Orthogonal Matching Pursuit
A Machine Learning Perspective

Slides: Team RAAAK

Outliers

Outliers in Linear Models

Samples that deviate strongly from the general pattern of our data

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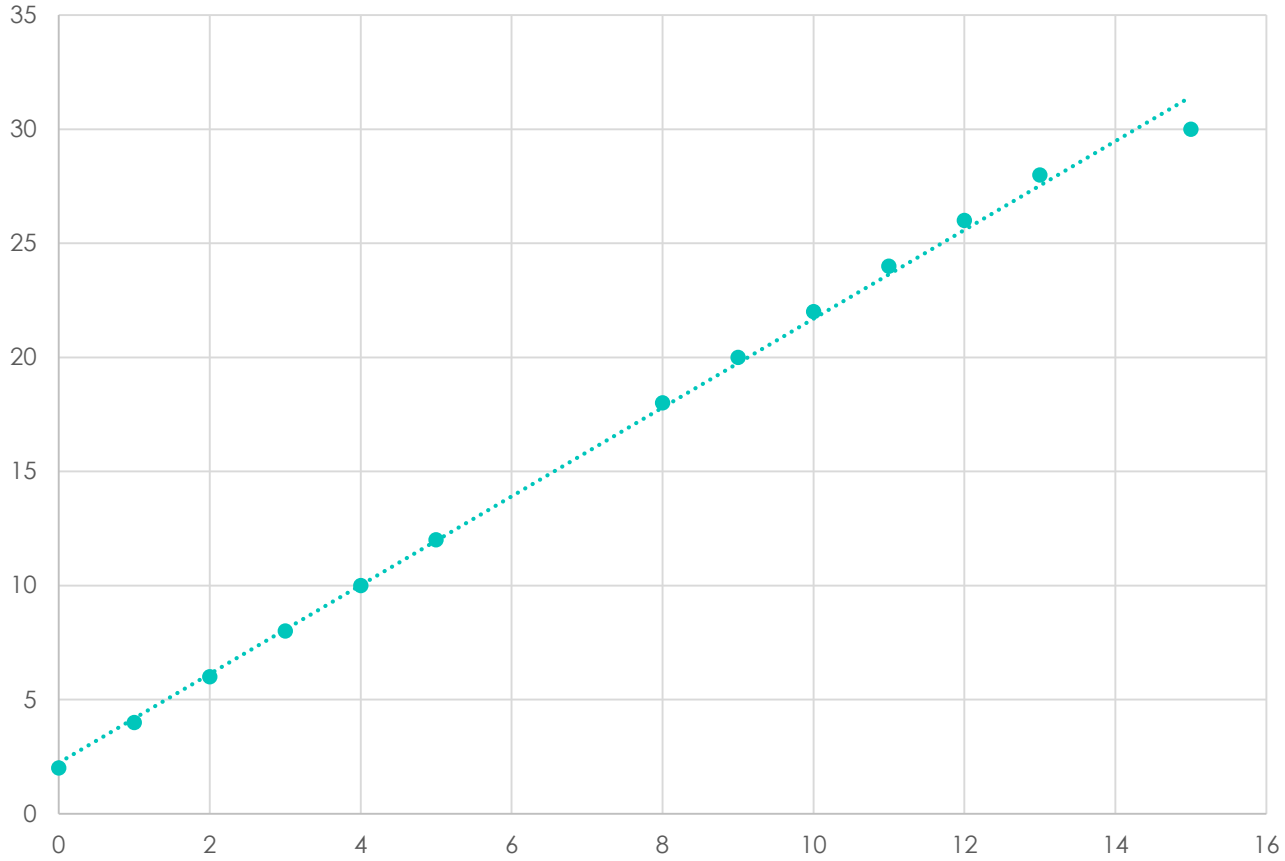
Sources of outliers include:

- Errors in measurement or data entry
- Sampling errors
- Noise in our data that corrupts our true observation

The Impact of Outliers

- Outliers can drive up the error of our model!
- Cause us to not represent the true pattern of our data



