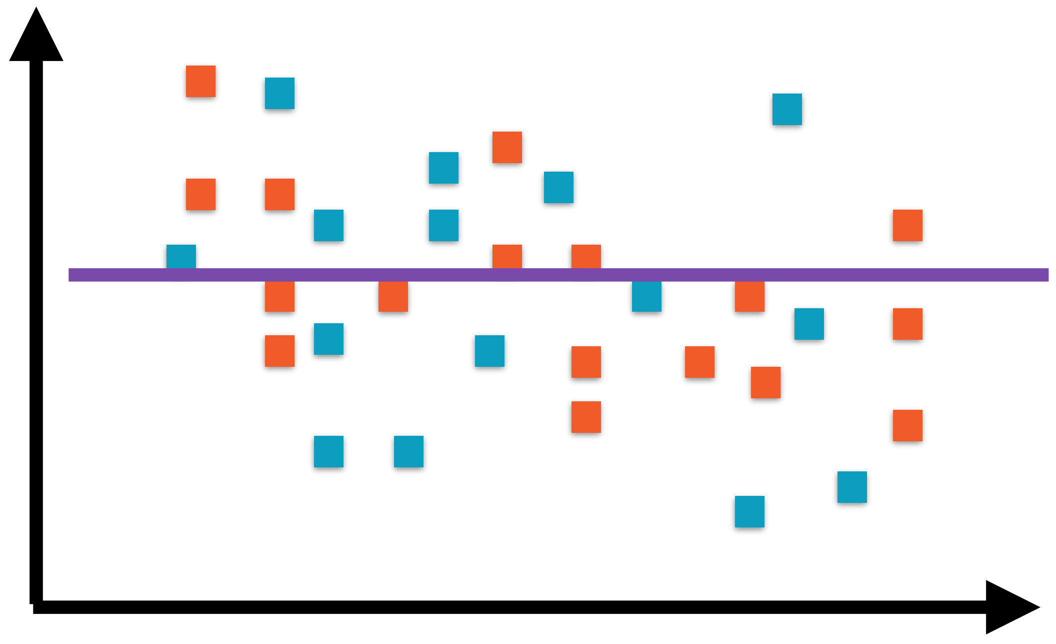
Model too complex	Model too simple
Model varies too much with changing training data	Model not very sensitive to training data

Bias-variance Trade-off



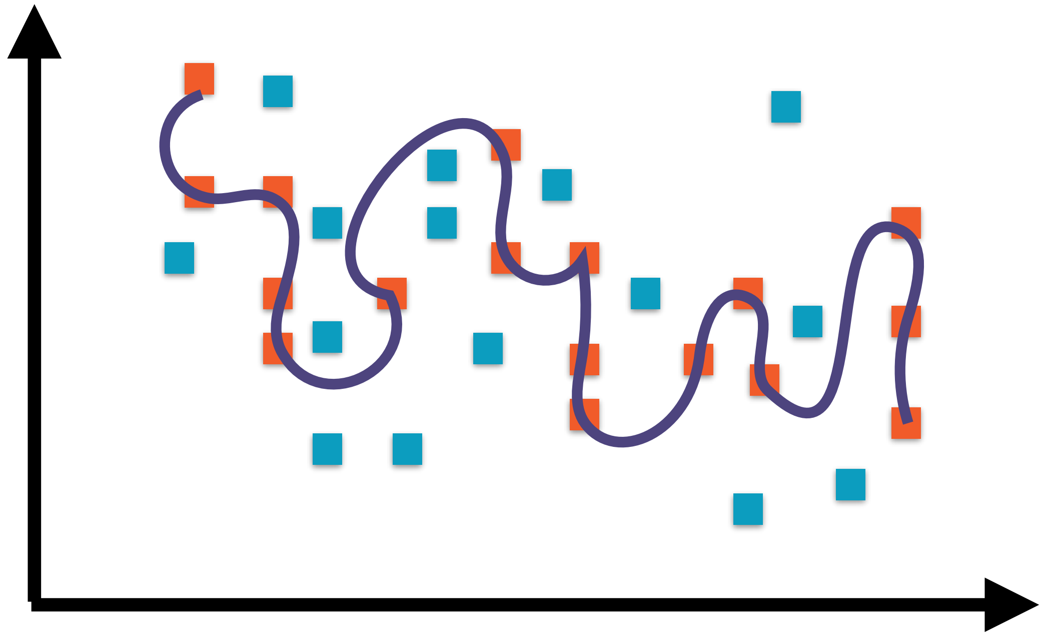
Model too complex

High variance error



Model too simple

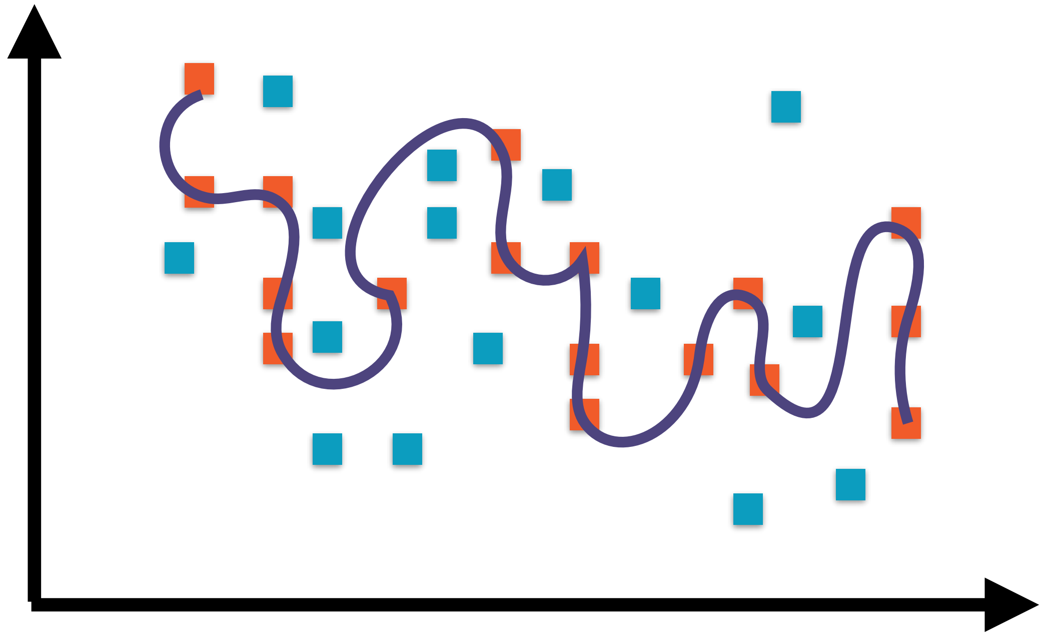
High bias error



Bias-variance Trade-off

- **High-bias algorithms: simple parameters**
  - **Regression**
- **High-variance algorithms: complex parameters**
  - **Decision trees**
  - **Dense neural networks**

Overfitting, Dropout and Regularization



Preventing Overfitting

- **Regularization**
- **Cross-validation**
- **Ensemble learning**
  - **Dropout**

Preventing Overfitting

Regularization - Penalize complex models

Cross-validation - Distinct training and validation phases

Dropout (NNs only) - Intentionally turn off some neurons during training

Regularization

Penalize complex models

Add penalty to objective function

Penalty as function of regression coefficients

Forces optimizer to keep it simple

Cross-Validation

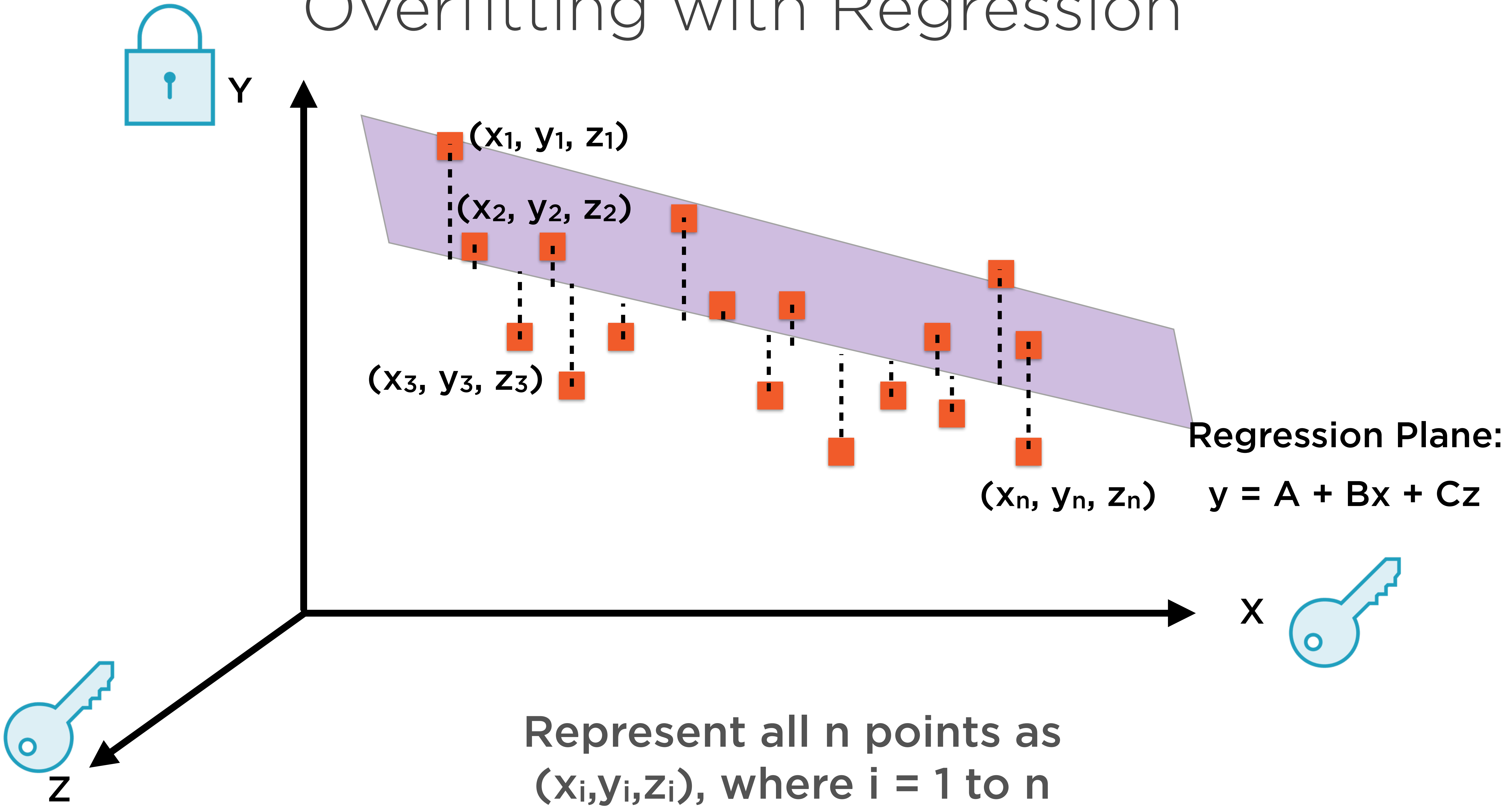
Distinct training and validation phases

Train different models (with training data only)

Select model that does best on validation data

“Hyperparameter tuning”

