

This presentation

- Intuition about linear algebra
- Matrix-vector and matrix-matrix multiplications
- Using linear algebra to express ML algorithms
- Worked example gradient descent in linear algebra

Language of ML: linear algebra

Language of ML: linear algebra – what is it?

- Calculations with vectors and matrices

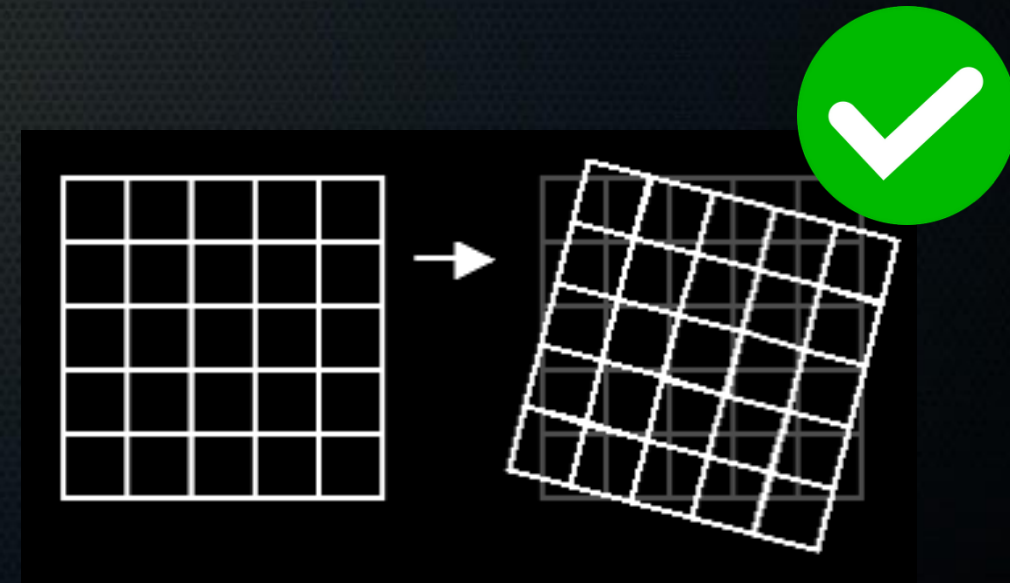
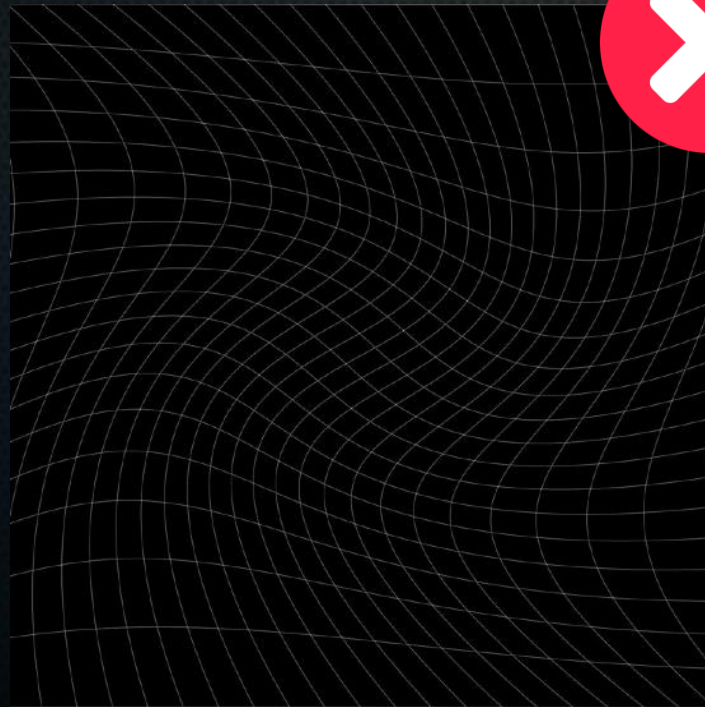
$$\begin{cases} 2x + 3y = 8 \\ x - y = 1 \end{cases}$$



$$\begin{bmatrix} 2 & 3 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 8 \\ 1 \end{bmatrix}$$

Language of ML: linear algebra – what is it?

- Calculations with vectors and matrices
- Should stay linear: just addition and scalar multiplication. No curves.



Language of ML: linear algebra – what is it?

