Section 7

Admin

- Office Hours: Wednesday 1-2PM!
- Homework 2 thoughts?
- Homework 3: **March 2nd**
- Course and Section Feedback?

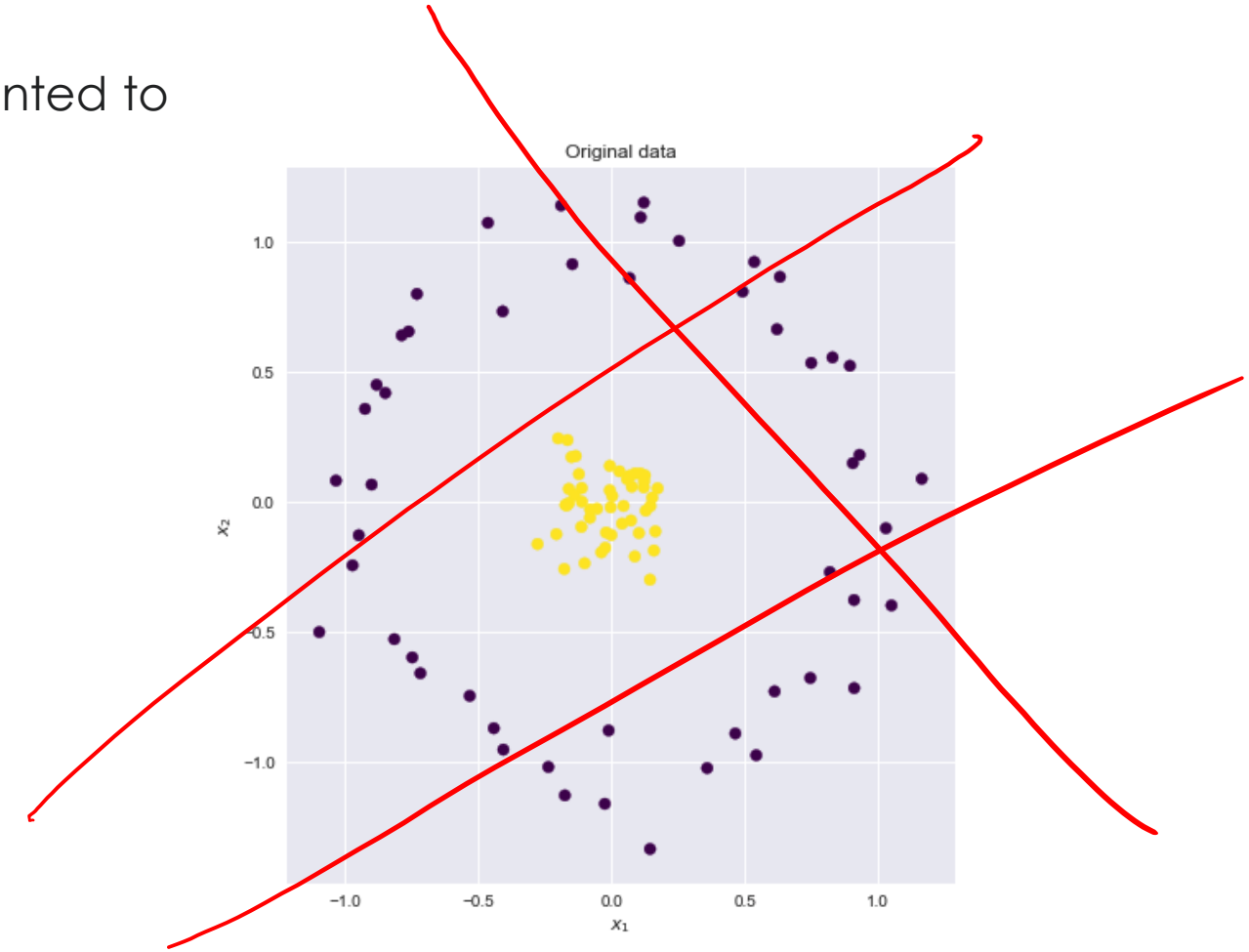
Agenda

- Kernels (~35 min)
  - Questions 1, 2, 3
- PyTorch Neural Network Edition (~15 min)
  - Notebook

