Language of ML: linear algebra

Language of ML: linear algebra – what is it?

- Calculations with vectors and matrices

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$$\begin{bmatrix} 3 \\ 4 \end{bmatrix}$$

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Language of ML: linear algebra – what is it?

- Calculations with vectors and matrices

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$$

Language of ML: linear algebra – what is it?

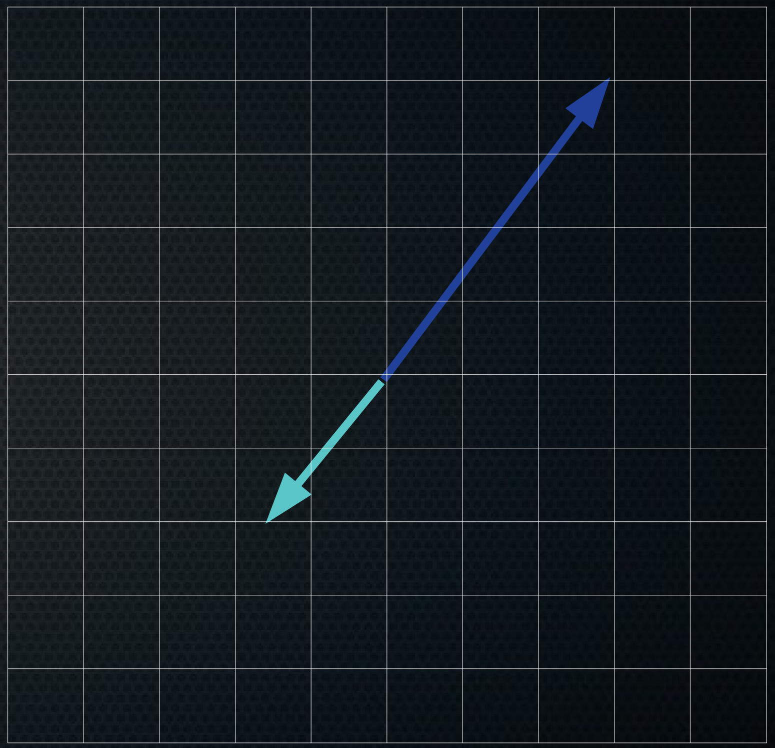
- Calculations with vectors and matrices
- For example, scaling a vector

$$0.5 \cdot \underline{\begin{bmatrix} 3 \\ 4 \end{bmatrix}} \longrightarrow \underline{\begin{bmatrix} 1.5 \\ 2 \end{bmatrix}}$$

Language of ML: linear algebra – what is it?

- Calculations with vectors and matrices
- For example, scaling a vector

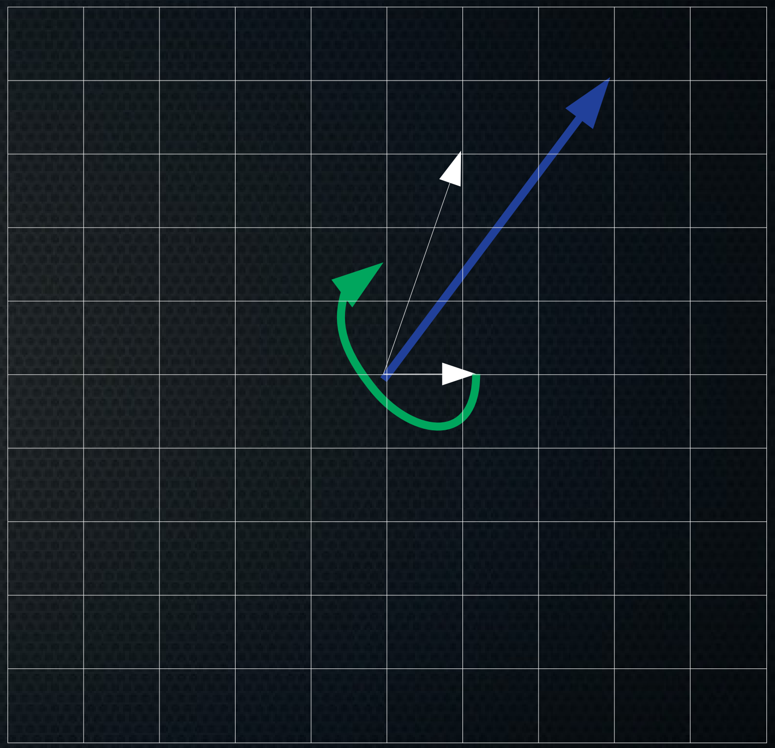
$$-0.5 \cdot \underline{\begin{bmatrix} 3 \\ 4 \end{bmatrix}} \longrightarrow \underline{\begin{bmatrix} -1.5 \\ -2 \end{bmatrix}}$$



Language of ML: linear algebra – what is it?