- Calculations with vectors and matrices

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



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Language of ML: linear algebra – what is it?

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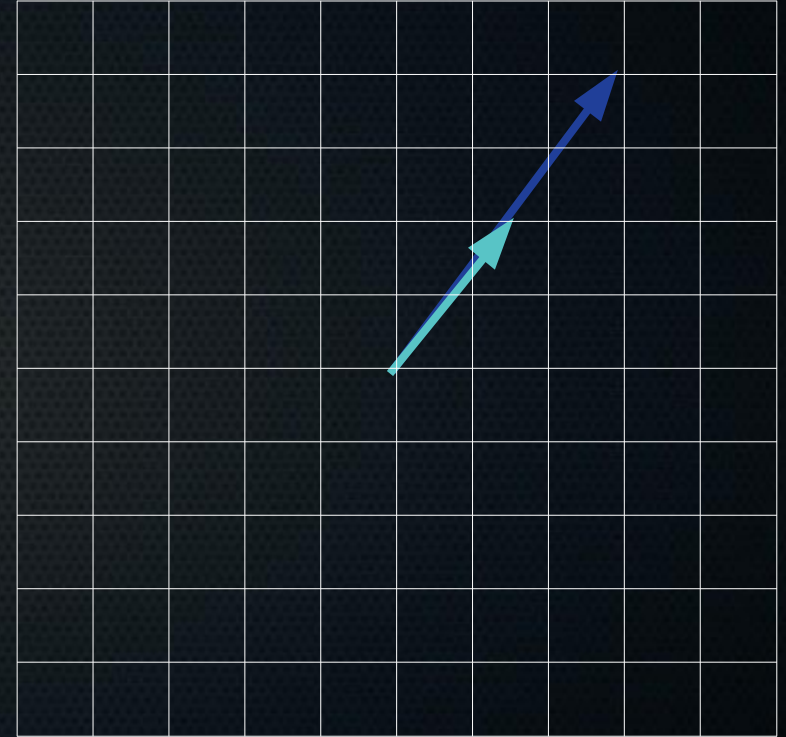
$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$$



Language of ML: linear algebra – what is it?

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

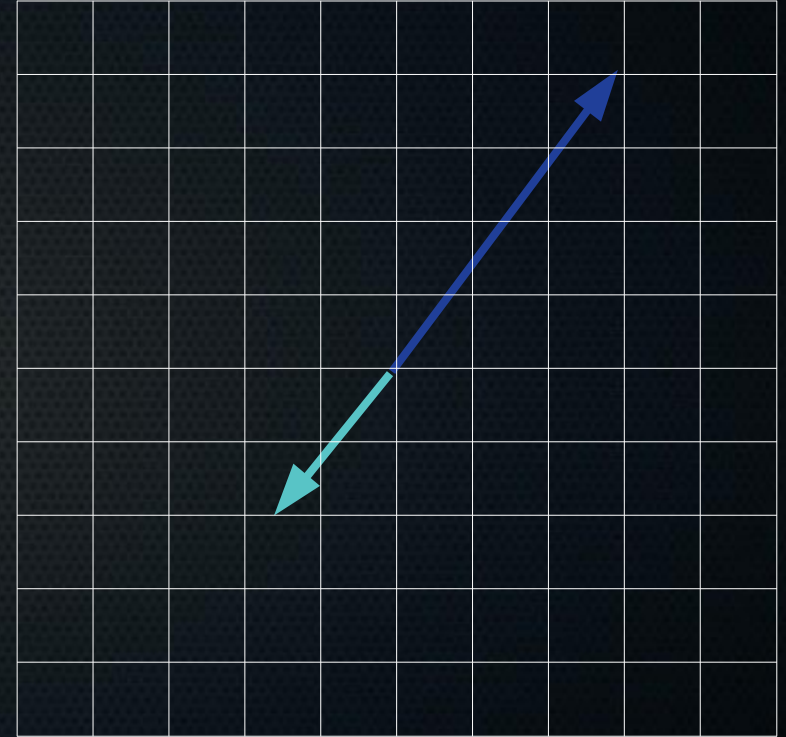
$$0.5 \cdot \begin{bmatrix} 3 \\ 4 \end{bmatrix} \longrightarrow \begin{bmatrix} 1.5 \\ 2 \end{bmatrix}$$



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



*



Language of ML: linear algebra – what is it?