Kernels

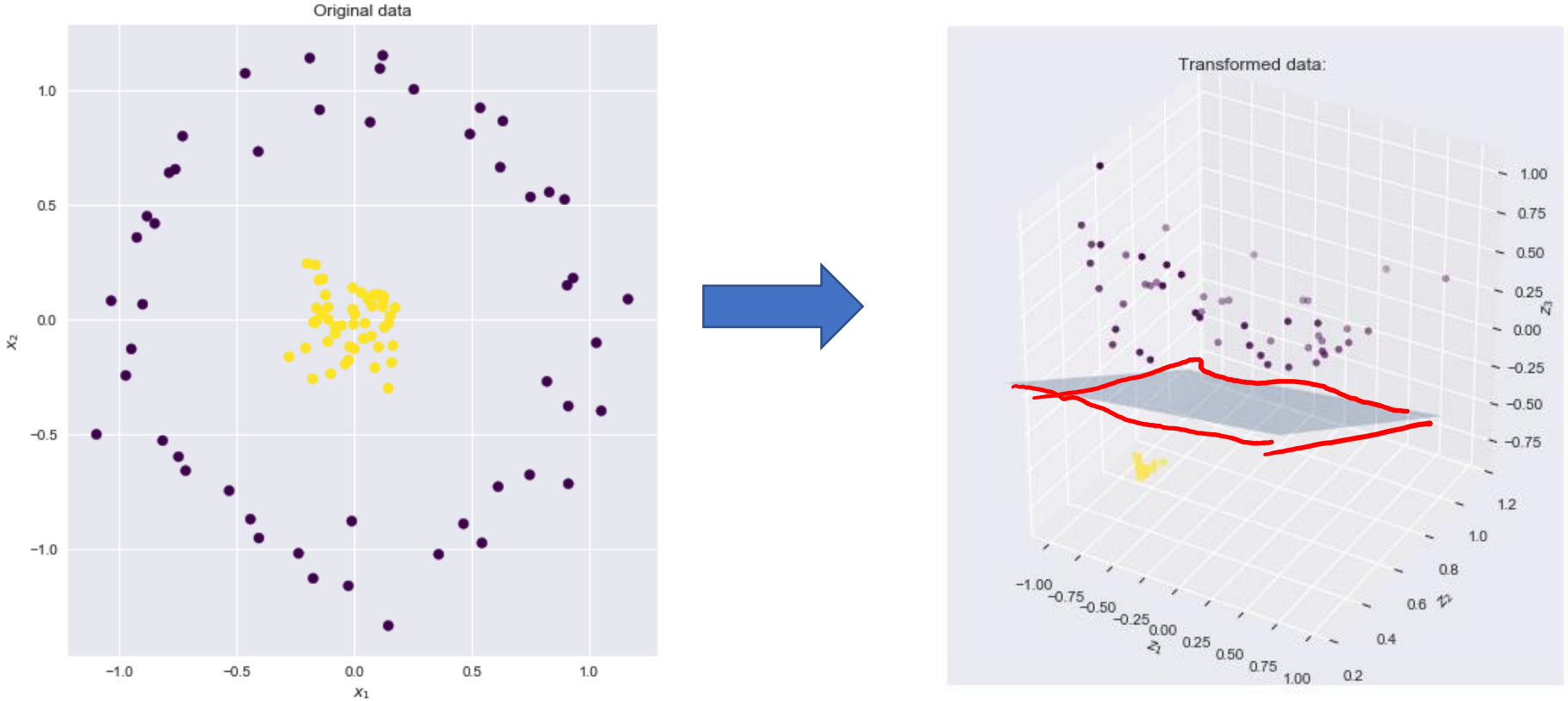
Kernels – Motivation

- Suppose we had input data and wanted to classify with a linear classifier (SVM)
- Clearly not linearly separable!
- What's the solution?