- Calculations with vectors and matrices
- Or matrix-vector multiplication

$$\begin{bmatrix} \boxed{\begin{matrix} 1 \\ 3 \end{matrix}} & \begin{matrix} 2 \\ 4 \end{matrix} \end{bmatrix} \cdot \begin{bmatrix} 3 \\ 4 \end{bmatrix} \rightarrow \begin{bmatrix} 11 \\ 25 \end{bmatrix}$$



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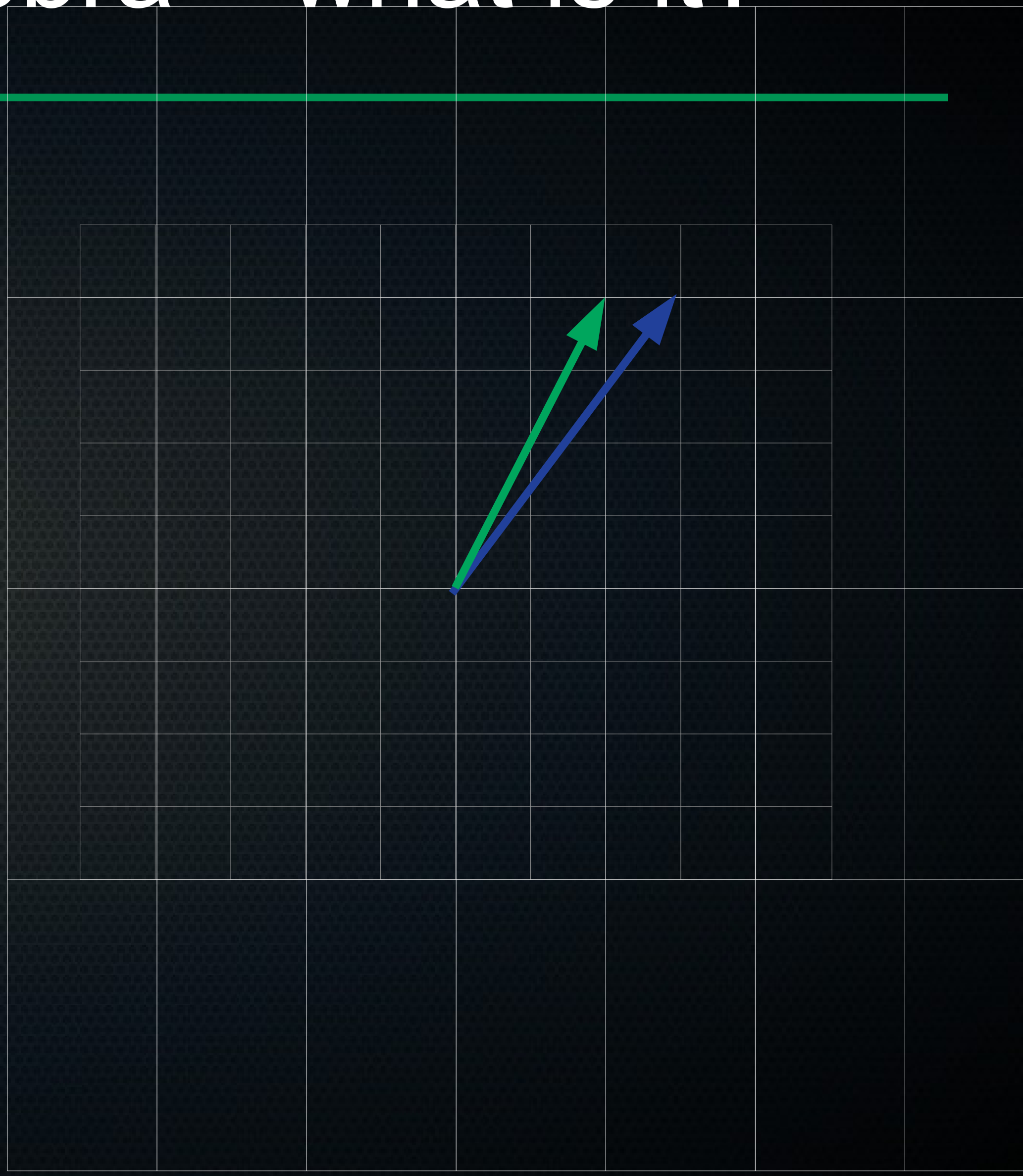