Overfitting with Regression



Represent all n points as (x_i,y_i,z_i), where i = 1 to n

Multiple Regression

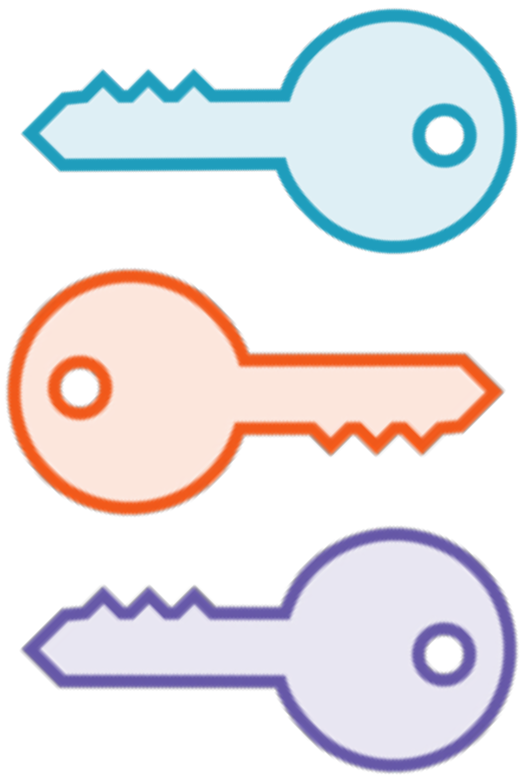
Regression Equation:

$$y = C_1 + C_2 x_1 + \ldots + C_{k+1} x_k$$

Linear regression involves finding k+1 coefficients, k for the explanatory variables, and 1 for the intercept

A big risk with regression is **multicollinearity**: X variables containing the same information

Success as a Salesperson



Causes

Number of cold calls, years of experience in sales jobs

Effect

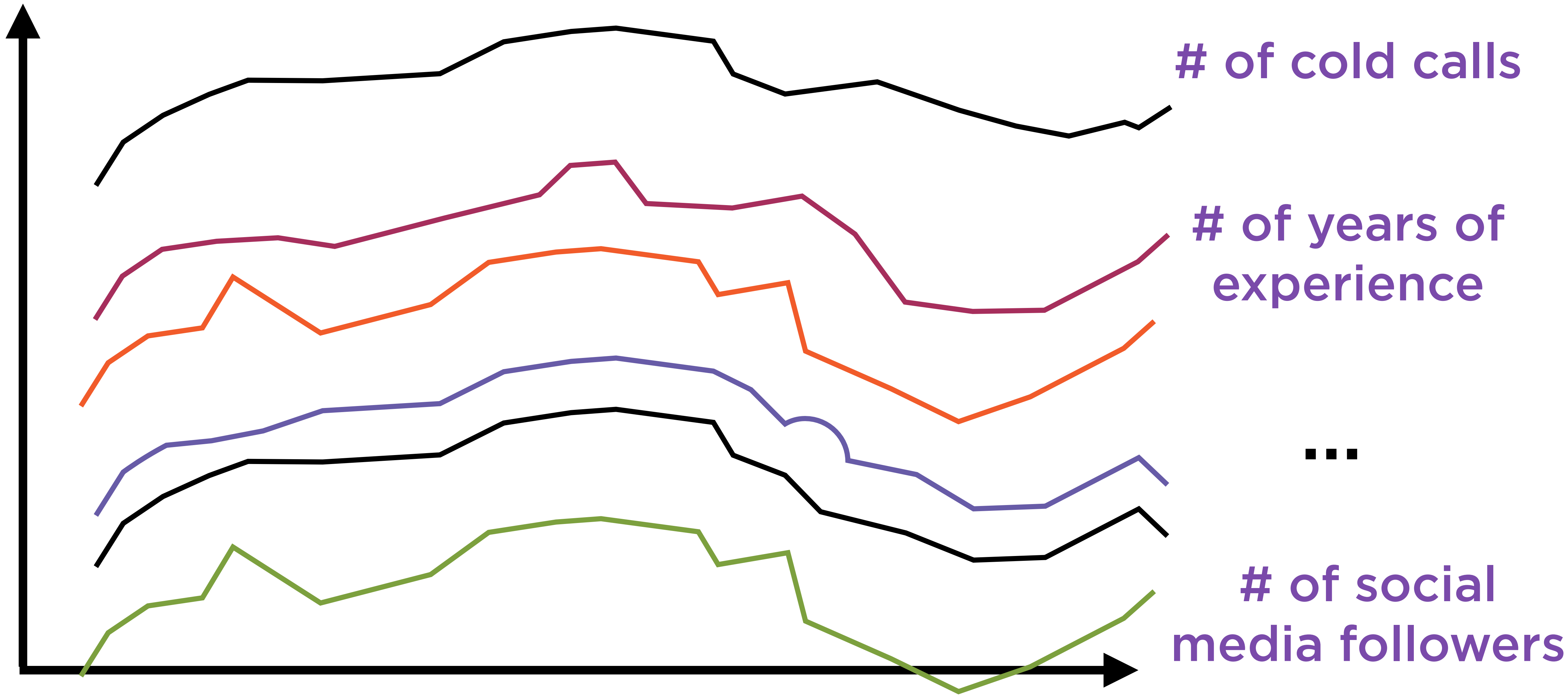
Bonus as member of sales team

Kitchen Sink Regression

Proposed Regression Equation:

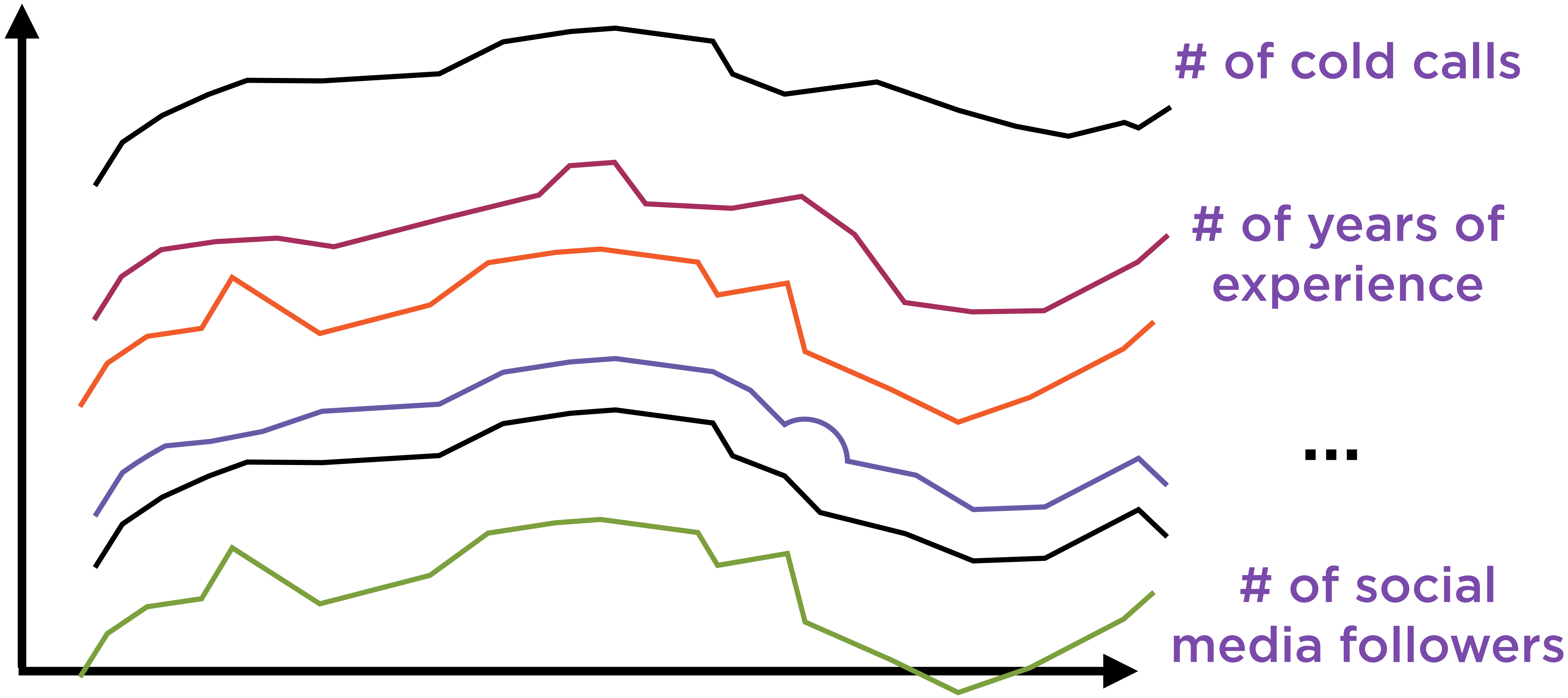
BONUS = A + B COLDCALLS + C EXPERIENCE + D NUMFOLLOWERS + E HONESTY + F PUNCTUALITY + ...

Bad News: Multicollinearity Detected



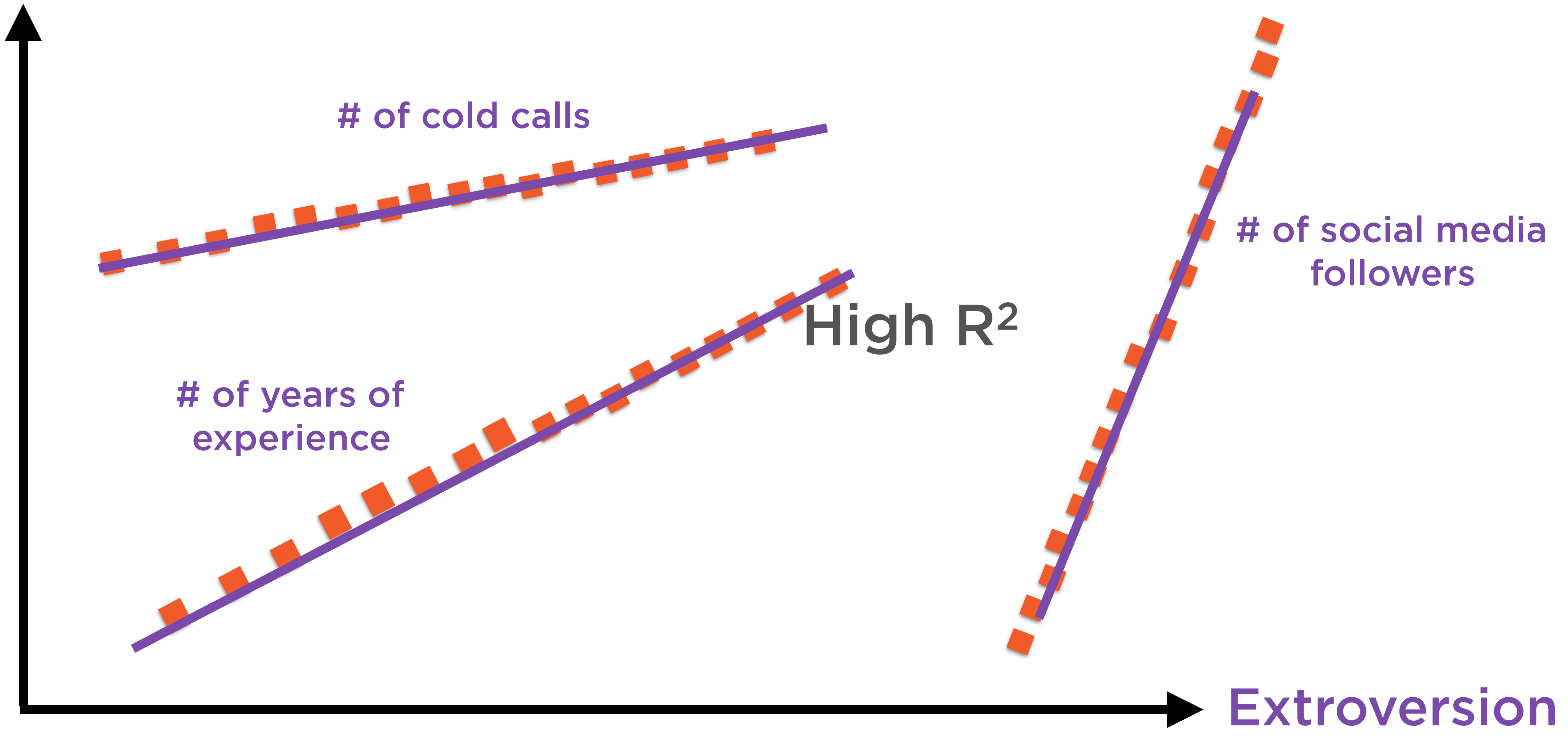
6 of 10 explanatory variables are highly correlated with each other