Kernels – Motivation

- Using a Kernel (polynomial):



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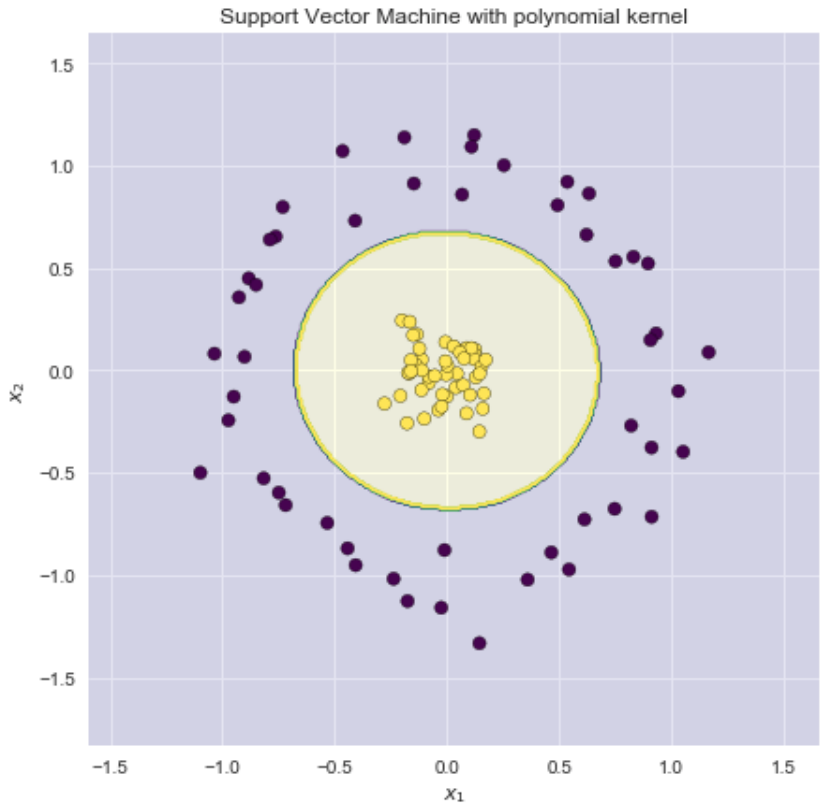
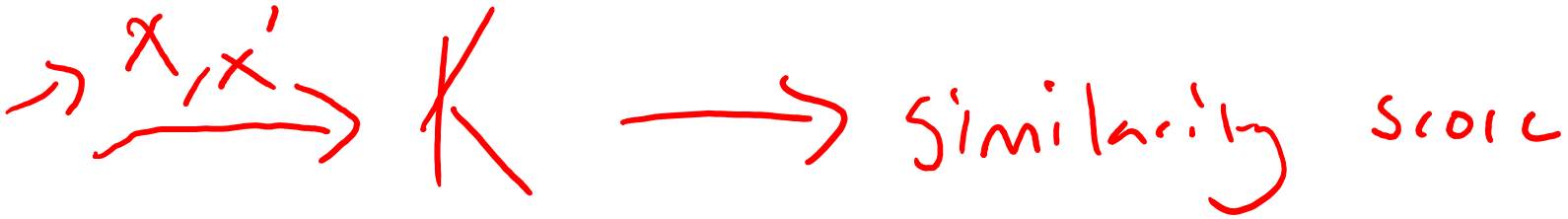


w/ SVM

Kernels – Math

- **Definition:** Let $\Phi: \mathbb{R}^k \to \mathbb{R}^d$, then a function $K: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a kernel for Φ if $K(x, x') = \phi(x) \cdot \phi(x')$ for all x, x'.
  - Can be thought of as a similarity metric for objects x, x'.



Kernels – Math

- **Definition:** Let $\Phi: \mathbb{R}^k \to \mathbb{R}^d$, then a function $K: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a kernel for Φ if $K(x, x') = \phi(x) \cdot \phi(x')$ for all x, x'.
  - Can be thought of as a similarity metric for objects x, x'.

We've justified why high dimensional data is important, but why is a kernel helpful?

Kernels – Math Intuition

Given dataset $x = (1, 2, 3), y = (3, 4, 5)$, and $\phi: z \to z \times z$, lets try and calculate $\langle \Phi(x), \Phi(y) \rangle$.