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

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \cdot \begin{bmatrix} 3 \\ 4 \end{bmatrix} \longrightarrow \begin{bmatrix} 11 \\ 25 \end{bmatrix}$$



Language of ML: linear algebra – what is it?

- Calculations with vectors and matrices
- Or matrix-vector multiplication
- Corresponds to a sort of squishing of space

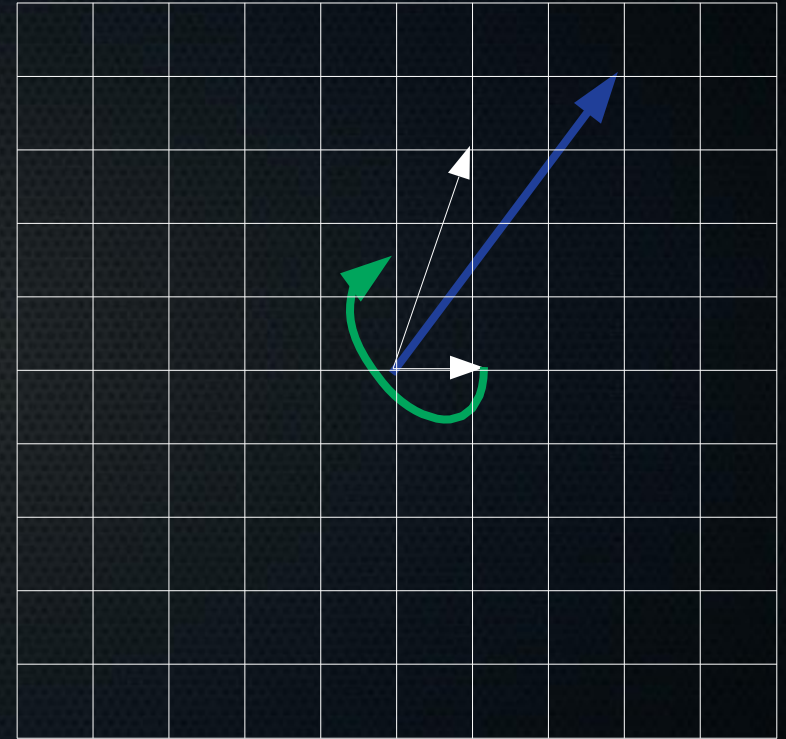
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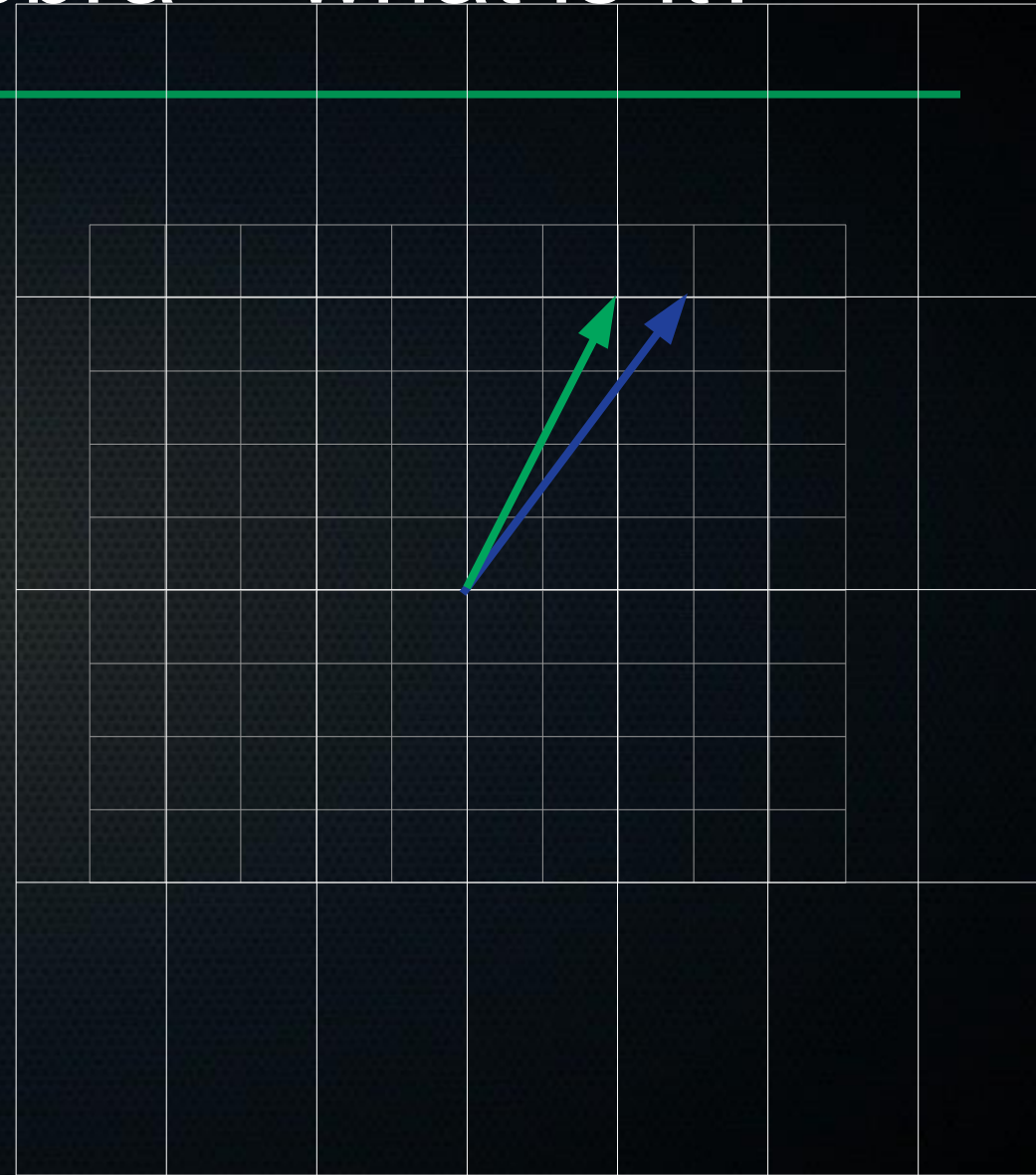
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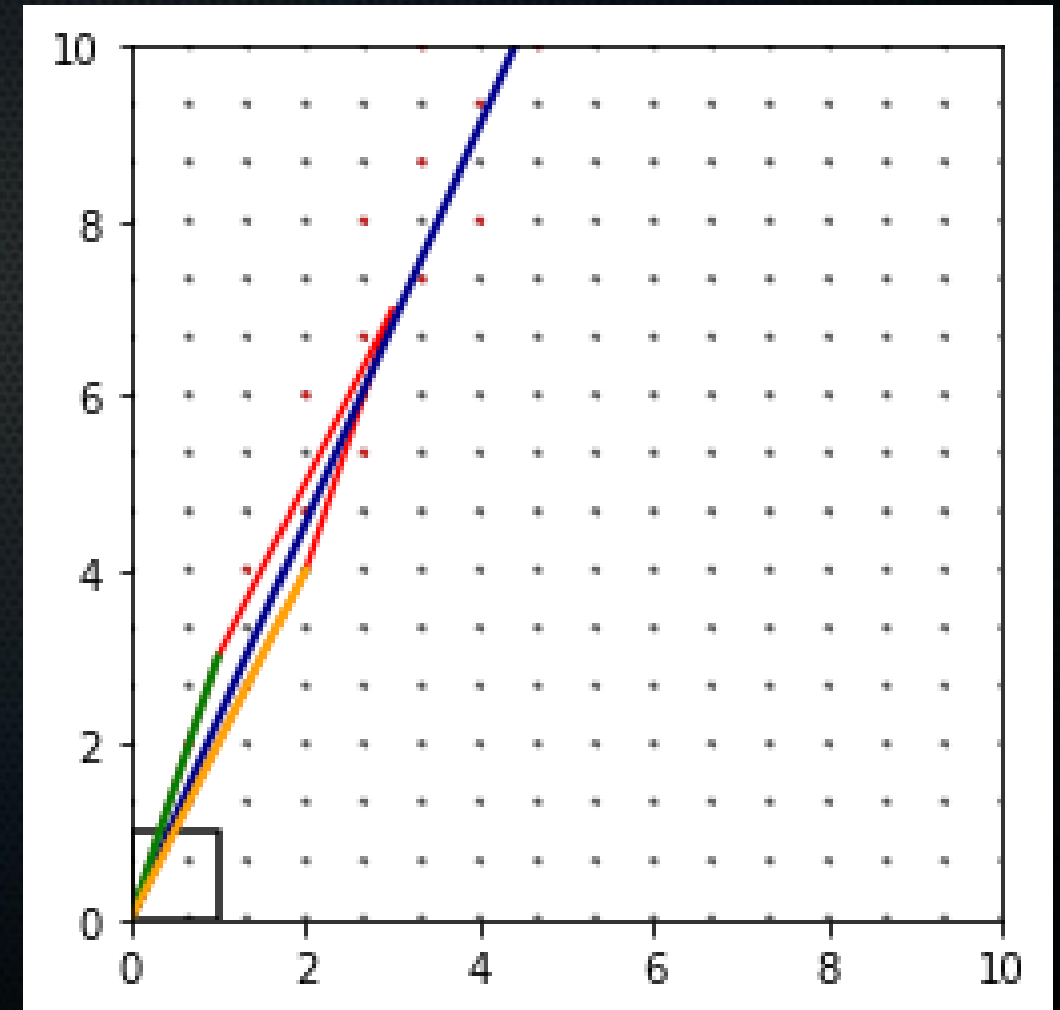
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Language of ML: linear algebra – why do we care?