Underlying Cause: Extroversion



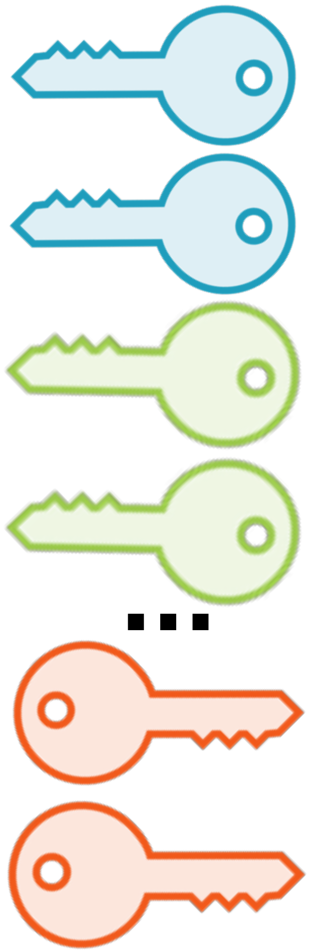
Each of these explanatory variables is caused by an underlying personality trait

Underlying Cause: Extroversion



Simply measure extroversion and use it instead of the correlated explanatory variables

Kitchen Sink Regression



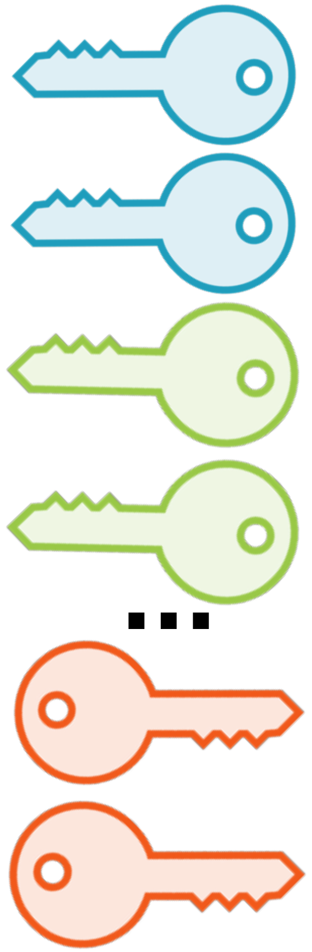
10 Causes

Cold calls, experience, social media followers, perceived honesty, billing punctuality...

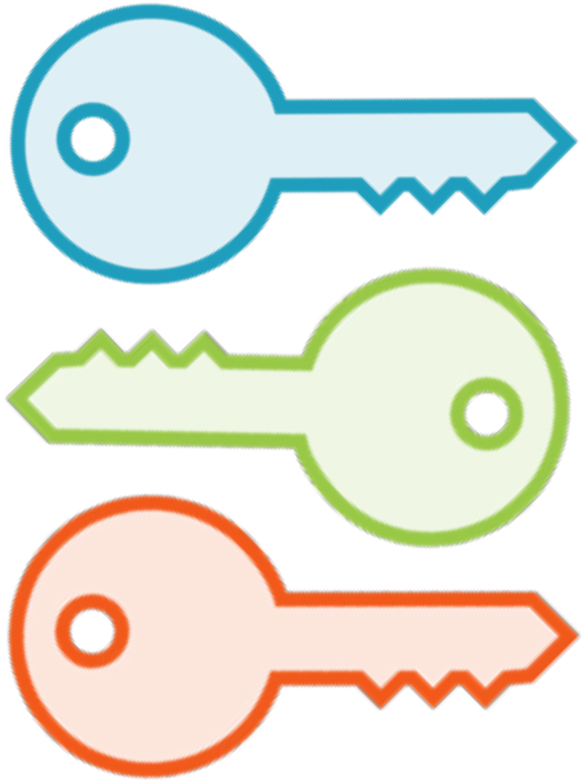
1 Effect

Bonus in sales team

Factor Analysis

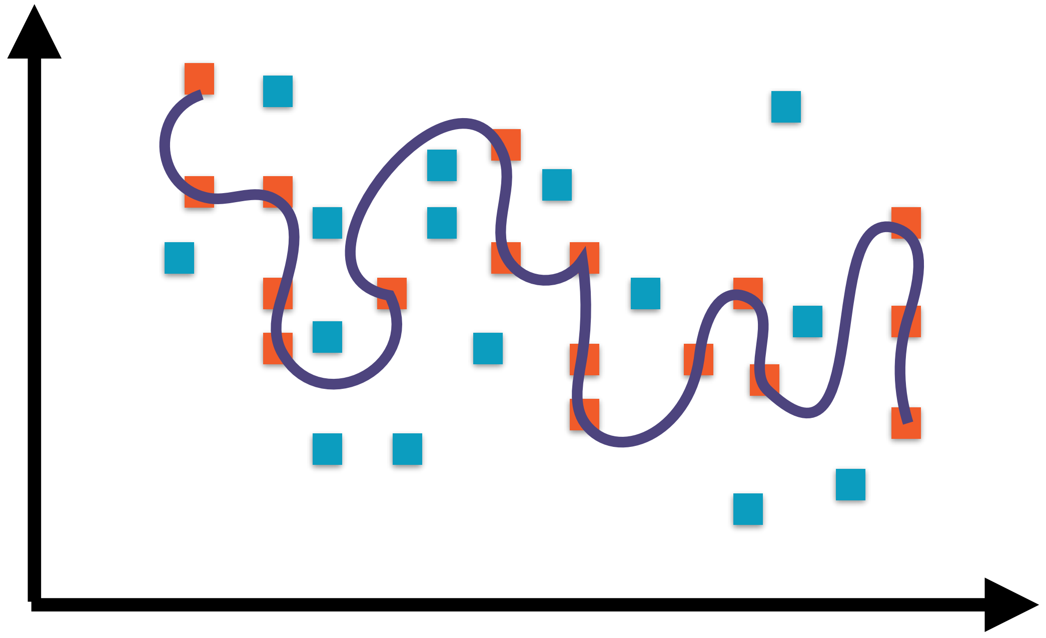


Many Observed Causes



Few Underlying Causes

One Effect



Overfitting in Regression

Multi-collinearity in regression leads to overfitting

Model performs well in training, poorly in prediction

Various techniques to improve regression algorithm

Preventing Overfitting

Regularized Regression Models

Lasso Regression

Penalizes large regression coefficients

Ridge Regression

Also penalizes large regression coefficients

Elastic Net Regression

Simply combines lasso and ridge

Regularization

Penalize complex models

Add penalty to objective function

Penalty as function of regression coefficients

Forces optimizer to keep it simple

Regularization

Regularization reduces variance error

But increases bias

Ordinary MSE Regression

Minimize

$$\sqrt{(y^{actual} - y^{predicted})^2}$$

To find

A, B

The value of A and B define the "best fit" line

y = A + Bx

Lasso Regression

Minimize $\sqrt{(y^{actual} - y^{predicted})^2}$ $+ \alpha\ (|A| + |B|)$

To find

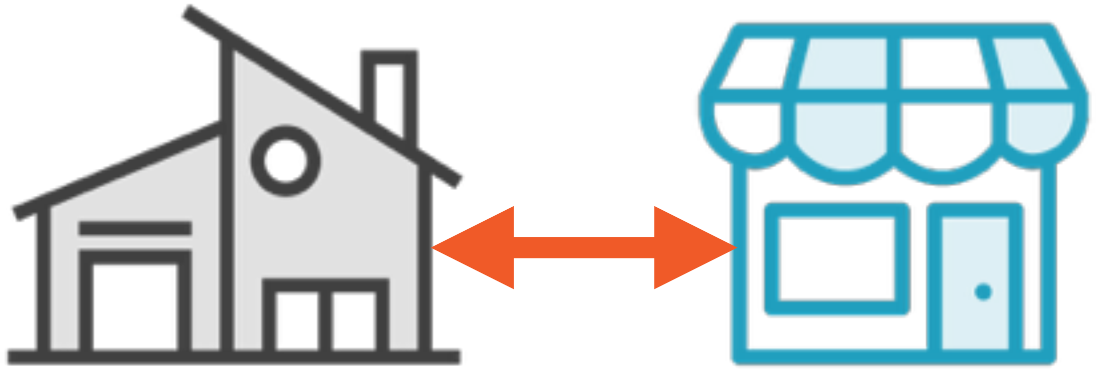
A, B

α is a hyperparameter

The value of A and B still define the "best fit" line

$y = A + Bx$

L-1 Norm



$$L1\text{-}Norm(A, B_1, B_2 \dots B_n) = |A|^1 + |B_1|^1 + |B_2|^1 \dots + |B_n|^1$$

Lasso Regression

Minimize $\sqrt{(y^{actual} - y^{predicted})^2}$ $+\alpha\ (|A| + |B|)$

To find

A, B

α is a hyperparameter

The value of A and B still define the "best fit" line

$$y = A + Bx$$

Lasso Regression

Minimize

$$\sqrt{(y^{actual} - y^{predicted})^2} + \alpha\,(|A| + |B|)$$

L-1 Norm of regression coefficients

To find

A, B

α is a hyperparameter

The value of A and B still define the “best fit” line

$y = A + Bx$

Ridge Regression

Minimize $\sqrt{(y^{actual} - y^{predicted})^2}$ $+ \alpha (|A|^2 + |B|^2)$

L-2 Norm of regression coefficients

To find

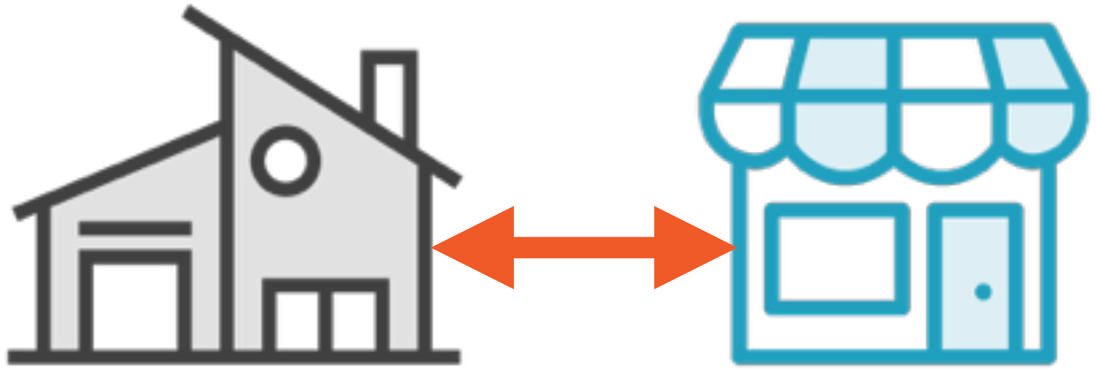
A, B

α is a hyperparameter

The value of A and B still define the “best fit” line

$y = A + Bx$

L-2 Norm



$$\text{L2-Norm}(A, B_1, B_2 \ldots B_n) = |A|^2 + |B_1|^2 + |B_2|^2 \ldots + |B_n|^2$$