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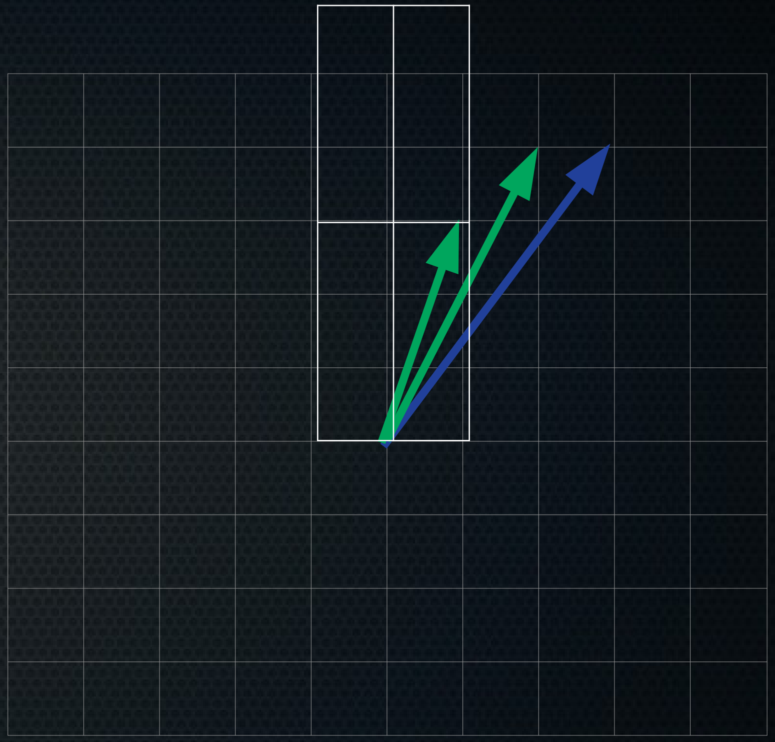

Language of ML: linear algebra – why do we care?

- Machine learning algorithms are implemented and defined in linear algebra. Linear regression prediction:

$$\hat{Y} = X^T \hat{\beta}$$

Language of ML: linear algebra – why do we care?

- Games require parallel calculations of many transformations of 3D vectors to rotate and show objects in 3D as you move around.
  - This has given us GPUs which are geared to do that immensely quickly and in parallel (GeForce GTX 690: ~5622 * 10^9/second)
  - And now TPUs or Tensor Processing Units which are geared more towards ML applications.
- Take advantage of that!

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

Language of ML: linear algebra – why do we care?

- Get rid of all the loops in your code *and* make it much faster. Win-win!

Language of ML: linear algebra – vectors

- Scalar multiplication (*scales* the vector):

$$5 \cdot \begin{bmatrix} 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 15 \\ 20 \end{bmatrix}$$

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- Vector addition:

$$\begin{bmatrix} 3 \\ 4 \end{bmatrix} + \begin{bmatrix} 2 \\ 8 \end{bmatrix} = \begin{bmatrix} 5 \\ 12 \end{bmatrix}$$

Language of ML: linear algebra – vectors

- Scalar multiplication (*scales* the vector):

$$5 \cdot \begin{bmatrix} 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 15 \\ 20 \end{bmatrix}$$

- Vector addition:

$$\begin{bmatrix} 3 \\ 4 \end{bmatrix} + \begin{bmatrix} 2 \\ 8 \end{bmatrix} = \begin{bmatrix} 5 \\ 12 \end{bmatrix}$$