Kernels – Math Intuition

Given dataset $x = (1, 2, 3), y = (3, 4, 5)$, and $\phi: z \to z \times z$, lets try and calculate $\langle \Phi(x), \Phi(y) \rangle$. Note that $K(x, y) = (\langle x, y \rangle)^2$.

Method 1:

$\Phi(z) = \langle z_1 z_1, z_1 z_2, z_1 z_3, z_2 z_1, z_2 z_2, z_2 z_3, z_3 z_1, z_3 z_2, z_3 z_3 \rangle$

$\Phi(x) = \langle 1,2,3,2,4,6,3,6,9 \rangle$

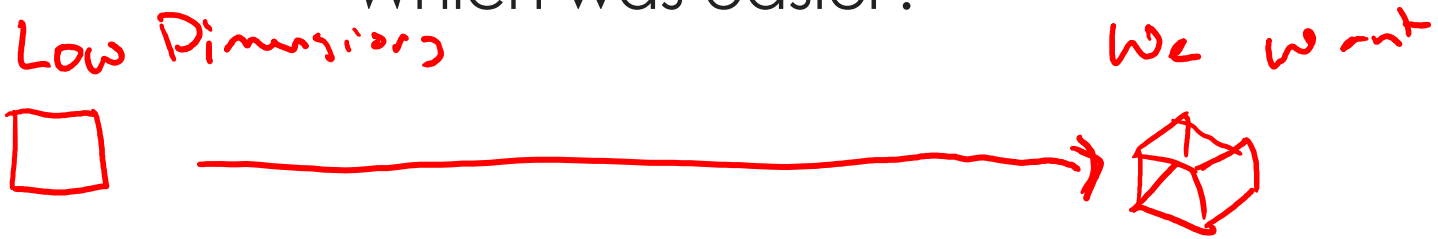
$\Phi(z) = \langle 16,20,24,20,25,30,24,30,36 \rangle$

$\langle \Phi(x), \Phi(y) \rangle = 16 + 40 + 72 + 40 + 100 + 180 + 72 + 180 + 324 = 1024$

Method 2:

$K(x, y) = (\langle x, y \rangle)^2 = (4 + 10 + 18)^2 = 1024$

Which was easier?



Kernels – Kernelized Regression (1)

Consider regularized linear regression (without a bias, for simplicity). We want to find the optimal parameters $\hat{w} = \arg\min_w L(w)$ for k-featured dataset $(x_i, y_i)_{i=1}^n$ (i.e. $X \in \mathbb{R}^{n \times k}$) that minimizes the following loss function:

$$L(w) = \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda ||w||_2^2$$

From class, we know there is an optimal $\hat{w}$ that lies in the span of the datapoints. Concretely, there exists $\alpha_1, ..., \alpha_n \in \mathbb{R}$ such that $\hat{w} = \sum_i^n \alpha_i x_i$.

Kernels – Kernelized Regression (1a)

Let $\alpha \in \mathbb{R}^n$, $\mathbf{K} \in \mathbb{R}^{n \times n}$, $\mathbf{y} \in \mathbb{R}^n$. Further, let us assume that we are using a linear kernel where $\mathbf{K}_{ij} = x_i^T x_j$. Express the loss function $L(w)$ in terms of $\mathbf{K}$ and α as $L(\alpha)$.

$$L(w) = \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda ||w||_2^2$$

want $L(\alpha)$

$$\hat{w} = \sum_i^n \alpha_i x_i.$$

$$w^T = \sum_j (\alpha_j x_j^T)$$

Kernels – Kernelized Regression (1a)

Let $\alpha \in \mathbb{R}^n$, $\mathbf{K} \in \mathbb{R}^{n \times n}$, $\mathbf{y} \in \mathbb{R}^n$. Further, let us assume that we are using a linear kernel where $\mathbf{K}_{ij} = x_i^T x_j$. Express the loss function $L(w)$ in terms of $\mathbf{K}$ and α as $L(\alpha)$.