Lasso Regression

Add penalty for large coefficients

Penalty term is L-1 norm of coefficients

Penalty weighted by hyperparameter α

Lasso Regression

$\alpha = 0$ ~ Regular (MSE regression)

$\alpha \to \infty$ ~ Force small coefficients to zero

Model selection by tuning α

Eliminates unimportant features

Lasso Regression

"Lasso" ~ *L*east *A*bsolute *S*hrinkage and *S*election *O*perator

Math is complex

No closed form, needs numeric solution

Ridge Regression

Minimize $\sqrt{(y^{actual} - y^{predicted})^2}$ $+ \alpha\,(|A|^2 + |B|^2)$

L-2 Norm of regression coefficients

To find

A, B

α is a hyperparameter

The value of A and B still define the "best fit" line

$y = A + Bx$

Ridge Regression

Add penalty for large coefficients

Penalty term is L-2 norm of coefficients

Penalty weighted by hyperparameter α

Ridge Regression

Unlike lasso, ridge regression has closed-form solution

Unlike lasso, ridge regression will not force coefficients to 0

- Does not perform model selection

Demo

Implementing Lasso and Ridge regression in scikit-lean

Setting Up the SVM Regression Problem

SVMs are typically used for classification problems

SVRs use the same underlying principles with a **different objective function**

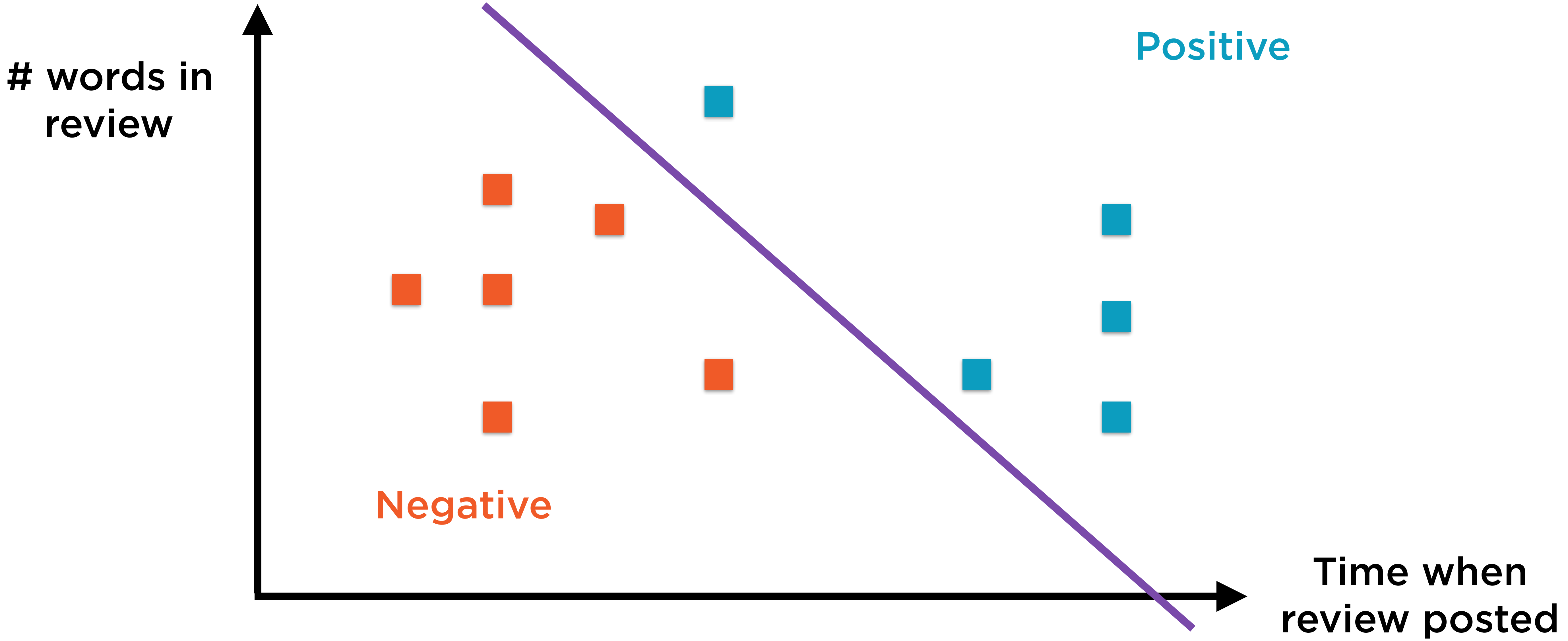
Data in One Dimension

Unidimensional data points can be represented using a line, such as a number line

Data in One Dimension

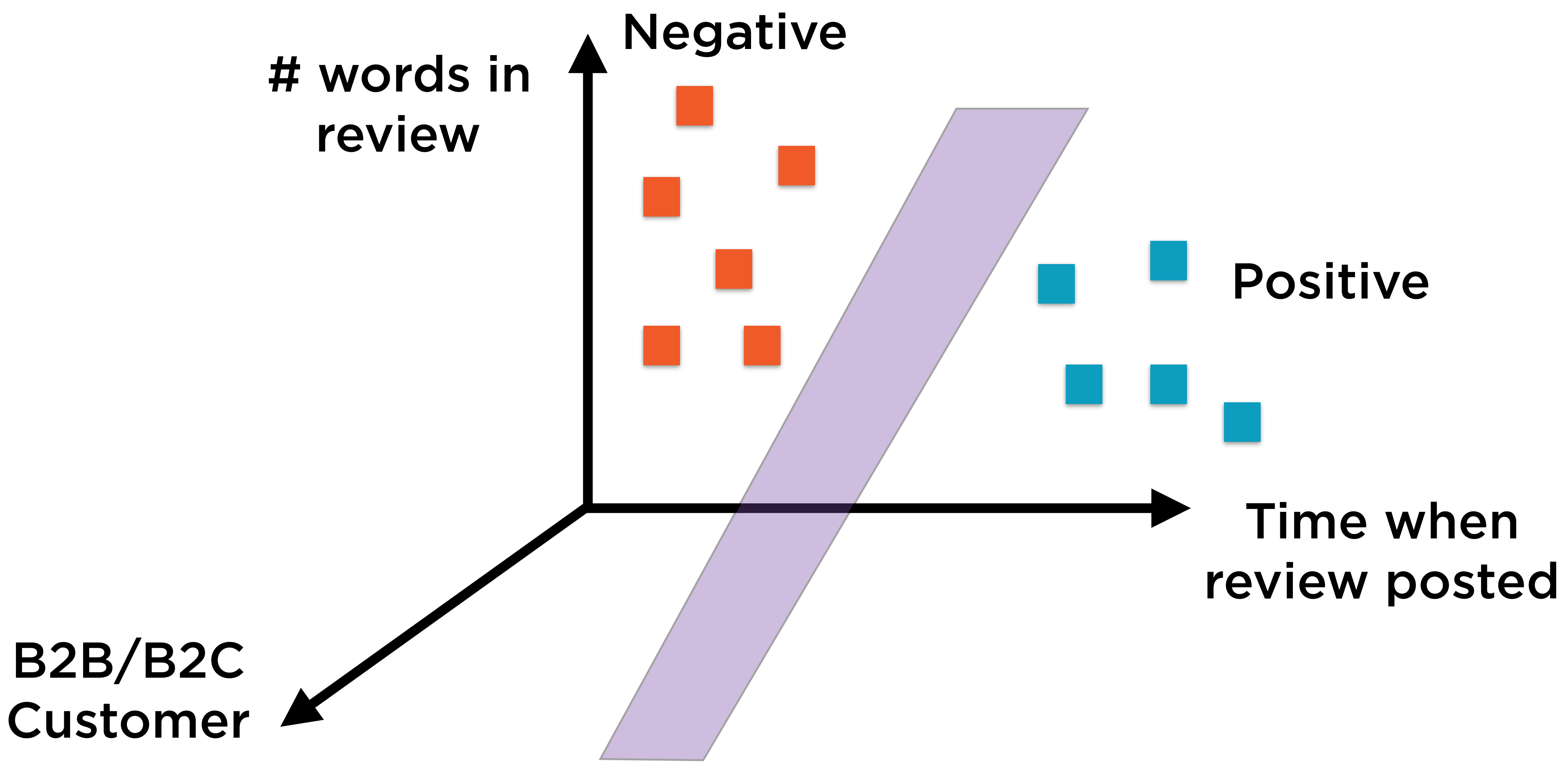
Unidimensional can also be separated, or classified, using a point

Data in Two Dimensions



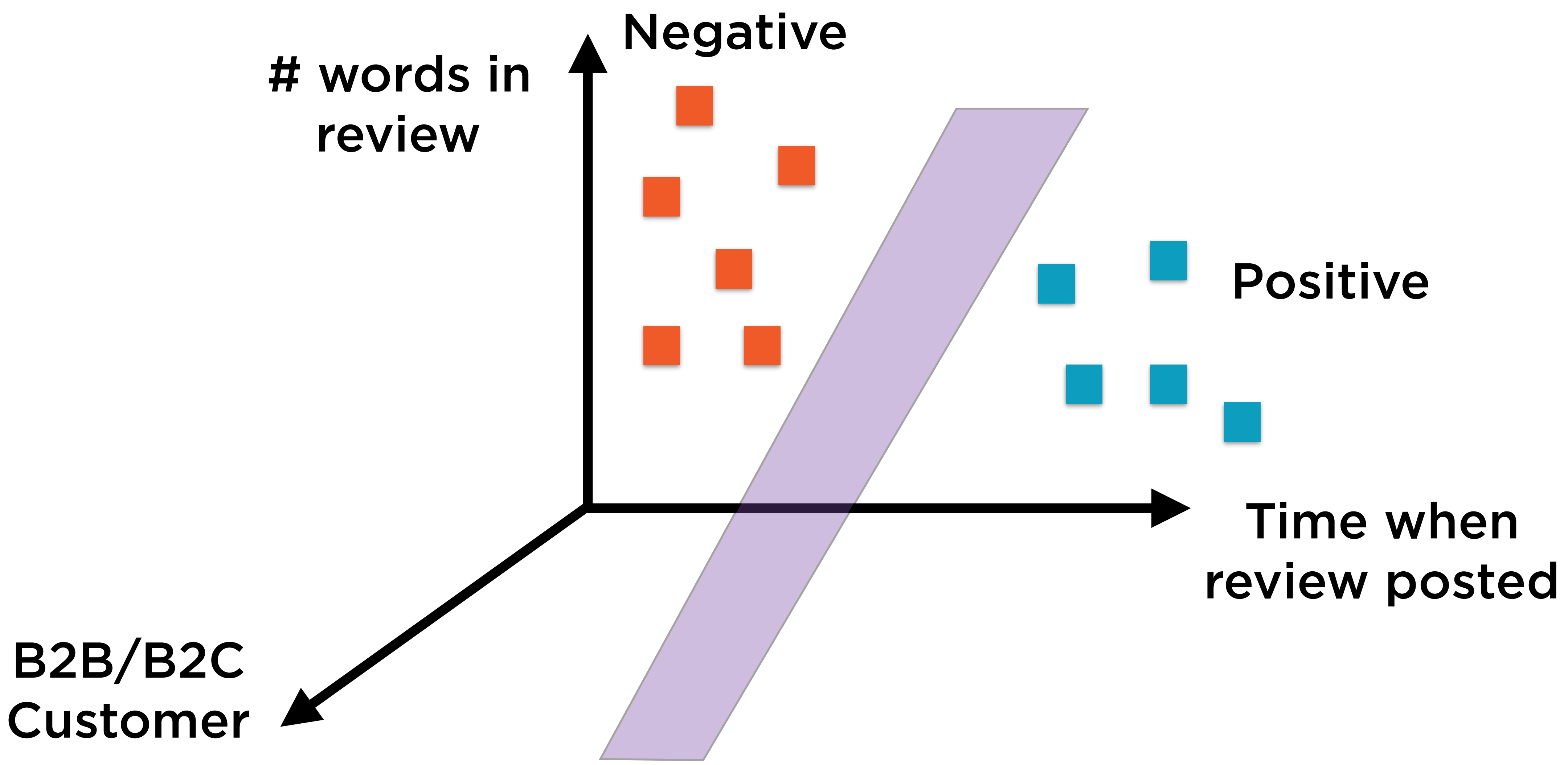
Bidimensional data points can be represented using a plane, and classified using a line