- Vector transpose (from column vector to row vector):

$$\begin{bmatrix} 3 \\ 4 \end{bmatrix}^T = \begin{bmatrix} 3 & 4 \end{bmatrix}$$

Language of ML: linear algebra – matrices

- Scalar multiplication (*scales* the matrix):

$$5 \cdot \begin{bmatrix} 2 & 3 \\ 8 & 9 \end{bmatrix} = \begin{bmatrix} 10 & 15 \\ 40 & 45 \end{bmatrix}$$

- Matrix addition:

$$\begin{bmatrix} 2 & 3 \\ 8 & 9 \end{bmatrix} + \begin{bmatrix} 10 & 15 \\ 40 & 45 \end{bmatrix} = \begin{bmatrix} 12 & 18 \\ 48 & 54 \end{bmatrix}$$

Language of ML: linear algebra – matrices

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$$\xcancel{\begin{bmatrix} 2 & 3 \\ 8 & 9 \end{bmatrix} + \begin{bmatrix} 10 & 15 & 1 \\ 40 & 45 & 9 \end{bmatrix} = ERROR}$$

Language of ML: linear algebra – matrices

- Scalar multiplication (*scales* the matrix):

$$5 \cdot \begin{bmatrix} 2 & 3 \\ 8 & 9 \end{bmatrix} = \begin{bmatrix} 10 & 15 \\ 40 & 45 \end{bmatrix}$$

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- Matrix transpose:

$$\begin{bmatrix} 2 & 3 \\ 8 & 9 \end{bmatrix}^T = \begin{bmatrix} 2 & 8 \\ 3 & 9 \end{bmatrix}$$

Language of ML: linear algebra – matrices

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Note: vector special case of matrix where one dimension is 1.

- Matrix transpose:

$$\begin{bmatrix} 2 & 3 \\ 8 & 9 \end{bmatrix}^T = \begin{bmatrix} 2 & 8 \\ 3 & 9 \end{bmatrix}$$

Language of ML: linear algebra – matrices

- Matrix-vector multiplication:

$$\begin{bmatrix} 2 & 3 \\ 8 & 9 \end{bmatrix} \cdot \begin{bmatrix} 10 \\ 8 \end{bmatrix} = \begin{bmatrix} 2 \cdot 10 + 3 \cdot 8 \\ 8 \cdot 10 + 9 \cdot 8 \end{bmatrix} = \begin{bmatrix} 44 \\ 152 \end{bmatrix}$$

Language of ML: linear algebra – matrices

- Matrix-vector multiplication:

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-Sum of each element in the *row* of the matrix * each element in the *column* of the vector
-2 by 2 matrix times 2 by 1 vector becomes 2 by 1 vector.

Language of ML: linear algebra – matrices

- Matrix-vector multiplication:

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-Sum of each element in the *row* of the matrix * each element in the *column* of the vector

-2 by $\underbrace{2 \text{ matrix times } 2}_{\text{\# of columns in A matches \# of rows in B}}$ by 1 vector becomes 2 by 1 vector.

of *columns* in A matches # of *rows* in B

Language of ML: linear algebra – matrices

- Matrix-vector multiplication:

$$\begin{bmatrix} \boxed{10} \\ 8 \end{bmatrix} \cdot \begin{bmatrix} 2 & 3 \\ 8 & 9 \end{bmatrix} = ERROR$$

-Sum of each element in the *row* of the matrix * each element in the *column* of the vector

-2 by 1 vector times 2 by 2 matrix is undefined

of *columns* in A **does not match**
of *rows* in B

Language of ML: linear algebra – matrices

- Matrix-vector multiplication:

$$\begin{bmatrix}2 & 3\\ 8 & 9\end{bmatrix}\cdot\begin{bmatrix}10\\ 8\end{bmatrix}=\begin{bmatrix}2\cdot 10+3\cdot 8\\ 8\cdot 10+9\cdot 8\end{bmatrix}=\begin{bmatrix}44\\ 152\end{bmatrix}$$

-Sum of each element in the *row* of the matrix * each element in the *column* of the vector
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Language of ML: linear algebra – matrices

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-Sum of each element in the *row* of the matrix * each element in the *column* of the vector