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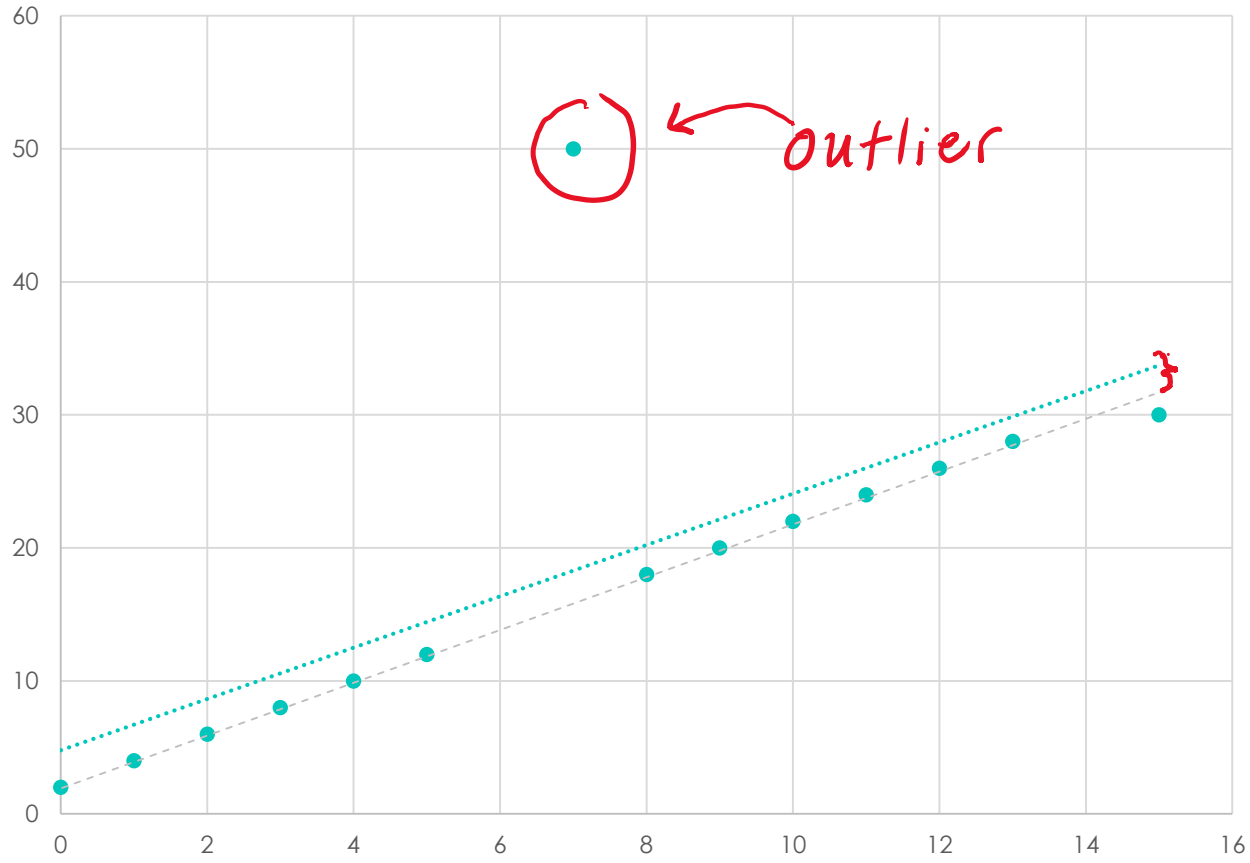

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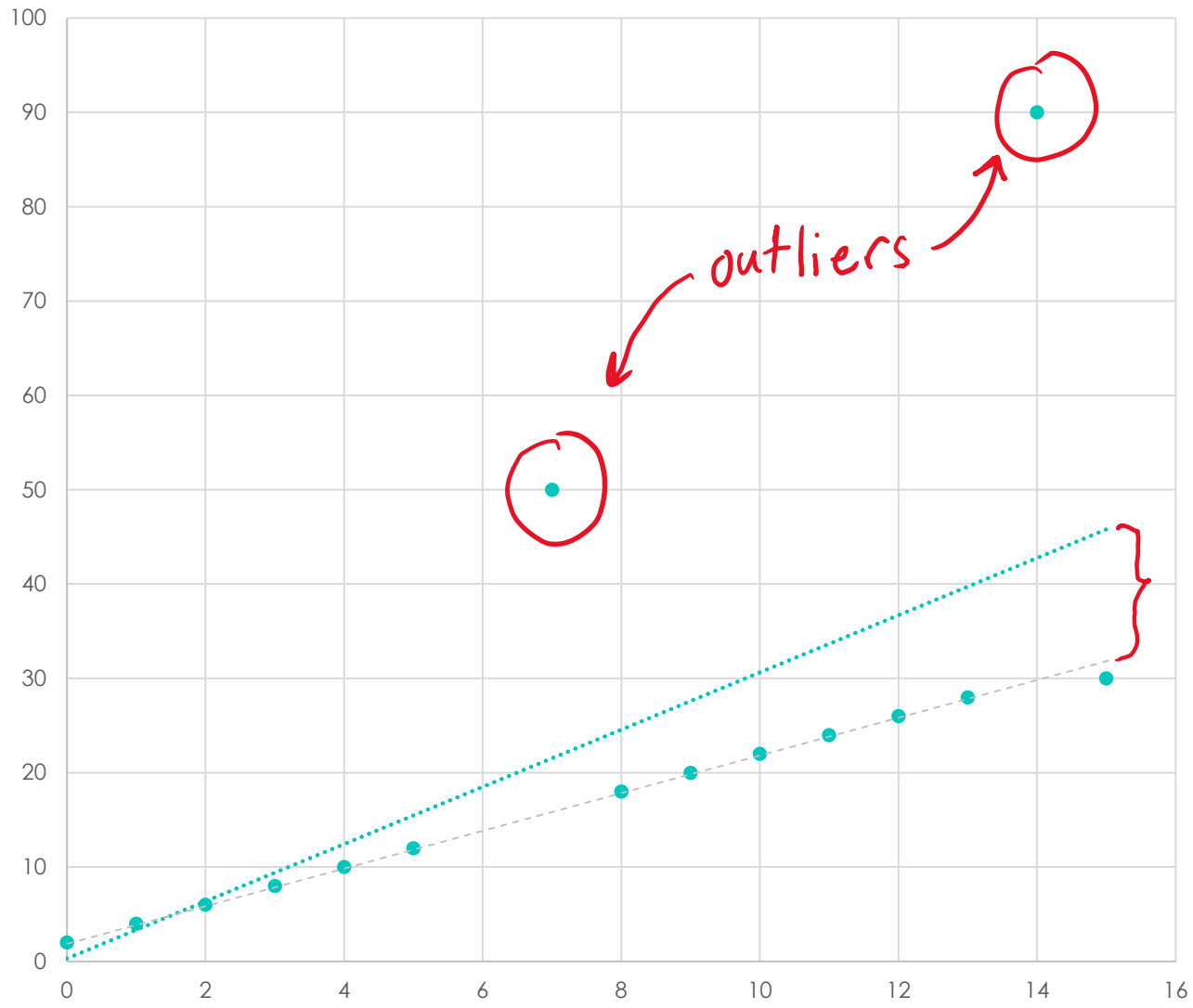