Data in N Dimensions



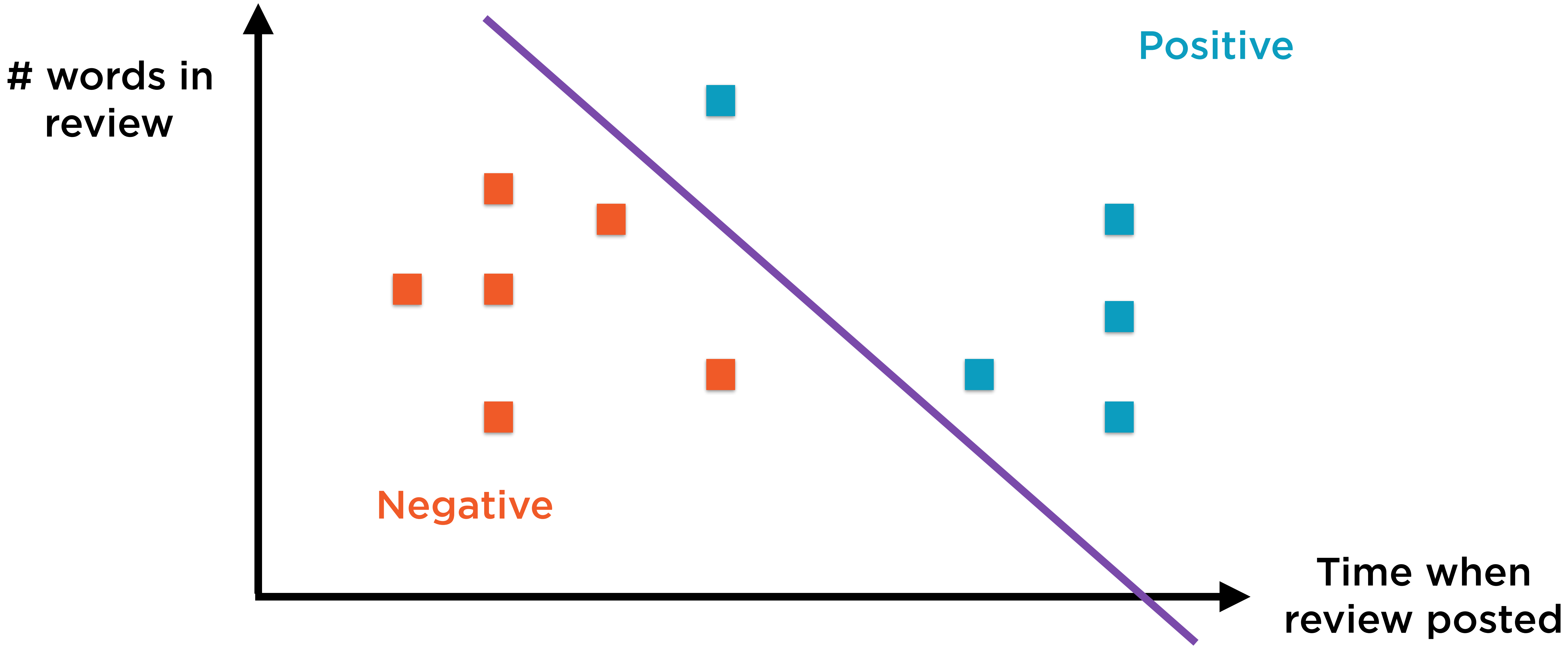
N-dimensional data can be represented in a hypercube, and classified using a hyperplane

Support Vector Machines



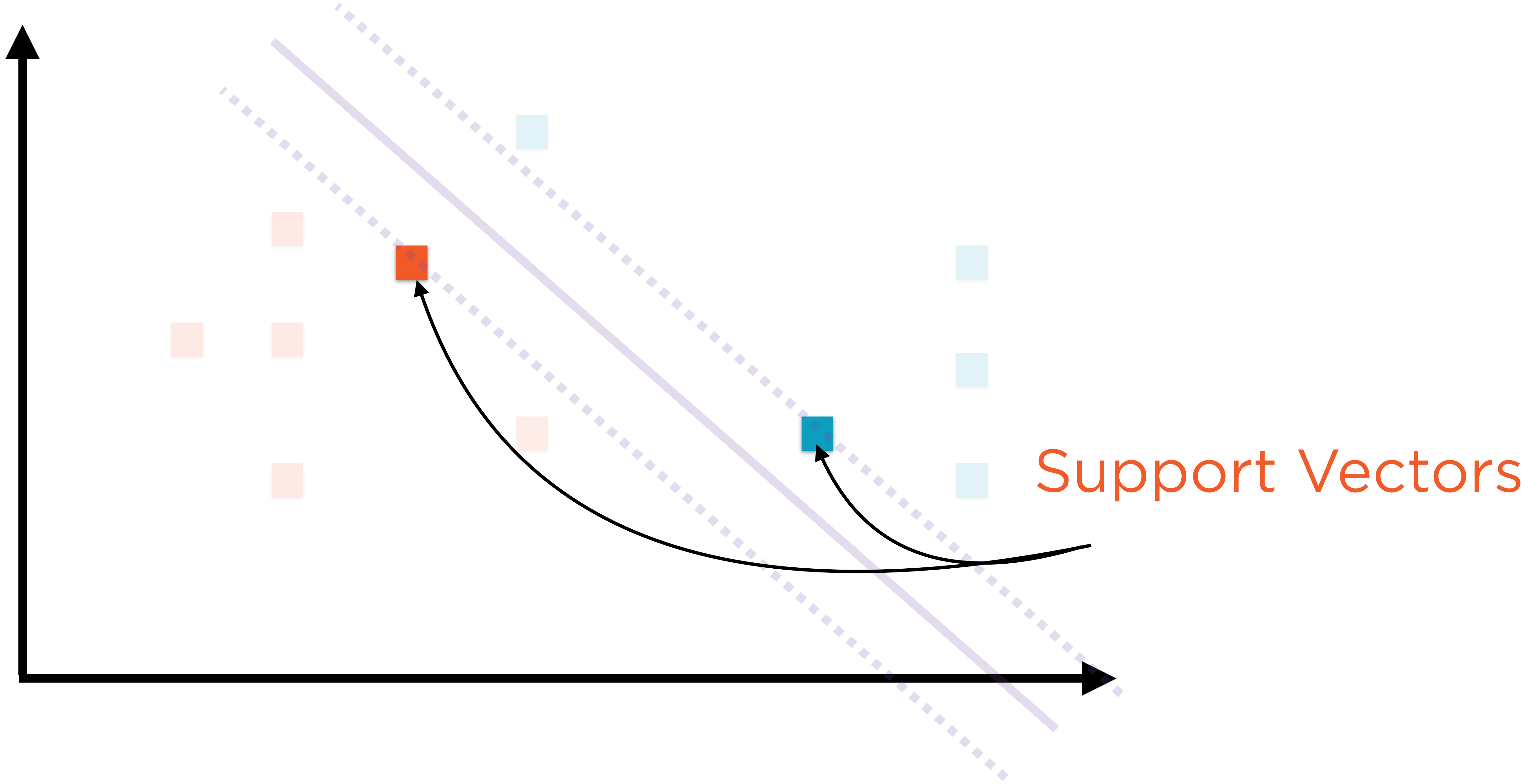
SVM classifiers find the hyperplane that best separates points in a hypercube

Classification



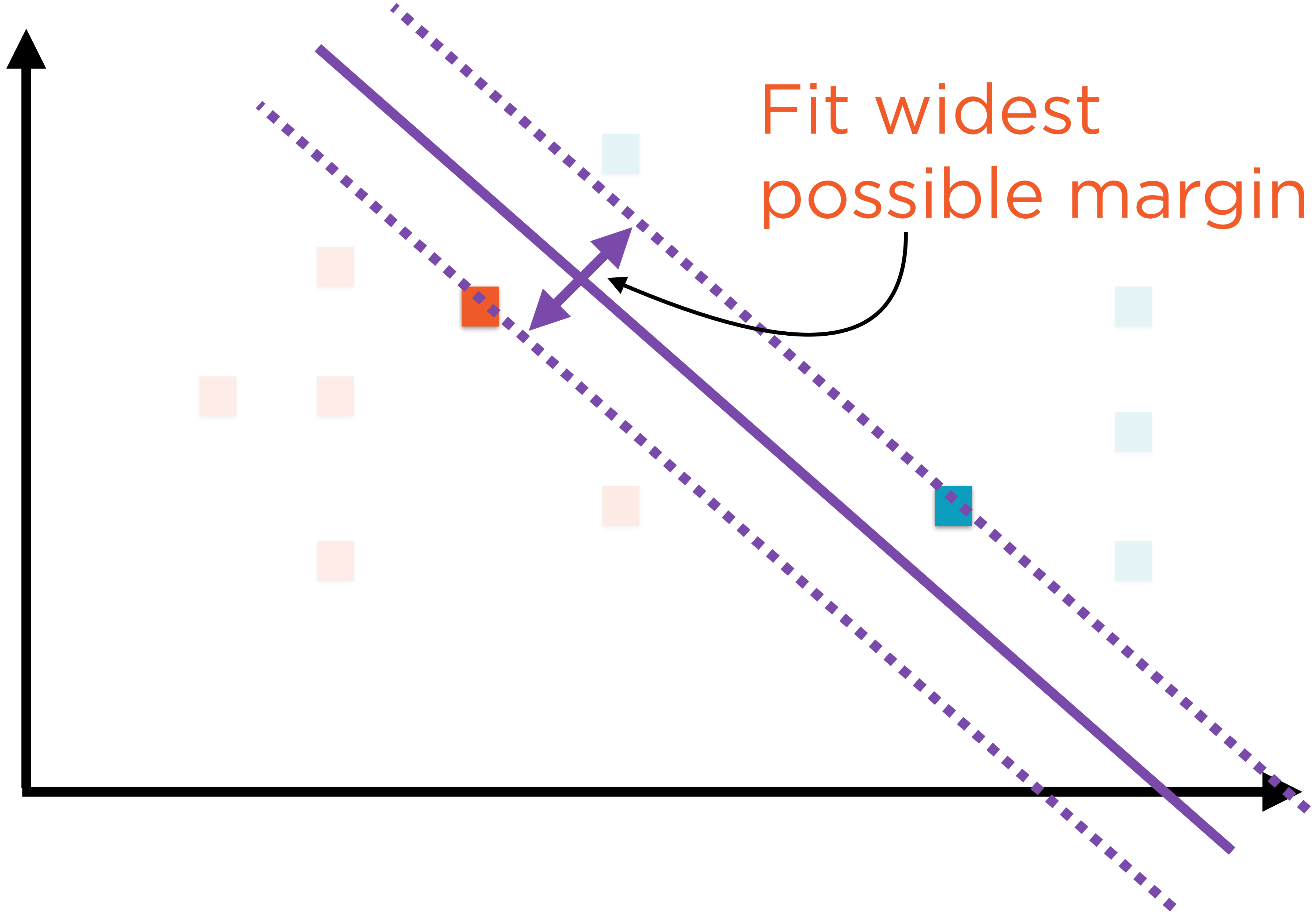
Ideally, data is linearly separable - hard decision boundary