-2 by 2 matrix times 2 by 1 vector becomes 2 by 1 vector.

of *rows* in matrix and number of *columns* in vector defines shape new vector

Language of ML: linear algebra – matrices

- Matrix-vector multiplication:

$$\begin{bmatrix} 2 & 3 \\ 8 & 9 \\ 0 & 4 \end{bmatrix} \cdot \begin{bmatrix} 10 \\ 8 \end{bmatrix} = \begin{bmatrix} 2 \cdot 10 + 3 \cdot 8 \\ 8 \cdot 10 + 9 \cdot 8 \\ 0 \cdot 10 + 4 \cdot 8 \end{bmatrix} = \begin{bmatrix} 44 \\ 152 \\ 32 \end{bmatrix}$$

-Sum of each element in the *row* of the matrix * each element in the *column* of the vector

-3 by 2 matrix times 2 by 1 vector becomes 3 by 1 vector.

\# of *rows* in matrix and number of *columns* in vector defines shape new vector

Language of ML: linear algebra – matrices

- Matrix-matrix multiplication:
  - Matrix really just concatenated vector, so similar process:

$$\begin{bmatrix} \boxed{2 \quad 3} \\ 8 \quad 9 \end{bmatrix} \cdot \begin{bmatrix} \boxed{\begin{matrix} 10 \\ 8 \end{matrix}} & \begin{matrix} 2 \\ 15 \end{matrix} \end{bmatrix} = \begin{bmatrix} \boxed{2\cdot 10+3\cdot 8} & 2\cdot 2+3\cdot 15 \\ 8\cdot 10+9\cdot 8 & 8\cdot 2+9\cdot 15 \end{bmatrix} = \begin{bmatrix} \boxed{44} & ? \\ ? & ? \end{bmatrix}$$

Language of ML: linear algebra – matrices

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  - Matrix really just concatenated vector, so similar process:

$$\begin{bmatrix} \boxed{2 \quad 3} \\ 8 \quad 9 \end{bmatrix} \cdot \begin{bmatrix} 10 & \boxed{\begin{matrix} 2 \\ 15 \end{matrix}} \\ 8 & \end{bmatrix} = \begin{bmatrix} 2 \cdot 10 + 3 \cdot 8 & \boxed{2 \cdot 2 + 3 \cdot 15} \\ 8 \cdot 10 + 9 \cdot 8 & 8 \cdot 2 + 9 \cdot 15 \end{bmatrix} = \begin{bmatrix} 44 & \boxed{49} \\ ? & ? \end{bmatrix}$$

Language of ML: linear algebra – matrices

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$$\begin{bmatrix} 2 & 3 \\ \boxed{8 \quad 9} \end{bmatrix} \cdot \begin{bmatrix} \boxed{\begin{matrix} 10 \\ 8 \end{matrix}} & \begin{matrix} 2 \\ 15 \end{matrix} \end{bmatrix} = \begin{bmatrix} 2\cdot 10+3\cdot 8 & 2\cdot 2+3\cdot 15 \\ \boxed{8\cdot 10+9\cdot 8} & 8\cdot 2+9\cdot 15 \end{bmatrix} = \begin{bmatrix} 44 & 49 \\ \boxed{152} & ? \end{bmatrix}$$

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-Sum of each element in the *row* of the matrix A * each element in the *column* of matrix B.

-2 by $\underbrace{2 \text{ matrix times } 2}_{\#\text{ of columns in A matches }\#\text{ of rows in B}}$ by 2 matrix becomes 2 by 2 matrix.

of *columns* in A matches # of *rows* in B

Language of ML: linear algebra – matrices

- Matrix-matrix multiplication is *non-commutative*: order matters!

$$\begin{bmatrix} 2 & 3 \\ 8 & 9 \end{bmatrix} \cdot \begin{bmatrix} 10 & 2 \\ 8 & 15 \end{bmatrix} = \begin{bmatrix} 44 & 49 \\ 152 & 151 \end{bmatrix}$$

$$2 \cdot 3 = 6$$

$$\begin{bmatrix} 10 & 2 \\ 8 & 15 \end{bmatrix} \cdot \begin{bmatrix} 2 & 3 \\ 8 & 9 \end{bmatrix} = \begin{bmatrix} 36 & 48 \\ 136 & 159 \end{bmatrix}$$

$$3 \cdot 2 = 6$$

Language of ML: linear algebra -application

- That‘s a lot of *mathiness.* How is this useful for linear regression?