Facts About OMP – A 16A Review

01

Goal: Solve a LS problem to get a sparse solution

02

Sparse: containing mostly zero entries

03

K-sparse vector: k controls the number of nonzero entries

04

Assumption: the columns of X (data matrix) are normalized

05

Property: OMP is a Greedy Algorithm

OMP Review – Signal Processing Context

- You have seen this interpretation in EECS16A
- Context:
  - m satellites that are potentially broadcasting unique signals
  - A received signal that is a linear combination of a subset of these signals

OMP Review – Signal Processing Context

- You have seen this interpretation in EECS16A
- What we're given:
  - m satellites that are potentially broadcasting unique signals
  - A received signal that is a linear combination of a subset of these signals
- Goal
  - find which k satellites are transmitting signals that are present in our received signal

$$\boldsymbol{y} = \sum_{i \in K} \alpha_i \boldsymbol{s_i}^{(\tau_i)}$$

OMP Review - Algorithm

Algorithm 1: OMP Algorithm from 16A

Input: Codes s_i, Received signal $\boldsymbol{y}$, Sparsity k, Residual Threshold ϵ
Output: The indices of the used codes F, the sent messages $\boldsymbol{x}$
$\boldsymbol{e} = \boldsymbol{y}$, j = 1, A = [], F = $\emptyset$;
while $j \leq k$ *and* $||\boldsymbol{e}|| \geq \epsilon$ **do**
    i, t = FindMaxCrossCorrelation();
    $F = F \bigcup \{i\}$;
    $A = [A|s_i^{(t)}]$;
    $\boldsymbol{x} = (A^T A)^{-1} A^T \boldsymbol{y}$;
    $\boldsymbol{e} = \boldsymbol{y} - A\boldsymbol{x}$;
    j = j + 1;
end
return $F, \boldsymbol{x}$

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    $e = y - Ax$;
    j = j + 1;
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return F, x

Recall: We find the code and time shift with the maximum cross-correlation to predict one satellite that contributes to our received signal

The Problem of Outlier Detection

We would like to **identify** and **remove** outlier data points to decrease model error

Outlier Detection: An Analogous Context

- Codes
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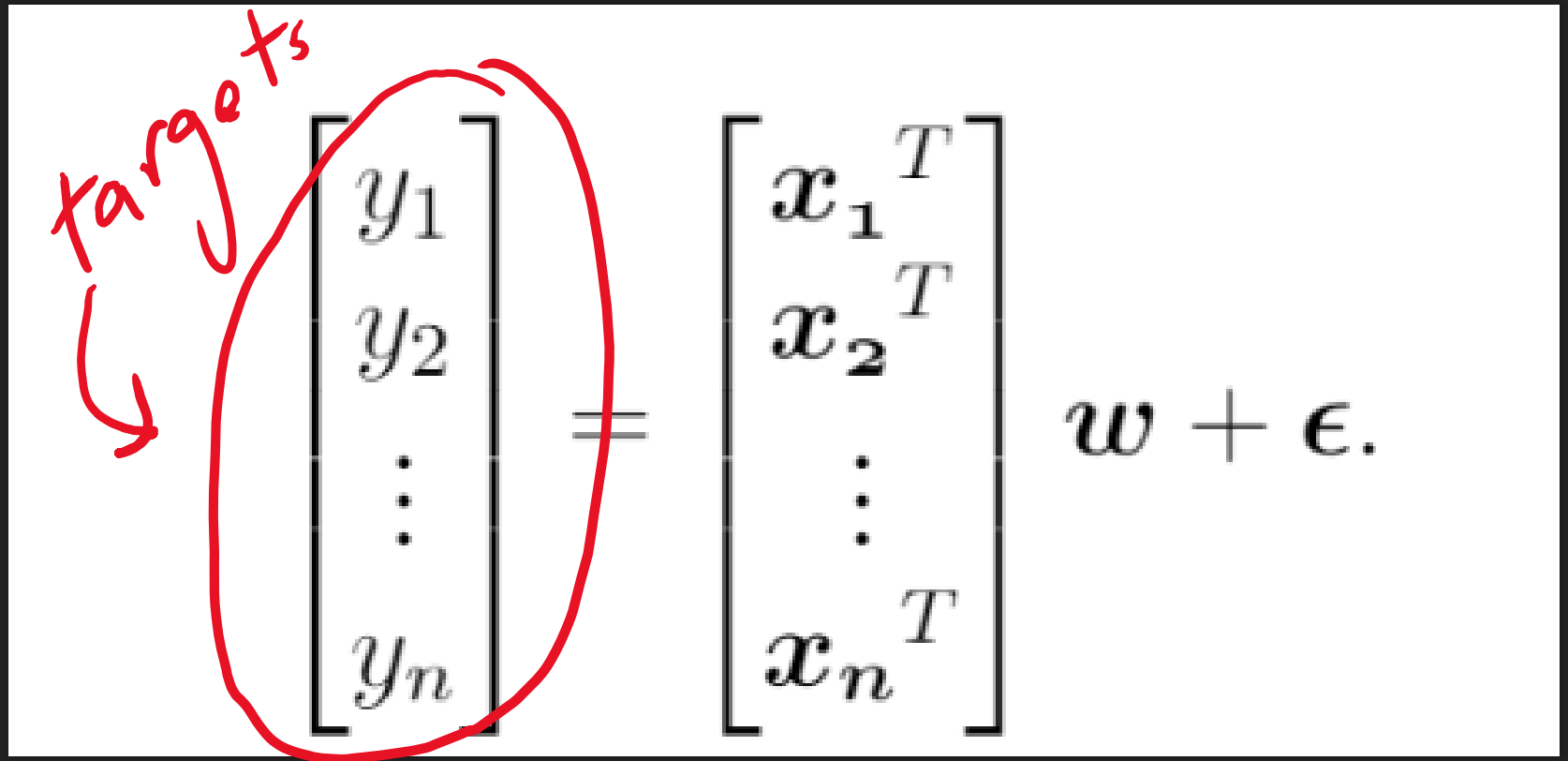
- Time shifts τ_i
  - In Outlier Detection, we no longer have the problem of time delays that we saw in the signal processing context
  - This means we no longer have to compute any cross-correlation values
- Meaning of k
  - Previously, we thought of k as related to the number of satellites transmitting unique codes
  - Now, k refers to the **number of outliers we aim to detect**