Classification



The nearest instances on either side of the boundary are called the support vectors

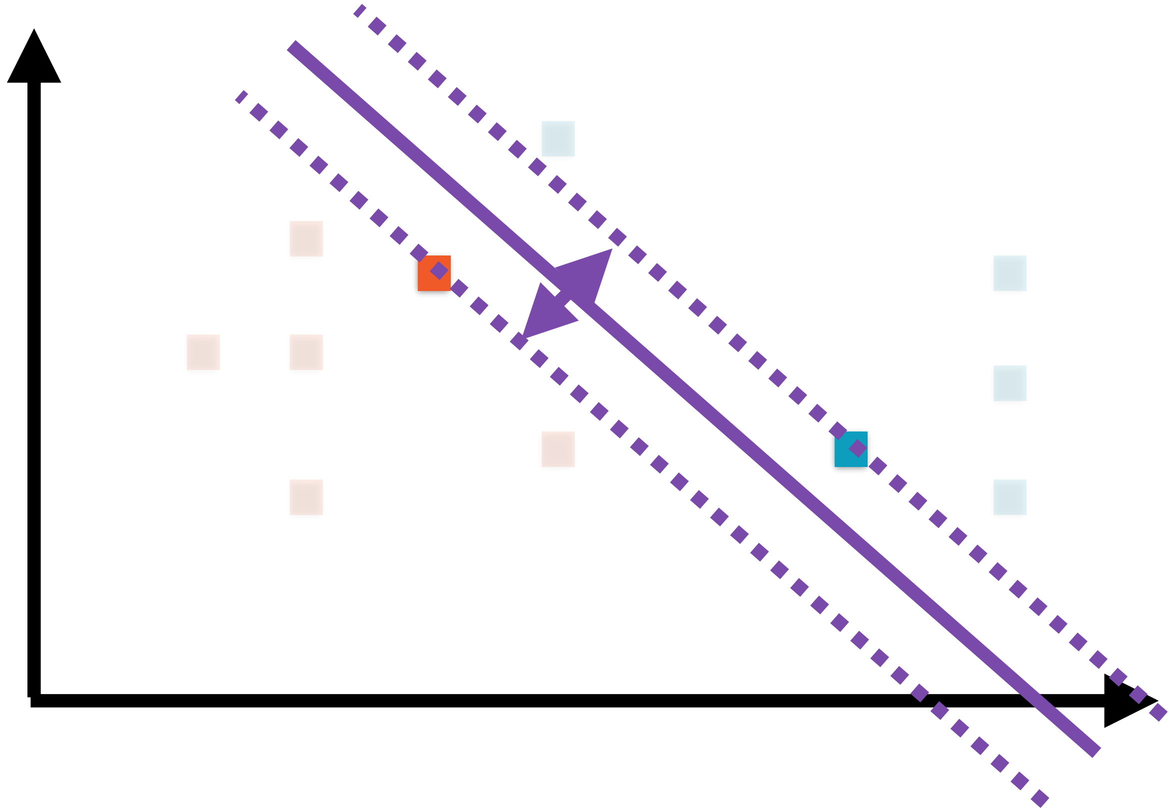
Classification



SVM finds the widest street between the nearest points on either side

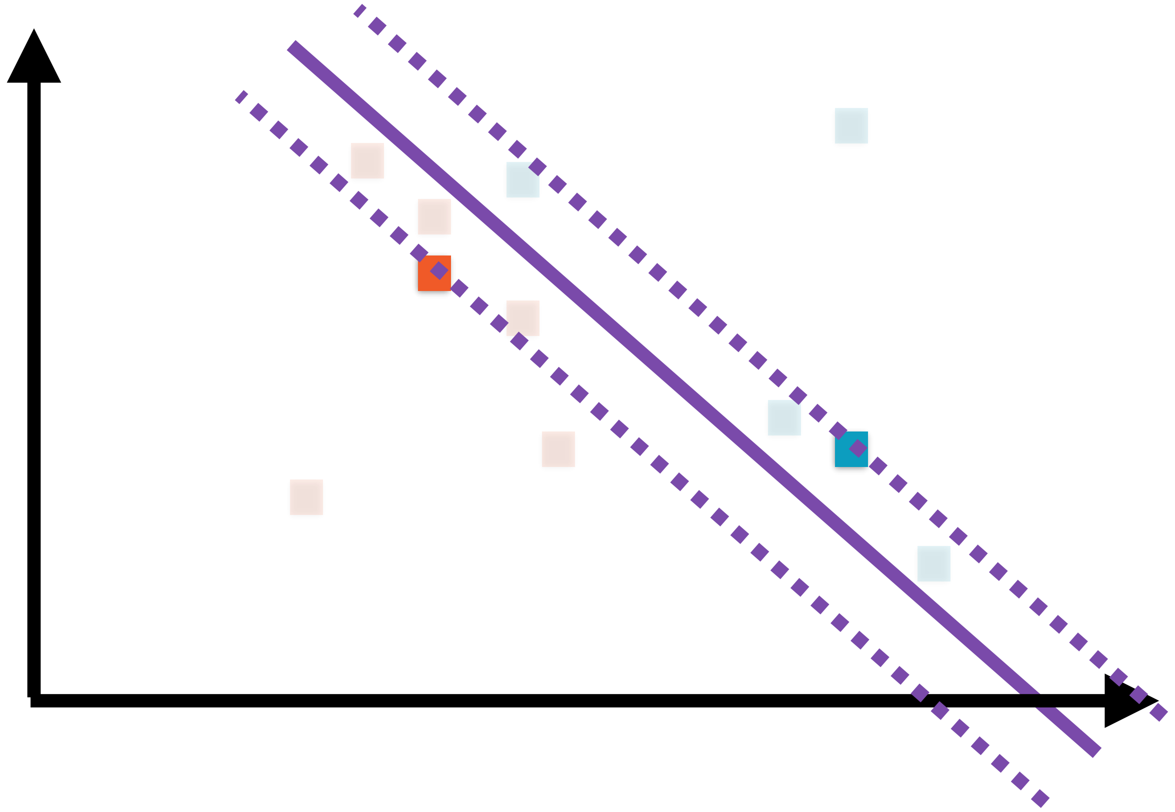
Similar, yet Different

SVM Classification



Find widest margin with most distance from nearest points (support vectors)