- 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: $\sim 5622 * 10^9$ /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):

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

Language of ML: linear algebra – vectors

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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

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

Language of ML: linear algebra – matrices

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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

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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

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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 *columns* in A matches # of
rows in B

Language of ML: linear algebra – matrices

- Matrix-vector multiplication:

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

-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:

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

Language of ML: linear algebra – matrices

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Language of ML: linear algebra – matrices

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Language of ML: linear algebra – matrices

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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 2 matrix times 2 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!

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

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



$2 \cdot 3 = 6$

$3 \cdot 2 = 6$

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

	Gene 1	Gene 2	Gene n
Sample 1	2	3	-2
Sample 2	8	9	1
Sample ...	0	4	5
Sample m	5	-2	2

Language of ML: linear algebra -application

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$$\begin{bmatrix} \theta_0 \\ \theta_1 \\ \dots \\ \theta_n \end{bmatrix}$$

Language of ML: linear algebra -application

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

Language of ML: linear algebra -application

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

	Intercept	Gene 1	Gene 2	Gene n		
Sample 1	1	2	3	-2	θ_0	3
Sample 2	1	8	9	1	θ_1	-0.5
Sample ...	1	0	4	5	...	5
Sample m	1	5	-2	2	θ_n	-1

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

θ_0	$\begin{bmatrix} 3 \\ -0.5 \\ 5 \\ -1 \end{bmatrix}$		$\begin{matrix} \text{Intercept} \\ \text{Gene 1} \\ \text{Gene 2} \\ \text{Gene } n \end{matrix}$	$\begin{bmatrix} 1 & 2 & 3 & -2 \\ 1 & 8 & 9 & 1 \\ 1 & 0 & 4 & 5 \\ 1 & 5 & -2 & 2 \end{bmatrix}$	$\longrightarrow ?$
θ_1		Sample 1			
θ_2		Sample 2			
\dots		Sample ...			
θ_n		Sample m			

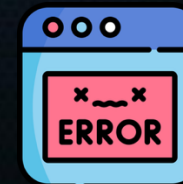
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θ_0	3	1	2	3	-2
θ_1	-0.5	1	8	9	1
...	5	1	0	4	5
θ_n	-1	1	5	-2	2

Wrong!
of columns A doesn't match
rows B!



Language of ML: linear algebra -application

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

Language of ML: linear algebra -application

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$$\begin{array}{c}
 \theta_0 \\
 \theta_1 \\
 \dots \\
 \theta_n
 \end{array}
 \begin{bmatrix}
 3 \\
 -0.5 \\
 5 \\
 -1
 \end{bmatrix}
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Language of ML: linear algebra -application

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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
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Sample3	18.0
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```
dtype: float64
```

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    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!

Summary

- In a very real way we are just using linear algebra as ✨fancy bookkeeping✨, and computer hardware is optimized for this as many operations can be expressed in terms of this bookkeeping.

Numpy details

- During the computer lab, try to make your basic unit a column vector. That is, a 2D array that looks like this:

```
array([[0],  
       [1],  
       [5]])
```
- When you subset things, numpy automatically makes single lists 1D. To make a 1D array 2D again, use `array[:, np.newaxis]`
- For your thetas, too, don't use a list like so: `[0.5, -0.3, 0.8]`, but make it 2D.
- To check whether something is the right form, you can check that `array.ndim == 2`, for instance.

Gradient descent in linear algebra

- Goal gradient descent: take a small step in every parameter such that you get closer to the minimum of the cost. Return new theta's.

$$\theta_{0_{new}} = \theta_0 - \frac{\alpha}{m} \sum_{i=1}^m ((h_{\theta}(x^{(i)}) - y^{(i)}) \cdot 1)$$

$$\theta_{1_{new}} = \theta_1 - \frac{\alpha}{m} \sum_{i=1}^m ((h_{\theta}(x^{(i)}) - y^{(i)}) \cdot x_1^{(i)})$$

$$\theta_{2_{new}} = \theta_2 - \frac{\alpha}{m} \sum_{i=1}^m ((h_{\theta}(x^{(i)}) - y^{(i)}) \cdot x_2^{(i)})$$

Gradient descent in linear algebra

We have data, known values, and initial theta's:

$$X = \begin{bmatrix} 1 & feat_1 val_1 & feat_2 val_1 \\ 1 & feat_1 val_2 & feat_2 val_2 \end{bmatrix}; y = \begin{bmatrix} 10.23 \\ -4 \end{bmatrix}; params = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix}$$

Get predicted values:

$$\begin{bmatrix} 1 & feat_1 val_1 & feat_2 val_1 \\ 1 & feat_1 val_2 & feat_2 val_2 \end{bmatrix} @ \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix} = \begin{bmatrix} 9.23 \\ -2.5 \end{bmatrix}$$

2 by 3 times 3 by 1 gives 2 by 1 (rows by columns)

Get errors:

$$errs = \begin{bmatrix} 9.23 \\ -2.5 \end{bmatrix} - y = \begin{bmatrix} 9.23 \\ -2.5 \end{bmatrix} - \begin{bmatrix} 10.23 \\ -4 \end{bmatrix} = \begin{bmatrix} -1 \\ 1.5 \end{bmatrix}$$

Where did the ² go?

$$J = \frac{1}{2m} \sum (\text{pred} - y)^2$$

$$\frac{\partial J}{\partial \text{pred}} = \frac{1}{m} (\text{pred} - y)$$

Gradient descent in linear algebra

$$errs = \begin{bmatrix} -1 \\ 1.5 \end{bmatrix}$$

$$\theta_{0new} = \theta_0 - \frac{a}{m} \sum_{i=1}^m ([h_{\theta}(x^{(i)}) - y^{(i)}] \cdot 1)$$

$$\theta_{1new} = \theta_1 - \frac{a}{m} \sum_{i=1}^m ([h_{\theta}(x^{(i)}) - y^{(i)}] \cdot x_1^{(i)})$$

$$\theta_{2new} = \theta_2 - \frac{a}{m} \sum_{i=1}^m ([h_{\theta}(x^{(i)}) - y^{(i)}] \cdot x_2^{(i)})$$

Gradient descent in linear algebra

Calculate, for each feature, sum of each error times that feature:

$$\begin{bmatrix} -1 \\ 1.5 \end{bmatrix}^T = [-1 \quad 1.5]$$

$$[-1 \quad 1.5] @ \begin{bmatrix} 1 & feat_1val_1 & feat_2val_1 \\ 1 & feat_1val_2 & feat_2val_2 \end{bmatrix} =$$

$$errs = \begin{bmatrix} -1 \\ 1.5 \end{bmatrix}$$

$$[-1 \cdot 1 + 1.5 \cdot 1 \quad -1 \cdot feat_1val_1 + 1.5 \cdot feat_1val_2 \quad -1 \cdot feat_2val_1 + 1.5 \cdot feat_2val_2]$$