$$
\begin{aligned}
L(\alpha) &= \sum_i^n \left(\sum_j^n (\alpha_j x_j^T) x_i - y_i \right)^2 + \lambda || \sum_i^n \alpha_i x_i ||^2 \\
&= \sum_i^n \left(\sum_j^n (\alpha_j x_j^T)\, x_i - y_i \right)^2 + \lambda (\sum_i^n \alpha_i x_i)^T (\sum_i^n \alpha_i x_i) \\
&= \sum_i^n \left(\sum_j^n \alpha_j (x_j, x_i) - y_i \right)^2 + \lambda \sum_i^n \sum_j^n \alpha_i \alpha_j x_i^T x_j \\
&= \sum_i^n \left(\sum_j^n \alpha_j K(x_j, x_i) - y_i \right)^2 + \lambda \sum_i^n \sum_j^n \alpha_i \alpha_j K(x_i, x_j) \\
&= ||\mathbf{y} - \mathbf{K}\alpha||_2^2 + \lambda \alpha^T \mathbf{K} \alpha
\end{aligned}
$$

Kernels – Kernelized Regression (1b)

Assuming that $\mathbf{K}$ is invertible, solve for the optimal $\hat{\alpha}$.

$L(\alpha)$ $||\mathbf{y} - \mathbf{K}\alpha||_2^2 + \lambda\alpha^T\mathbf{K}\alpha$

$\nabla L(\alpha) = 0$

Kernels – Kernelized Regression (1b)

Assuming that $\mathbf{K}$ is invertible, solve for the optimal $\hat{\alpha}$. $\|\mathbf{y} - \mathbf{K}\alpha\|_2^2 + \lambda\alpha^T\mathbf{K}\alpha$

Set the gradient of $L(\alpha) = 0$:

$$\nabla L(\alpha) = 0$$

So then,

$$\begin{aligned}
-2\mathbf{K}(\mathbf{y} - \mathbf{K}\alpha) + 2\lambda\mathbf{K}\alpha &= 0 \\
-\mathbf{K}(\mathbf{y} - \mathbf{K}\alpha) + \lambda\mathbf{K}\alpha &= 0 \\
\mathbf{K}(\mathbf{K}\alpha - \mathbf{y} + \lambda\alpha) &= 0 \\
\mathbf{K}((\mathbf{K} + \lambda I)\alpha - \mathbf{y}) &= 0 \\
\mathbf{K}(\mathbf{K} + \lambda I)\alpha &= \mathbf{K}\mathbf{y} \\
\hat{\alpha} &= (\mathbf{K} + \lambda I)^{-1}\mathbf{y}
\end{aligned}$$

Kernels – Kernelized Regression (1c)

Suppose after training our model on $\mathbf{X}_{\text{train}}$ we seek to make predictions on $\mathbf{X}_{\text{test}}$. Express these predictions $\hat{\mathbf{Y}}$ in terms of $\mathbf{K}_{train} = \mathbf{X}_{train}\mathbf{X}_{train}^T$, $\mathbf{y}_{train}$, $\mathbf{X}_{\text{train}}$, and $\mathbf{X}_{\text{test}}$. What would the general prediction formula look like if we are not using a linear kernel? Express the solution in terms of $\mathbf{K}_{\text{train, test}} = \Phi(\mathbf{X}_{test})\Phi(\mathbf{X}_{train}^T)$ and $\hat{\alpha}$, where for arbitrary d, we have $\Phi : \mathbb{R}^k \to \mathbb{R}^d$.

$$\hat{\alpha} = (K + \lambda I)^{-1} y$$

Kernels – Kernelized Regression (1c)

Suppose after training our model on $\mathbf{X}_{\text{train}}$ we seek to make predictions on $\mathbf{X}_{\text{test}}$. Express these predictions $\hat{\mathbf{Y}}$ in terms of $\mathbf{K}_{train} = \mathbf{X}_{train}\mathbf{X}_{train}^T$, $\mathbf{y}_{train}$, $\mathbf{X}_{\text{train}}$, and $\mathbf{X}_{\text{test}}$. What would the general prediction formula look like if we are not using a linear kernel? Express the solution in terms of $\mathbf{K}_{\text{train, test}} = \Phi(\mathbf{X}_{test})\Phi(\mathbf{X}_{train}^T)$ and $\hat{\alpha}$, where for arbitrary d, we have $\Phi : \mathbb{R}^k \to \mathbb{R}^d$.