Language of ML: linear algebra -application

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$$h_\theta(x) = \theta_0 + \theta_1 \cdot Gene\,1 + \theta_2 \cdot Gene\,2 + \theta_n \cdot Gene\,n$$

$$\begin{array}{rc} & \begin{array}{ccc} \text{Gene 1} & \text{Gene 2} & \text{Gene m} \end{array} \\ \begin{array}{r} \text{Sample 1} \\ \text{Sample 2} \\ \\ \text{Sample n} \end{array} & \begin{bmatrix} 2 & 3 & -2 \\ 8 & 9 & 1 \\ 0 & 4 & 5 \\ 5 & -2 & 2 \end{bmatrix} \end{array}$$

Language of ML: linear algebra -application

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$$\begin{array}{l} \\ \text{Sample 1} \\ \text{Sample 2} \\ \text{Sample ...} \\ \text{Sample n} \end{array}
\begin{array}{c} \begin{array}{ccc} \text{Gene 1} & \text{Gene 2} & \text{Gene m} \end{array} \\ \begin{bmatrix} 2 & 3 & -2 \\ 8 & 9 & 1 \\ 0 & 4 & 5 \\ 5 & -2 & 2 \end{bmatrix} \end{array}
\qquad
\begin{array}{c} \theta_0 \\ \theta_1 \\ \dots \\ \theta_n \end{array}
\begin{bmatrix} 3 \\ -0.5 \\ 5 \\ -1 \end{bmatrix}$$

Language of ML: linear algebra -application

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$$h_\theta(x)=\theta_0+\theta_1\cdot Gene\,1+\theta_2\cdot Gene\,2+\theta_n\cdot Gene\,n$$

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To get vector of predictions from vector of thetas and matrix of data, want to multiply them

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$$\begin{array}{r} \\ \text{Sample 1} \\ \text{Sample 2} \\ \text{Sample ...} \\ \text{Sample n} \end{array}
\begin{array}{c} \begin{array}{cccc} \text{Intercept} & \text{Gene 1} & \text{Gene 2} & \text{Gene m} \end{array} \\ \begin{bmatrix} 1 & 2 & 3 & -2 \\ 1 & 8 & 9 & 1 \\ 1 & 0 & 4 & 5 \\ 1 & 5 & -2 & 2 \end{bmatrix} \end{array}
\begin{array}{c} \theta_0 \\ \theta_1 \\ \dots \\ \theta_n \end{array}
\begin{bmatrix} 3 \\ -0.5 \\ 5 \\ -1 \end{bmatrix}$$

To get vector of predictions from vector of thetas and matrix of data, want to multiply them

Dimensions don‘t match, easy fix: new feature

Language of ML: linear algebra -application

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$$h_\theta(x)=\theta_0+\theta_1\cdot Gene\,1+\theta_2\cdot Gene\,2+\theta_n\cdot Gene\,n$$

$$\begin{array}{c} \theta_0 \\ \theta_1 \\ \dots \\ \theta_n \end{array} \begin{bmatrix} 3 \\ -0.5 \\ 5 \\ -1 \end{bmatrix} \cdot \begin{array}{r} \\ \text{Sample 1} \\ \text{Sample 2} \\ \text{Sample ...} \\ \text{Sample n} \end{array} \begin{array}{c} \begin{array}{cccc} \text{Intercept} & \text{Gene 1} & \text{Gene 2} & \text{Gene m} \end{array} \\ \begin{bmatrix} 1 & 2 & 3 & -2 \\ 1 & 8 & 9 & 1 \\ 1 & 0 & 4 & 5 \\ 1 & 5 & -2 & 2 \end{bmatrix} \end{array} \longrightarrow ?$$

Language of ML: linear algebra -application

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$$\begin{array}{c} \theta_0 \\ \theta_1 \\ \dots \\ \theta_n \end{array} \begin{bmatrix} \boxed{3} \\ -0.5 \\ 5 \\ -1 \end{bmatrix} \cdot \begin{array}{cc} & \begin{matrix}\text{Intercept} & \text{Gene 1} & \text{Gene 2} & \text{Gene m}\end{matrix} \\ \begin{matrix}\text{Sample 1}\\ \text{Sample 2}\\ \text{Sample ...}\\ \text{Sample n}\end{matrix} & \begin{bmatrix} 1 & 2 & 3 & -2 \\ 1 & 8 & 9 & 1 \\ 1 & 0 & 4 & 5 \\ 1 & 5 & -2 & 2 \end{bmatrix} \end{array} \longrightarrow$$

Wrong!
# of columns A doesn‘t match
rows B!