OMP for Outlier Detection – Initial Setup



OMP for Outlier Detection – Initial Setup

Recall: We are given data in $(\vec{x}_i, y_i)$ pairs

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} \boldsymbol{x}_1{}^T \\ \boldsymbol{x}_2{}^T \\ \vdots \\ \boldsymbol{x}_n{}^T \end{bmatrix} \boldsymbol{w} + \boldsymbol{\epsilon}.$$

→ data matrix X

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weights we aim to learn through Least Squares

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$\begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$

noise!

OMP for Outlier Detection – Error & Residuals

- Consider an error term ϵ_i added to each predicted output

$$y_i = \boldsymbol{x}_i^T \boldsymbol{w} + \boldsymbol{\epsilon}_i$$

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$$y_i = \boldsymbol{x_i^T w} + \boldsymbol{\epsilon_i}$$

- Constructing the error vector $\boldsymbol{\epsilon}$

$$\boldsymbol{y} = \boldsymbol{Xw} + \sum \epsilon_i \boldsymbol{e_i}$$

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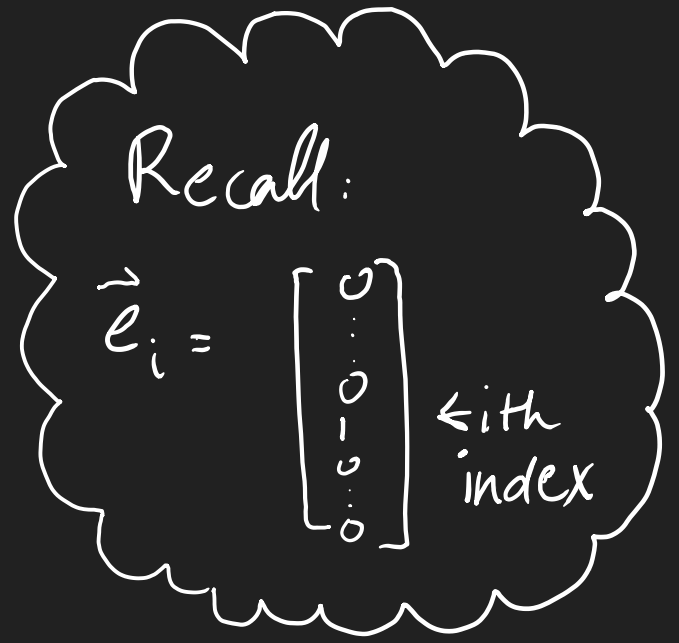
$$\boldsymbol{y} = \boldsymbol{Xw} + \sum \epsilon_i \boldsymbol{e_i}$$

- Matrix-vector product form

$$[\boldsymbol{X}\ \boldsymbol{I}]\begin{bmatrix}\boldsymbol{w}\\ \boldsymbol{\epsilon}\end{bmatrix}$$



OMP for Outlier Detection – Error & Residuals

$$[\boldsymbol{X}\ \boldsymbol{I}]\begin{bmatrix}\boldsymbol{w}\\ \boldsymbol{\epsilon}\end{bmatrix}$$

Note: We assume there are only a few outliers, so $\boldsymbol{\epsilon}$ contains only a few large values