General Solution for Kernel Ridge

$$\begin{aligned}\hat{\mathbf{Y}} &= \mathbf{X}_{\text{test}}\hat{w} \\ &= \mathbf{X}_{\text{test}}\mathbf{X}_{\text{Train}}^T\hat{\alpha} \\ &= \mathbf{X}_{\text{test}}\mathbf{X}_{\text{train}}^T\left(\mathbf{K}_{\text{train}} + \lambda I\right)^{-1}\mathbf{y}_{\text{train}}\end{aligned}$$

$$\begin{aligned}\hat{\mathbf{Y}} &= \Phi(\mathbf{X}_{\text{test}})\Phi(\mathbf{X}_{\text{train}}^T)\left(\mathbf{K}_{\text{train}} + \lambda I\right)^{-1}\mathbf{y}_{\text{train}} \\ &= \mathbf{K}_{\text{train, test}}\hat{\alpha}\end{aligned}$$

Kernels – Proving $\hat{w} \in Span(x_1, \ldots, x_n)$ (2)

Why is this something we need to show?

$\Updownarrow$

$\hat{w} = \sum a_i x_i$

K

Kernels – Proving $\hat{w} \in Span(x_1, ..., x_n)$ (2)

Why is this something we need to show?

We will prove this through contradiction. Assume $\hat{w} \notin Span(x_1, ..., x_n)$ solves $\arg\min_w L(w)$ where $L(w)$ is defined above. Then, there exists a component of $\hat{w}$ that is perpendicular to the span, which we will call $w^{\perp}$. Concretely,

$$\hat{w} = \bar{w} + w^{\perp}$$

Where $\bar{w} = \sum_i^n \alpha_i x_i$ is the component of $\hat{w}$ in the span of the datapoints.

Kernels – Proving $\hat{w} \in Span(x_1, ..., x_n)$ (2a)

Show that $\hat{w} \cdot x_i = \bar{w} \cdot x_i$, for every x_i. (Hint: what is the relationship of $w^{\perp}$ and x_i)

Kernels – Proving $\hat{w} \in Span(x_1, \ldots, x_n)$ (2a)

Show that $\hat{w} \cdot x_i = \bar{w} \cdot x_i$, for every x_i. (Hint: what is the relationship of $w^\perp$ and x_i)

$$\begin{aligned}
\hat{w} \cdot x_i &= (\bar{w} + w^\perp) \cdot x_i \\
&= \bar{w} \cdot x_i + w^\perp \cdot x_i \\
&= \bar{w} \cdot x_i + 0 \\
&= \bar{w} \cdot x_i
\end{aligned}$$

$w^\perp$ is perpindicular to each x_i

Kernels – Proving $\hat{w} \in Span(x_1, ..., x_n)$ (2b)

Now, show that $||\hat{w}||_2^2 \geq ||\bar{w}||_2^2$. (Hint: Use the Pythagorean Theorem)

$$||\hat{w}||_2^2 = ||\bar{w} + w^{\perp}||_2^2$$

$$= ||\bar{w}||_2^2 + ||w^{\perp}||_2^2 \quad (2)$$

$$\geq ||\bar{w}||_2^2 \quad (1)$$

Why?

Kernels – Proving $\hat{w} \in Span(x_1, ..., x_n)$ (2b)

Now, show that $||\hat{w}||_2^2 \geq ||\bar{w}||_2^2$. (Hint: Use the Pythagorean Theorem)

$$
\begin{aligned}
||\hat{w}||_2^2 &= ||\bar{w} + w^{\perp}||_2^2 \\
&= ||\bar{w}||_2^2 + ||w^{\perp}||_2^2 \qquad \text{Pythagorean Theorem} \\
&\geq ||\bar{w}||_2^2
\end{aligned}
$$

Kernels – Proving $\hat{w} \in Span(x_1, ..., x_n)$ (2c)

Finally, show that $\hat{w} \in Span(x_1, ..., x_n)$. (Hint: Think about the regularization term)