Language of ML: linear algebra -application

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\cdot
\begin{array}{c} \theta_0 \\ \theta_1 \\ \dots \\ \theta_n \end{array}
\begin{bmatrix} 3 \\ -0.5 \\ 5 \\ -1 \end{bmatrix}
\begin{bmatrix} \boxed{1\cdot 3+2\cdot -0.5+3\cdot 5+-2\cdot -1=19} \\ 43 \\ 18 \\ -11.5 \end{bmatrix}$$

Language of ML: linear algebra -application

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$$h_\theta(x) = \theta_0 + \theta_1 \cdot Gene\,1 + \theta_2 \cdot Gene\,2 + \theta_n \cdot Gene\,n$$

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\cdot
\begin{array}{c} \theta_0 \\ \theta_1 \\ \ldots \\ \theta_n \end{array}
\boxed{\begin{bmatrix} 3 \\ -0.5 \\ 5 \\ -1 \end{bmatrix}}
\quad
\begin{bmatrix} 1 \cdot 3 + 2 \cdot -0.5 + 3 \cdot 5 + -2 \cdot -1 = 19 \\ \boxed{43} \\ 18 \\ -11.5 \end{bmatrix}$$

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\cdot
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\begin{bmatrix} 1 & 2 & 3 & -2 \\ 1 & 8 & 9 & 1 \\ 1 & 0 & 4 & 5 \\ 1 & 5 & -2 & 2 \end{bmatrix}
\end{array}
\cdot
\begin{array}{c} \theta_0 \\ \theta_1 \\ \ldots \\ \theta_n \end{array}
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\begin{bmatrix} 1 \cdot 3 + 2 \cdot -0.5 + 3 \cdot 5 + -2 \cdot -1 = 19 \\ 43 \\ 18 \\ -11.5 \end{bmatrix}$$

Code comparison

```
#data setup
thetas = np.array([3, -0.5, 5, -1], np.newaxis)

featureDataFrame = pd.DataFrame({"Intercept" : [1,1,1,1],
                                 "Gene1" : [2,8,0,5],
                                 "Gene2" : [3,9,4,-2],
                                 "Gene3" : [-2, 1, 5, 2]})
featureDataFrame.index = (["Sample" + str(num) for num in range(1,5)] )

print(featureDataFrame)
print(thetas)
```

```
         Intercept  Gene1  Gene2  Gene3
Sample1          1      2      3     -2
Sample2          1      8      9      1
Sample3          1      0      4      5
Sample4          1      5     -2      2
[ 3.  -0.5  5.  -1. ]
```

```
#not vectorised
totalPredictions = []
for sample, sampleData in featureDataFrame.iterrows():
    thisPrediction = 0
    for index, feature in enumerate(sampleData):
      thisPrediction += feature * thetas[index]
    totalPredictions.append(thisPrediction)

print(totalPredictions)
```

```
[19.0, 43.0, 18.0, -11.5]
```

```
#vectorised
totalPredictionsLA = featureDataFrame @ thetas
print(totalPredictionsLA)
```

```
Sample1    19.0
Sample2    43.0
Sample3    18.0
Sample4   -11.5
dtype: float64
```