OMP for Outlier Detection – Inputs

- Data
  - Given in the form of a data matrix $\boldsymbol{X}$
  - And targets $\boldsymbol{y}$
- Desired sparsity k of our solution
- Potentially also a desired threshold (more on this later)

OMP for Outlier Detection – Outputs

- A set of indices in our data that correspond to outlier data points
  - We'll call this F

The Algorithm: Initialization

Residual r

Matrix A

Outlier Set F

OMP: Initial Values

- **Residual:** difference of target and predicted value (using OLS)
  - $\boldsymbol{r = y - X(X^T X)^{-1} X^T y}$
- **A:** matrix that is updated after each iteration based on the standard basis vector we have considered
  - $\boldsymbol{A = X}$
- **Outlier Set:** We haven't found any outlier data points yet, so this will be initialized to the empty set
- We also set our index j to be 1 initially, and add 1 at each iteration

OMP: The Algorithm So Far

Algorithm 2: OMP to Detect Outliers

Input: Data matrix X, Predictions $\boldsymbol{y}$, Sparsity k, Residual Threshold ϵ

Output: Set of data indices F where the outliers are

$\boldsymbol{r} = \boldsymbol{y} - X(X^T X)^{-1} X^T \boldsymbol{y}$, j = 1, A = X, F = $\emptyset$;

while **do**

  j = j + 1;

end

return F

Identifying an index

- We'd like to pinpoint the index i with the largest error value (captured by our residual)
- How would we do this?
- Check for understanding: what should replace the red question mark below?

$$i = \underset{i}{\operatorname{argmax}} \left| \langle \boldsymbol{r}, \boldsymbol{?} \rangle \right|$$

Identifying an index

- We'd like to pinpoint the index i with the largest error value (captured by our residual)
- How would we do this?
- **We take the inner product of the residual with the i'th standard basis vector**

$$i = \underset{i}{\operatorname{argmax}} \left| \langle \boldsymbol{r}, \boldsymbol{e}_i \rangle \right|$$

$$i = \underset{i}{\operatorname{argmax}} \left| \langle \boldsymbol{r}, \boldsymbol{e_i} \rangle \right| = \underset{i}{\operatorname{argmax}} \left| \boldsymbol{r}[i] \right|$$

This simplifies to the i'th index of the residual, which we add to our set of outlier indices

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  i = $\text{argmax}_i \, |\boldsymbol{r}[i]|$;

  $F = F \bigcup \{i\}$;

  j = j + 1;

end

return F

Augmenting A

- We've pinpointed the i'th standard basis vector to have the maximum inner product with our residual
- So, we augment A by appending the i'th standard basis vector as follows:

$$A = [A | e_i];$$

Recomputing the Residual

- The next step to generate a new value of the residual, taking into account the fact that we've identified one new outlier data point
- To do this, we first perform OLS to generate a new prediction with our augmented version of A
  - Define $\boldsymbol{x} = \left(\boldsymbol{A}^{\boldsymbol{T}}\boldsymbol{A}\right)^{-\mathbf{1}}\boldsymbol{A}^{\boldsymbol{T}}\boldsymbol{y}$
- Our updated prediction of the targets is $\boldsymbol{Ax}$

Recomputing the Residual

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$$\text{Define } \boldsymbol{x} = \left(\boldsymbol{A}^{\boldsymbol{T}}\boldsymbol{A}\right)^{-\boldsymbol{1}}\boldsymbol{A}^{\boldsymbol{T}}\boldsymbol{y}$$

- Our updated prediction of the targets is $\boldsymbol{Ax}$
- We then redefine our residual exactly as we did in the initial step, as the difference between the target vector and our prediction

$$\boldsymbol{r} = \boldsymbol{y} - \boldsymbol{Ax}$$

OMP: The Algorithm So Far

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  $\boldsymbol{x} = (A^T A)^{-1} A^T \boldsymbol{y}$;

  $\boldsymbol{r} = \boldsymbol{y} - A\boldsymbol{x}$;