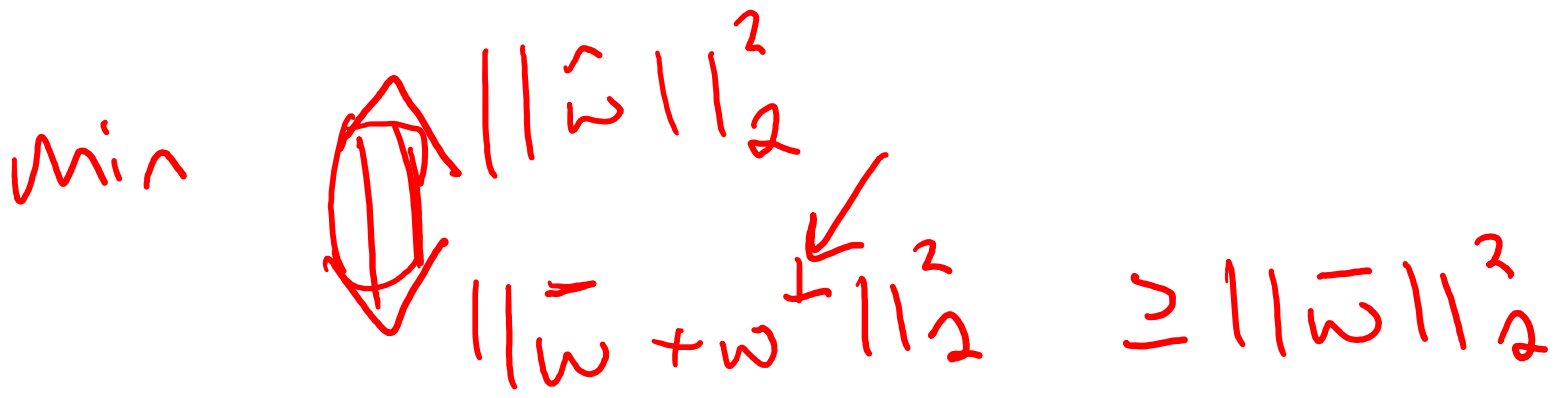
$\hat{w} \cdot x_i = \bar{w} \cdot x_i$

$\|\hat{w}\|_2^2 \geq \|\bar{w}\|_2^2$

Kernels – Proving $\hat{w} \in Span(x_1, ..., x_n)$ (2c)

Finally, show that $\hat{w} \in Span(x_1, ..., x_n)$. (Hint: Think about the regularization term)

Note that in the loss function we're trying to minimize the magnitude of w (with the regularization term $\lambda||w||_2^2$). Note that if $\forall_i \hat{w}^T x_i = \bar{w}^T x_i$, and $||\hat{w}||_2^2 \geq ||\bar{w}||_2^2$, then our optimization will always choose $w^\perp = 0$, meaning that $\hat{w} = \bar{w}$ and $\hat{w} \in Span(x_1, ..., x_n)$, which completes the contradiction.



Kernels – Kernel Proofs (3a)

Let $\phi : d \to k$ be a feature map, and define K to be the kernel matrix of ϕ. Prove that the kernel matrix is symmetric. That is, show $K_{i,j} = K_{j,i}$.

Kernels – Kernel Proofs (3a)

Let $\phi : d \to k$ be a feature map, and define K to be the kernel matrix of ϕ. Prove that the kernel matrix is symmetric. That is, show $K_{i,j} = K_{j,i}$.

Let $\phi(x_i)$ and $\phi(x_j)$ be the feature maps for x_i and x_j, respectively. Then $K_{i,j} = \phi(x_i)^T \phi(x_j) = \phi(x_j)^T \phi(x_i) = K_{j,i}$.

A is symmetric and

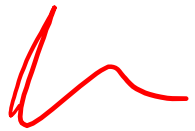
A is a kernel

Kernels – Kernel Proofs (3b)

Let $\phi : d \to k$ be a feature map, and define K to be the kernel matrix of ϕ.

Recall that a matrix M is positive semi-definite if $x^T Mx \geq 0, \forall x \in \mathbb{R}^n$.

Show that K is positive semi-definite. (Hint: consider the matrix B where the i^{th} [illegible] B is $\phi(x_i)$.