Code comparison

```
#data setup
thetas = np.array([3, -0.5, 5, -1], np.newaxis)

featureDataFrame = pd.DataFrame({"Intercept" : [1,1,1,1],
                                  "Gene1" : [2,8,0,5],
                                  "Gene2" : [3,9,4,-2],
                                  "Gene3" : [-2, 1, 5, 2]})
featureDataFrame.index = (["Sample" + str(num) for num in range(1,5)] )

print(featureDataFrame)
print(thetas)
```

```
         Intercept  Gene1  Gene2  Gene3
Sample1          1      2      3     -2
Sample2          1      8      9      1
Sample3          1      0      4      5
Sample4          1      5     -2      2
[ 3.  -0.5  5.  -1. ]
```

```
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totalPredictions = []
for sample, sampleData in featureDataFrame.iterrows():
    thisPrediction = 0
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      thisPrediction += feature * thetas[index]
    totalPredictions.append(thisPrediction)

print(totalPredictions)
```

```
[19.0, 43.0, 18.0, -11.5]
```

```
#vectorised
totalPredictionsLA = featureDataFrame @ thetas
print(totalPredictionsLA)
```

```
Sample1    19.0
Sample2    43.0
Sample3    18.0
Sample4   -11.5
dtype: float64
```

Code comparison

```
#data setup
thetas = np.array([3, -0.5, 5, -1], np.newaxis)

featureDataFrame = pd.DataFrame({"Intercept" : [1,1,1,1],
                                 "Gene1" : [2,8,0,5],
                                 "Gene2" : [3,9,4,-2],
                                 "Gene3" : [-2, 1, 5, 2]})
featureDataFrame.index = (["Sample" + str(num) for num in range(1,5)] )

print(featureDataFrame)
print(thetas)
```

```
         Intercept  Gene1  Gene2  Gene3
Sample1          1      2      3     -2
Sample2          1      8      9      1
Sample3          1      0      4      5
Sample4          1      5     -2      2
[ 3.  -0.5  5.  -1. ]
```

```
#not vectorised
totalPredictions = []
for sample, sampleData in featureDataFrame.iterrows():
    thisPrediction = 0
    for index, feature in enumerate(sampleData):
      thisPrediction += feature * thetas[index]
    totalPredictions.append(thisPrediction)

print(totalPredictions)
```

```
[19.0, 43.0, 18.0, -11.5]
```

```
#vectorised
totalPredictionsLA = featureDataFrame @ thetas
print(totalPredictionsLA)
```

```
Sample1    19.0
Sample2    43.0
Sample3    18.0
Sample4   -11.5
dtype: float64
```

Summary

- Linear algebra is the basis of ML: algorithms are defined in it and run quickly due to hardware optimised for matrix and vector operations
- Using linear algebra cuts down on code complexity
- You always add a „dummy“ feature that is 1 to multiply with θ_0
- We covered how to multiply and add matrices and vectors, and showed that matrix multiplication is *non-commutative*: order matters!

Practical

- Practicing vector and matrix operations with numpy
- Changing cost function, hypothesis function, and gradient descent to work with matrices and vectors
- Working with a real biological dataset

HAVE FUN!

Language of ML: linear algebra -application

- That‘s a lot of *mathiness.* How is this useful for linear regression?

$$h_\theta(x)=\theta_0+\theta_1\cdot Gene\,1+\theta_2\cdot Gene\,2+\theta_n\cdot Gene\,n$$

$$\begin{array}{c} \\ \text{Sample 1} \\ \text{Sample 2} \\ \text{Sample ...} \\ \text{Sample n} \end{array}
\begin{array}{c} \begin{array}{cccc} \text{Intercept} & \text{Gene 1} & \text{Gene 2} & \text{Gene m} \end{array} \\ \begin{bmatrix} 1 & 2 & 3 & -2 \\ 1 & 8 & 9 & 1 \\ 1 & 0 & 4 & 5 \\ 1 & 5 & -2 & 2 \end{bmatrix}^T \end{array}
=
\begin{array}{c} \begin{array}{cccc} \text{Sample 1} & \text{Sample 2} & \text{Sample ...} & \text{Sample n} \end{array} \\ \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 8 & 0 & 5 \\ 3 & 9 & 4 & -2 \\ -2 & 1 & 5 & 2 \end{bmatrix} \end{array}
\begin{array}{l} \\ \text{Intercept} \\ \text{Gene 1} \\ \text{Gene 2} \\ \text{Gene m} \end{array}$$

$$\begin{array}{c} \theta_0 \\ \theta_1 \\ \dots \\ \theta_n \end{array} \begin{bmatrix} 3 \\ -0.5 \\ 5 \\ -1 \end{bmatrix}$$