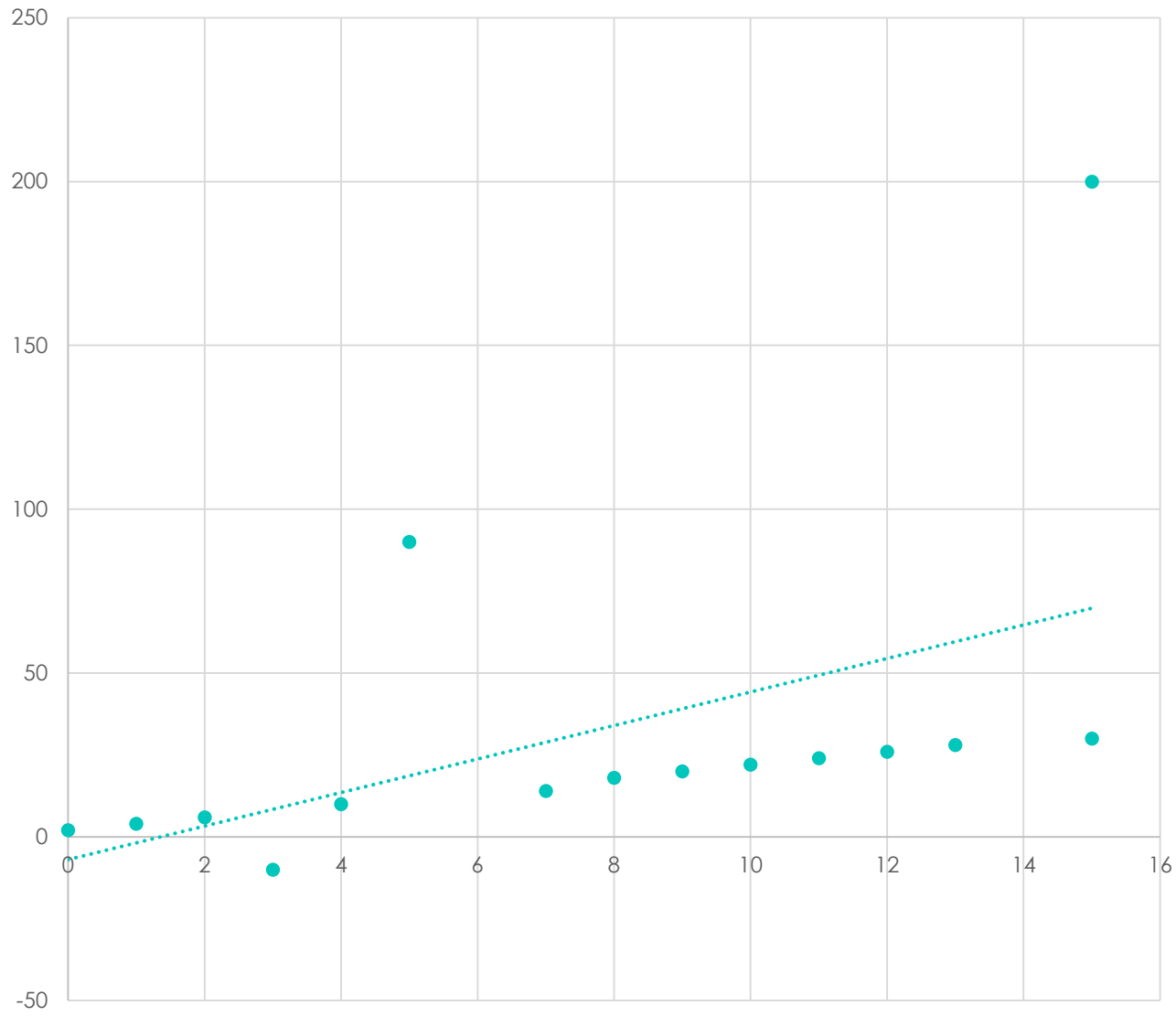
  j = j + 1;