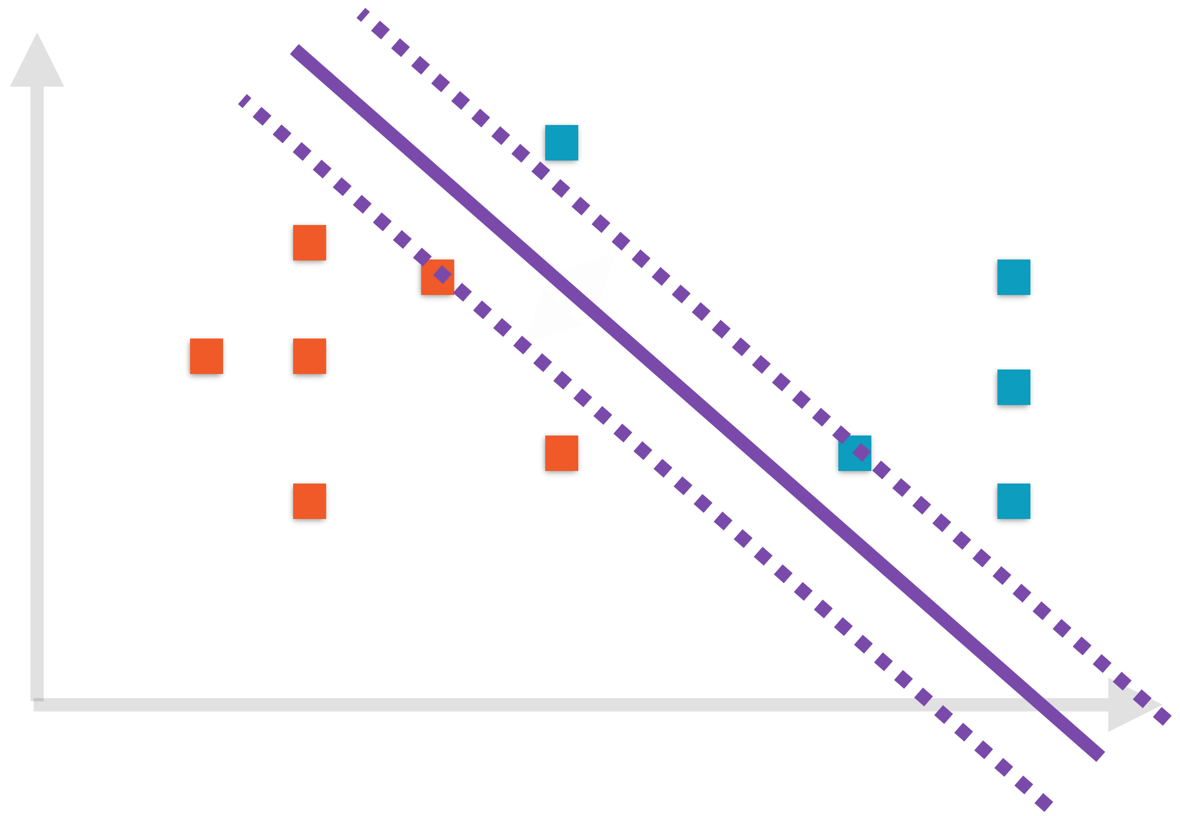
SVM Regression



Find line that "best fits" the points

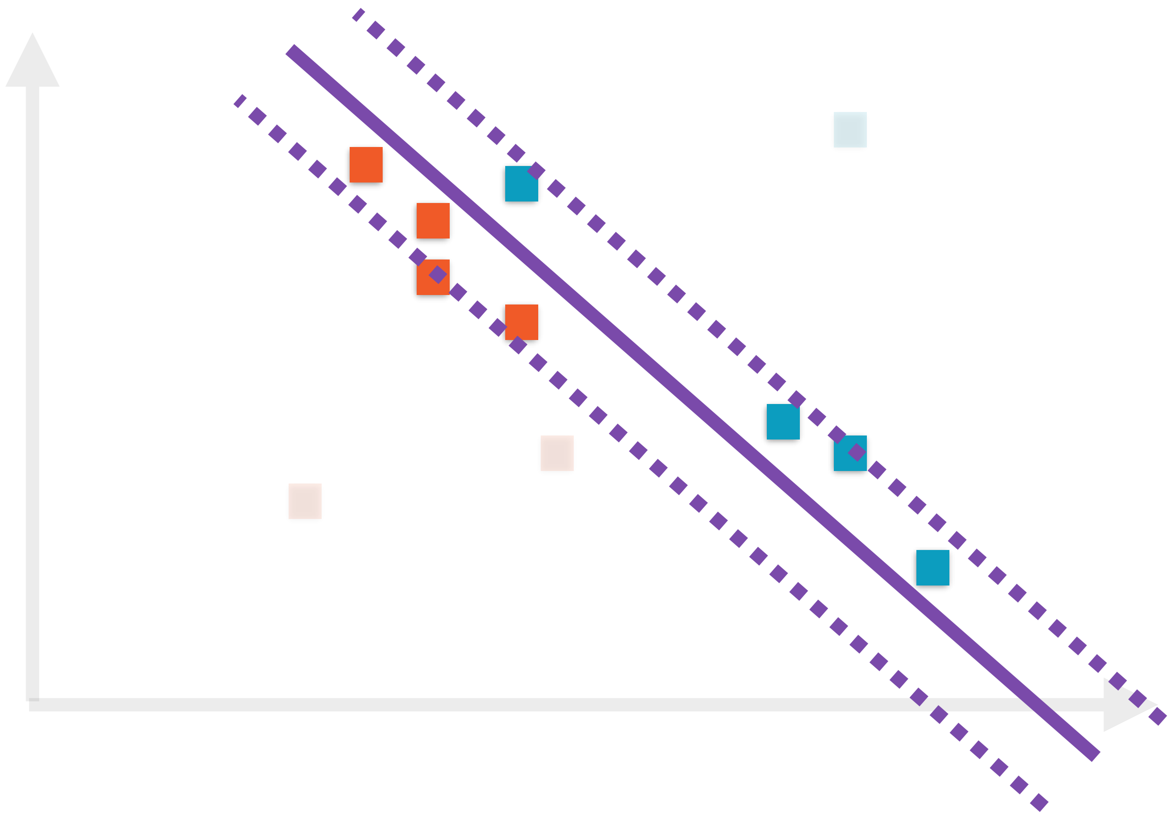
Similar, yet Different

SVM Classification



No points are inside the margin

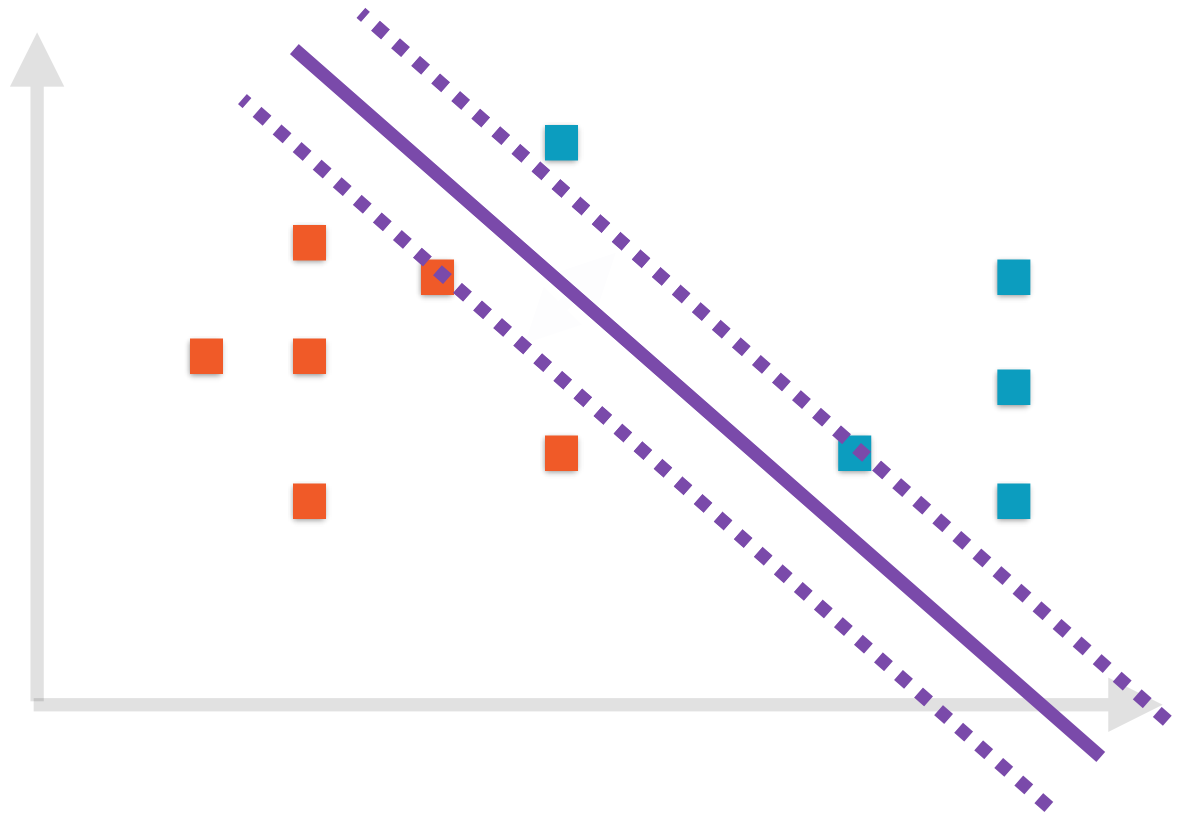
SVM Regression



Seek to maximize the number of points inside the margin

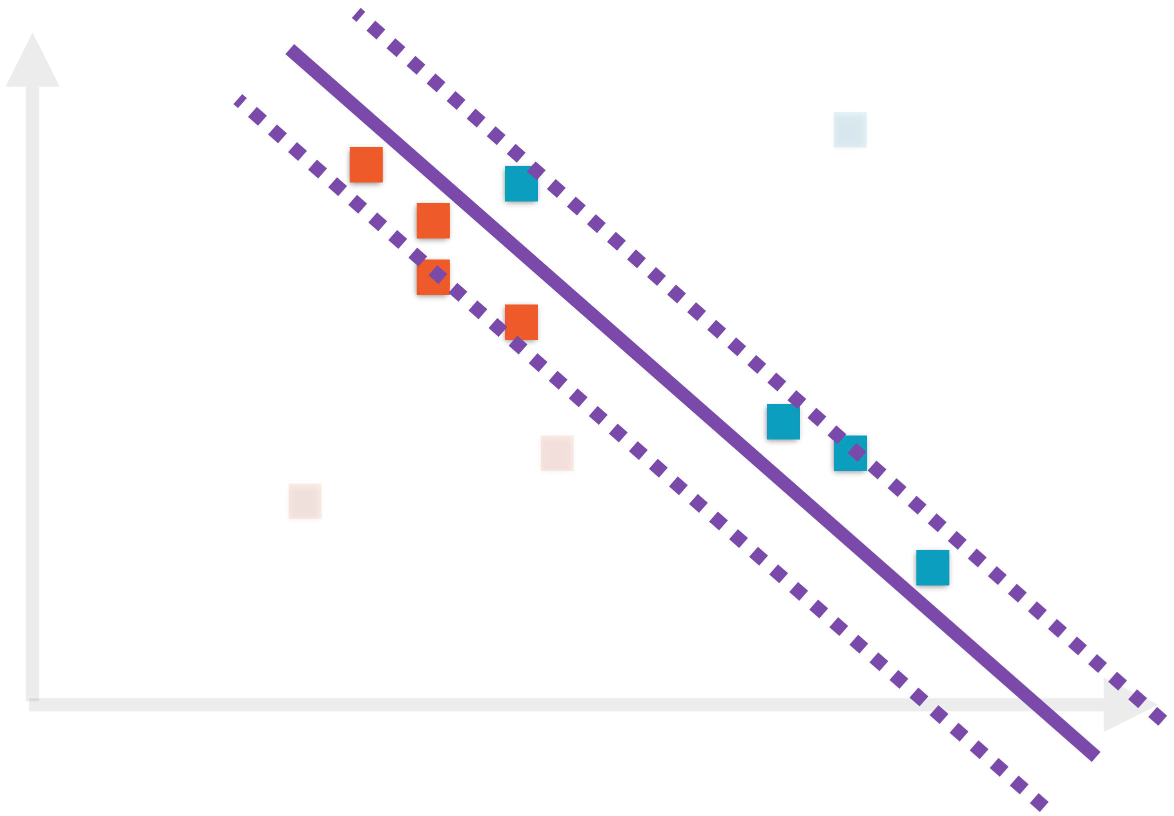
Similar, yet Different

SVM Classification



Points far from the margin are "good" (improve objective function value)

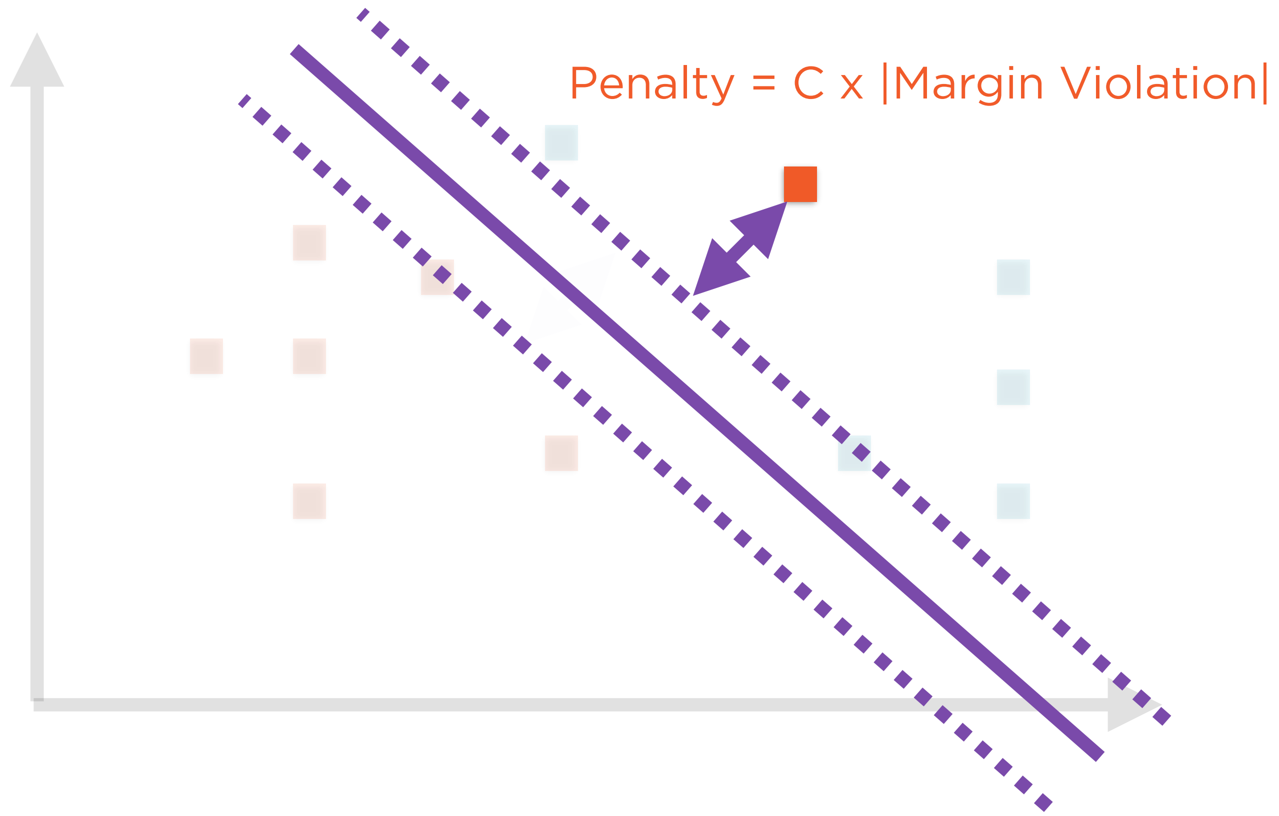
SVM Regression



Points far from the margin are "bad" (worsen objective function value)