Gradient descent in linear algebra

Calculate, for each feature, sum of each error times that feature:

$$\begin{bmatrix} -1 \\ 1.5 \end{bmatrix}^T = \begin{bmatrix} -1 & 1.5 \end{bmatrix}$$

$$errs = \begin{bmatrix} -1 \\ 1.5 \end{bmatrix}$$

$$\begin{bmatrix} -1 & 1.5 \end{bmatrix} @ \begin{bmatrix} 1 & feat_1val_1 & feat_2val_1 \\ 1 & feat_1val_2 & feat_2val_2 \end{bmatrix} =$$

$$\begin{bmatrix} -1 \cdot 1 + 1.5 \cdot 1 & -1 \cdot feat_1val_1 + 1.5 \cdot feat_1val_2 & -1 \cdot feat_2val_1 + 1.5 \cdot feat_2val_2 \end{bmatrix}$$

$$\theta_{0new} = \theta_0 - \frac{a}{m} \sum_{i=1}^m ((h_{\theta}(x^{(i)}) - y^{(i)}) \cdot 1)$$

$$\theta_{1new} = \theta_1 - \frac{a}{m} \sum_{i=1}^m ((h_{\theta}(x^{(i)}) - y^{(i)}) \cdot x_1^{(i)}) \quad \theta_{2new} = \theta_2 - \frac{a}{m} \sum_{i=1}^m ((h_{\theta}(x^{(i)}) - y^{(i)}) \cdot x_2^{(i)})$$

Gradient descent in linear algebra

Now all that we need to do is multiply with α/m and subtract from our old theta's:

$$\begin{aligned} & \alpha/m \cdot \begin{bmatrix} -1 \cdot 1 + 1.5 \cdot 1 & -1 \cdot feat_1 val_1 + 1.5 \cdot feat_1 val_2 & -1 \cdot feat_2 val_1 + 1.5 \cdot feat_2 val_2 \end{bmatrix} \\ &= \begin{bmatrix} \frac{\alpha}{m}(-1 \cdot 1 + 1.5 \cdot 1) & \frac{\alpha}{m}(-1 \cdot feat_1 val_1 + 1.5 \cdot feat_1 val_2) & \frac{\alpha}{m}(-1 \cdot feat_2 val_1 + 1.5 \cdot feat_2 val_2) \end{bmatrix} \end{aligned}$$

Transpose it:

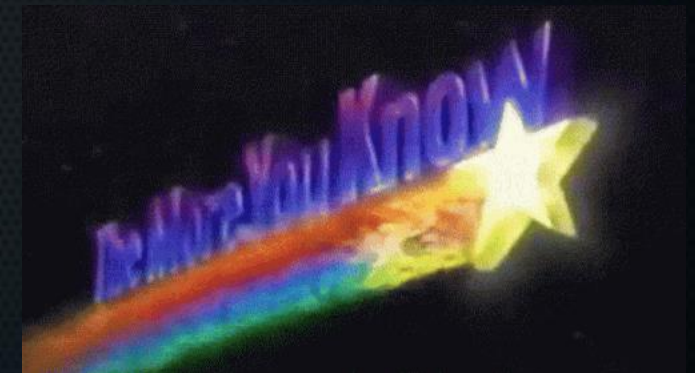
$$\begin{bmatrix} \frac{\alpha}{m}(-1 \cdot 1 + 1.5 \cdot 1) & \frac{\alpha}{m}(-1 \cdot feat_1 val_1 + 1.5 \cdot feat_1 val_2) & \frac{\alpha}{m}(-1 \cdot feat_2 val_1 + 1.5 \cdot feat_2 val_2) \end{bmatrix}^T = \begin{bmatrix} \frac{\alpha}{m}(-1 \cdot 1 + 1.5 \cdot 1) \\ \frac{\alpha}{m}(-1 \cdot feat_1 val_1 + 1.5 \cdot feat_1 val_2) \\ \frac{\alpha}{m}(-1 \cdot feat_2 val_1 + 1.5 \cdot feat_2 val_2) \end{bmatrix}$$

So finally:

$$\begin{bmatrix} \theta_{0old} \\ \theta_{1old} \\ \theta_{2old} \end{bmatrix} - \begin{bmatrix} \frac{\alpha}{m}(-1 \cdot 1 + 1.5 \cdot 1) \\ \frac{\alpha}{m}(-1 \cdot feat_1 val_1 + 1.5 \cdot feat_1 val_2) \\ \frac{\alpha}{m}(-1 \cdot feat_2 val_1 + 1.5 \cdot feat_2 val_2) \end{bmatrix} = \begin{bmatrix} \theta_{0new} \\ \theta_{1new} \\ \theta_{2new} \end{bmatrix}$$

$$\theta_{1new} = \theta_{1old} - \frac{\alpha}{m} \sum_{i=1}^m ((h_{\theta}(x^{(i)}) - y^{(i)}) \cdot x_1^{(i)})$$

Relevant XKCD



Computer Lab

- 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!

(and/or suffer if it's too hard... but then tell me and I shall try to ease your suffering)