end

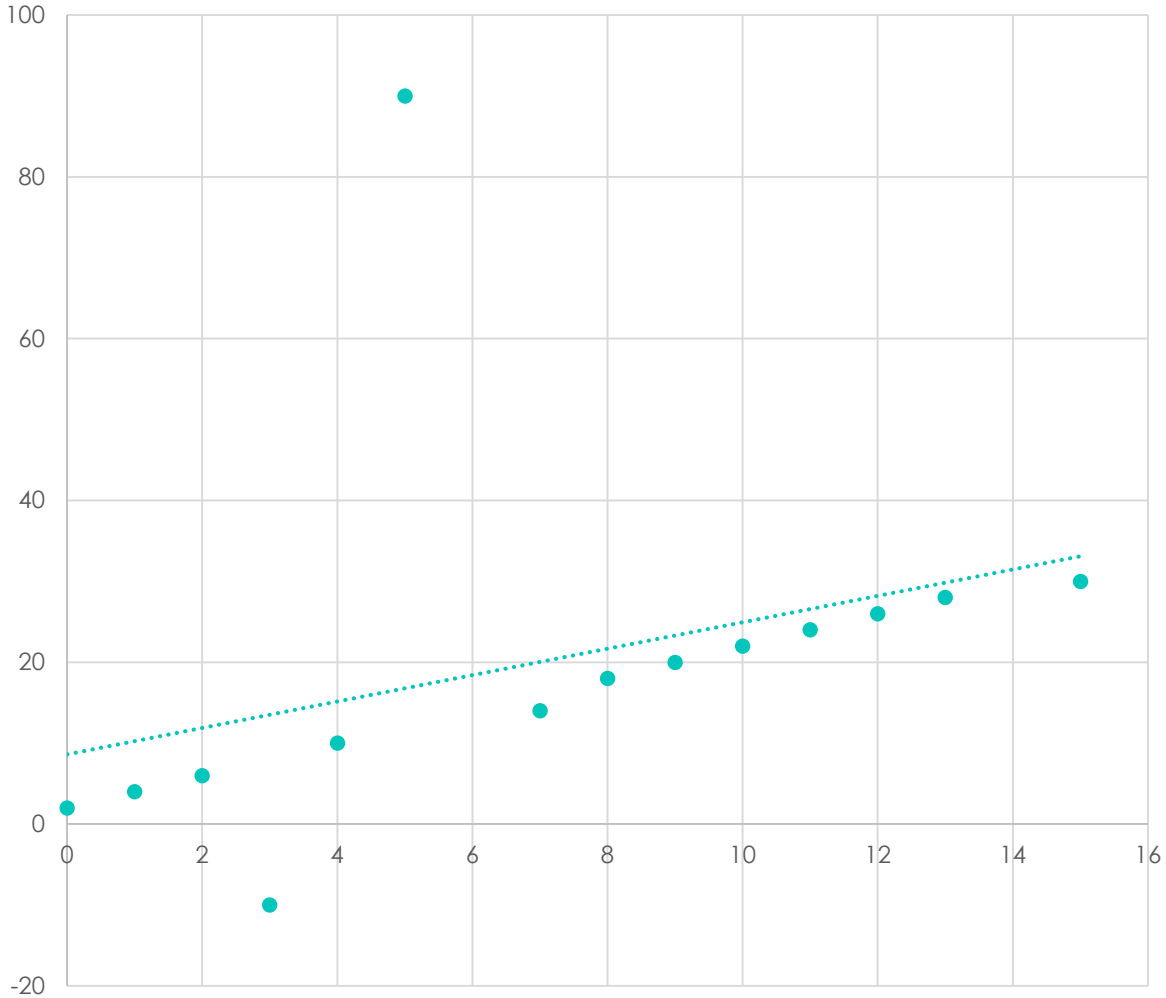
return F

OMP for Outlier Detection – Big Picture

- Each iteration pinpoints one outlier to be removed
- Goal: finding the vectors in a given basis (e.g. the standard basis consisting of vectors e_i) that can best capture the pattern in our data, while excluding those directions that increase error in our predictions



OMP for Outlier Detection and Removal - Visualization



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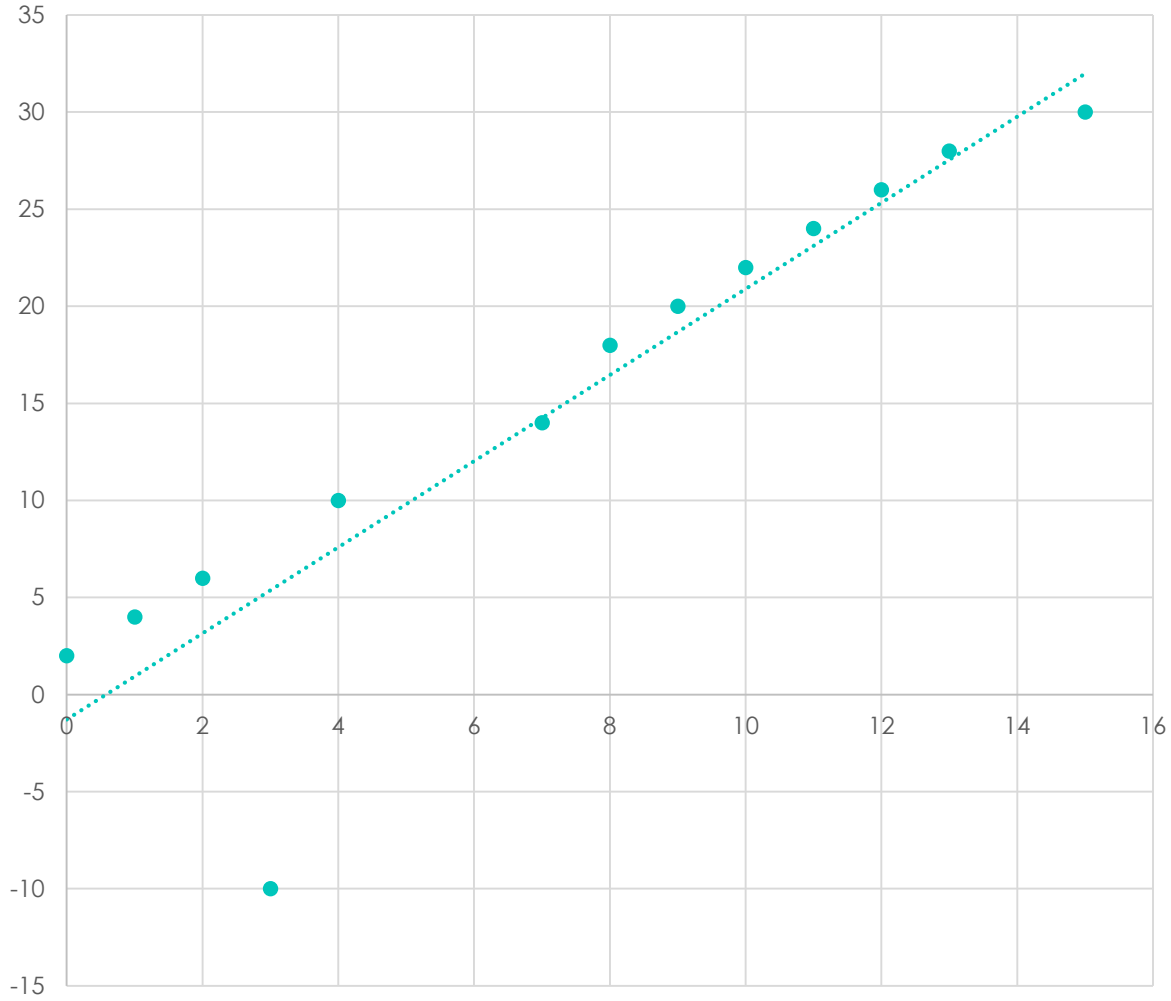