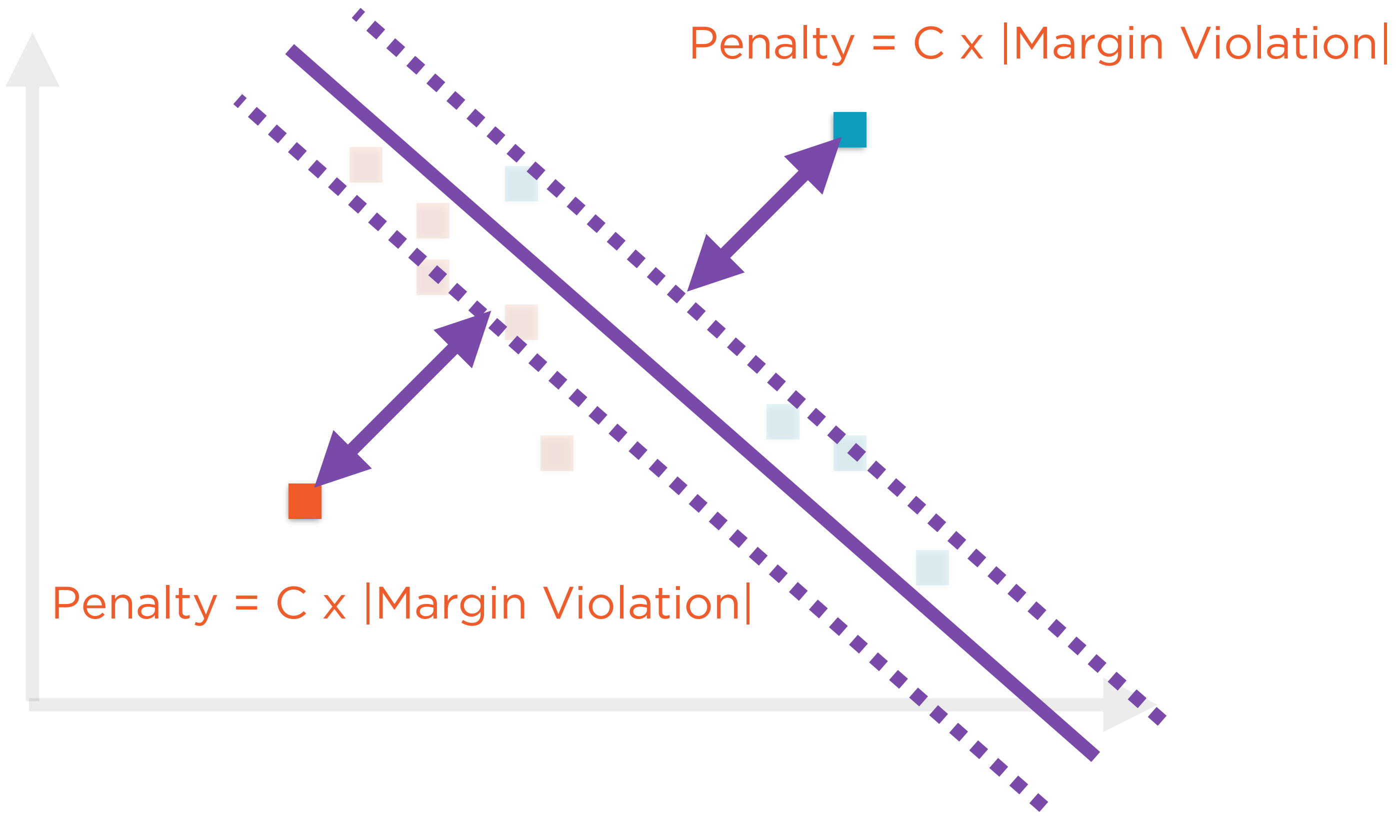
Similar, yet Different

SVM Classification



Outliers on “wrong” side of line are penalised

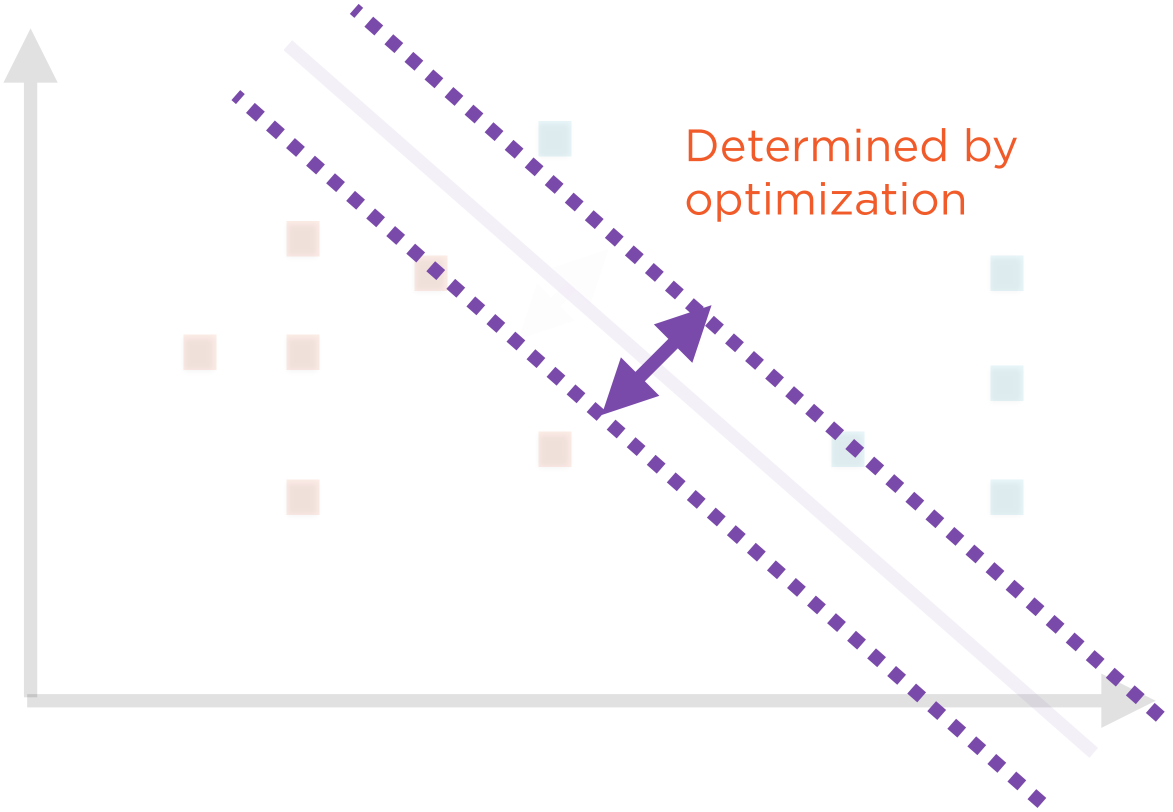
SVM Regression



Points far from the margin are penalized

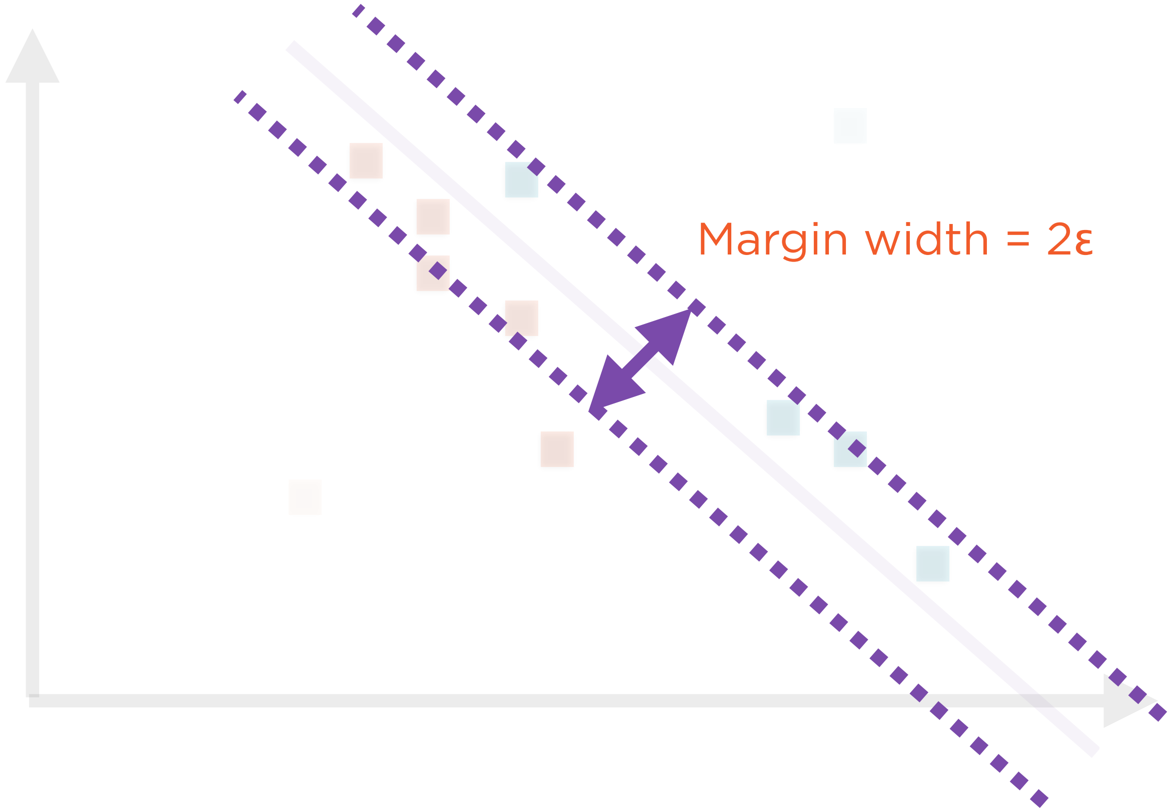
Similar, yet Different

SVM Classification



Width of margin found by optimizer (make as wide as possible)

SVM Regression



Width of margin specified in model (requires another hyperparameter ε)

Demo

Implementing Support Vector Regression in scikit-learn

Summary

Regression models and R^2 for measuring model fit

The bias-variance trade-off and overfitted models

Lasso and Ridge regression to mitigate overfitting

Support vector regression models