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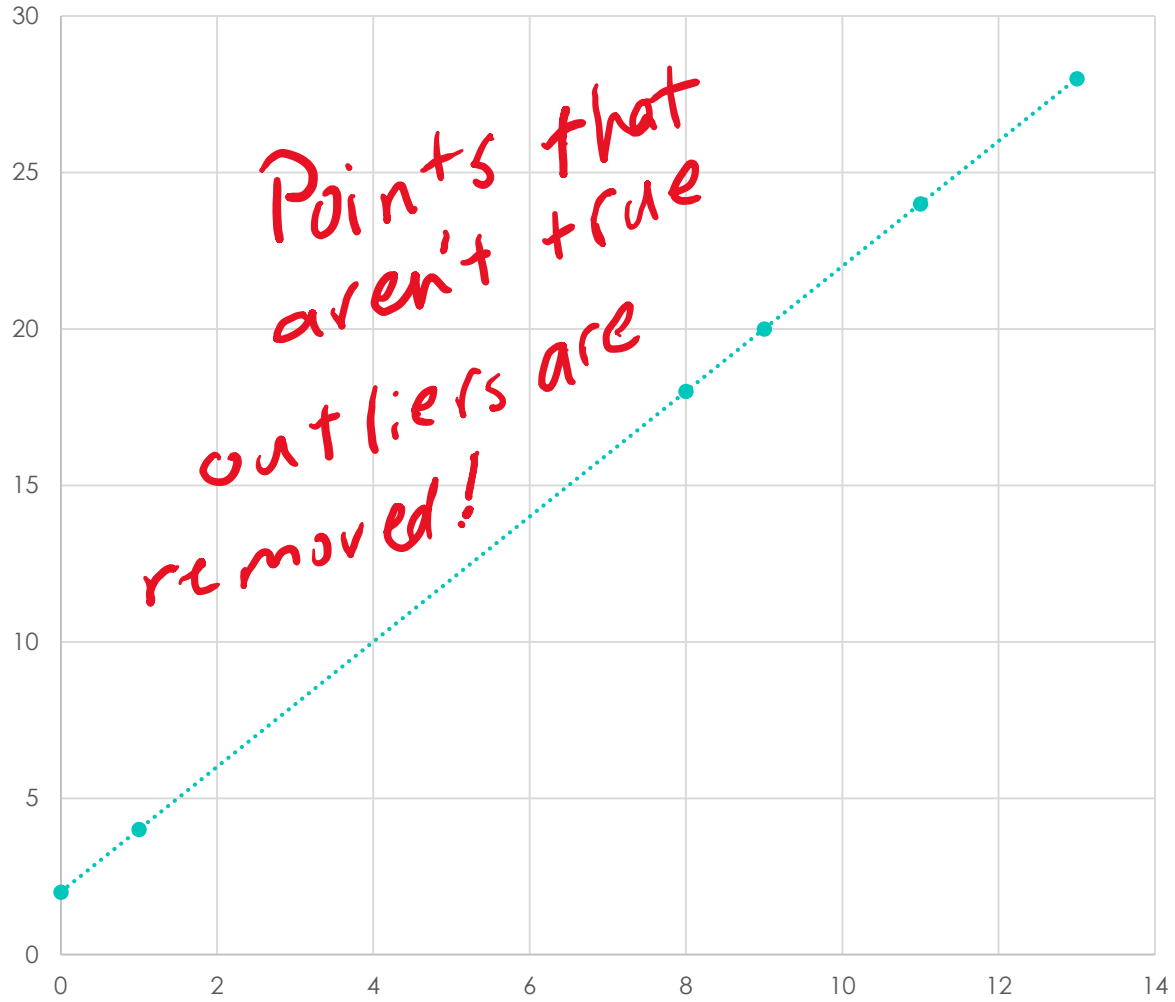

After Several Iterations…

Question

How do we know when to stop running Orthogonal Matching Pursuit for outlier detection?

Stopping Conditions

- Option 1: Stop after a certain number of outliers are removed
  - This is especially helpful when we have an idea of how many outliers exist in our data
  - How does this affect our algorithm?
    - For k outliers, iterate while $j \leq k$

Stopping Conditions

- Option 1: Stop after a certain number of outliers are removed
  - This is especially helpful when we have an idea of how many outliers exist in our data
  - How does this affect our algorithm?
    - For k outliers, iterate while $j \leq k$
- Option 2: stop once we've reached a certain residual threshold
  - Stop iterating when the norm of our residual r falls below a predefined value ϵ
  - How does this affect our algorithm?
    - Iterate while $||r|| \geq \epsilon$

Note: the values of k and epsilon are set **by us**, and are not a quantity determined by the OMP algorithm.

This means we can tune them!

Tuning our Stopping Condition

- Last week, you learned about validation (and more specifically, cross-validation) as a method to turn hyperparameters so that our model performs well on our test dataset
- We can use this for finding an OMP stopping condition as well!
- Option 1
  - Cross-validation to set our residual threshold ϵ
  - We choose the value of ϵ for which the error on our validation set is lowest
- Option 2
  - Tuning our number of removed points k
  - We choose the value of k for which the error on our validation set is lowest
- Option 3
  - We stop when there are only two points left in our dataset (the minimum needed to create our linear model)

OMP for Outlier Detection – Putting it all together

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