Kernels – Kernel Proofs (3b)

PSD

$x^T A x \geq 0$

Let $\phi : d \to k$ be a feature map, and define K to be the kernel matrix of ϕ.
Recall that a matrix M is positive semi-definite if $x^T M x \geq 0, \forall x \in \mathbb{R}^n$.
Show that K is positive semi-definite. (Hint: consider the matrix B where the i^{th} column of B is $\phi(x_i)$.

Recall that $K_{i,j} = \phi(x_i)^T \phi(x_j)$. Observe that $K = B^T B$, as $(B^T B)_{i,j} = \phi(x_i)^T \phi(x_j)$. Now consider an arbitrary vector y. To show K is PSD it suffices to show $y^T K y$ is non-negative. We have:

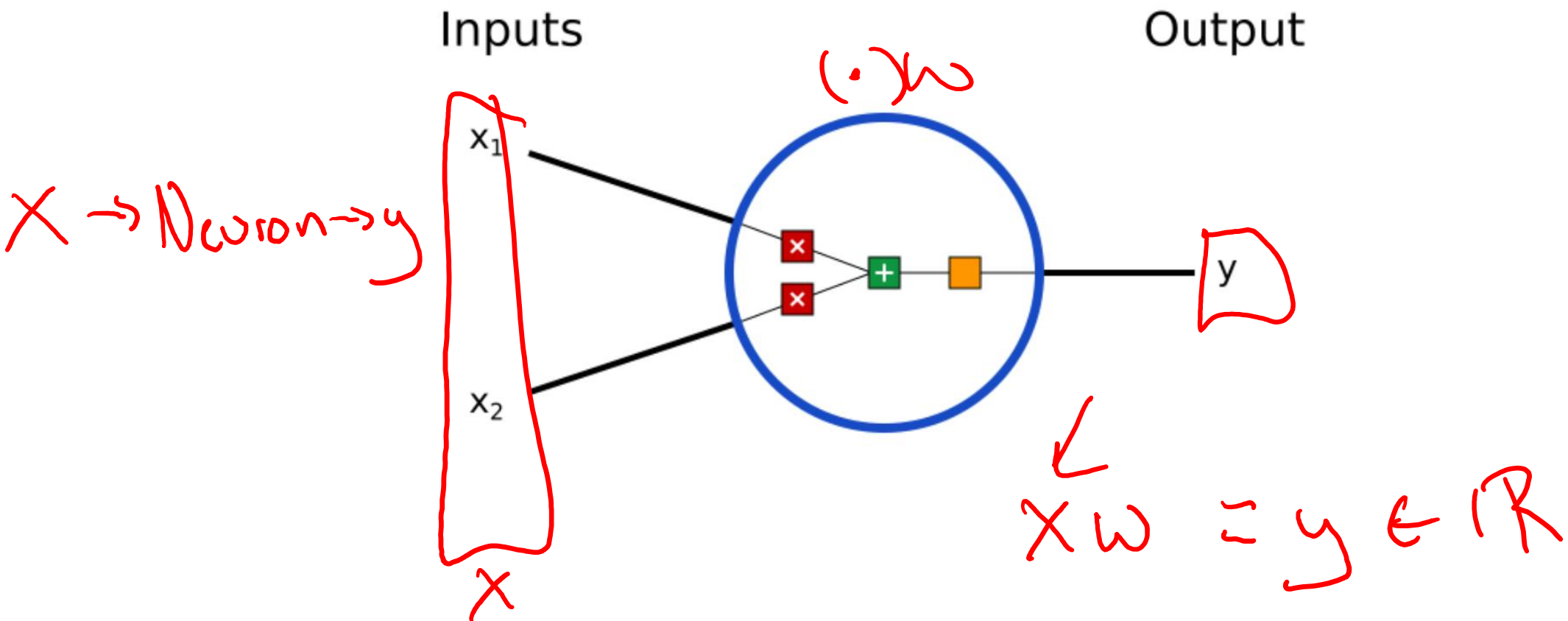
$$y^T K y = y^T B^T B y = (By)^T (By) = ||By||_2^2 \geq 0$$

if A is (symmetric, PSD) $\Rightarrow$ A is a kernel

PyTorch Neural Network Edition

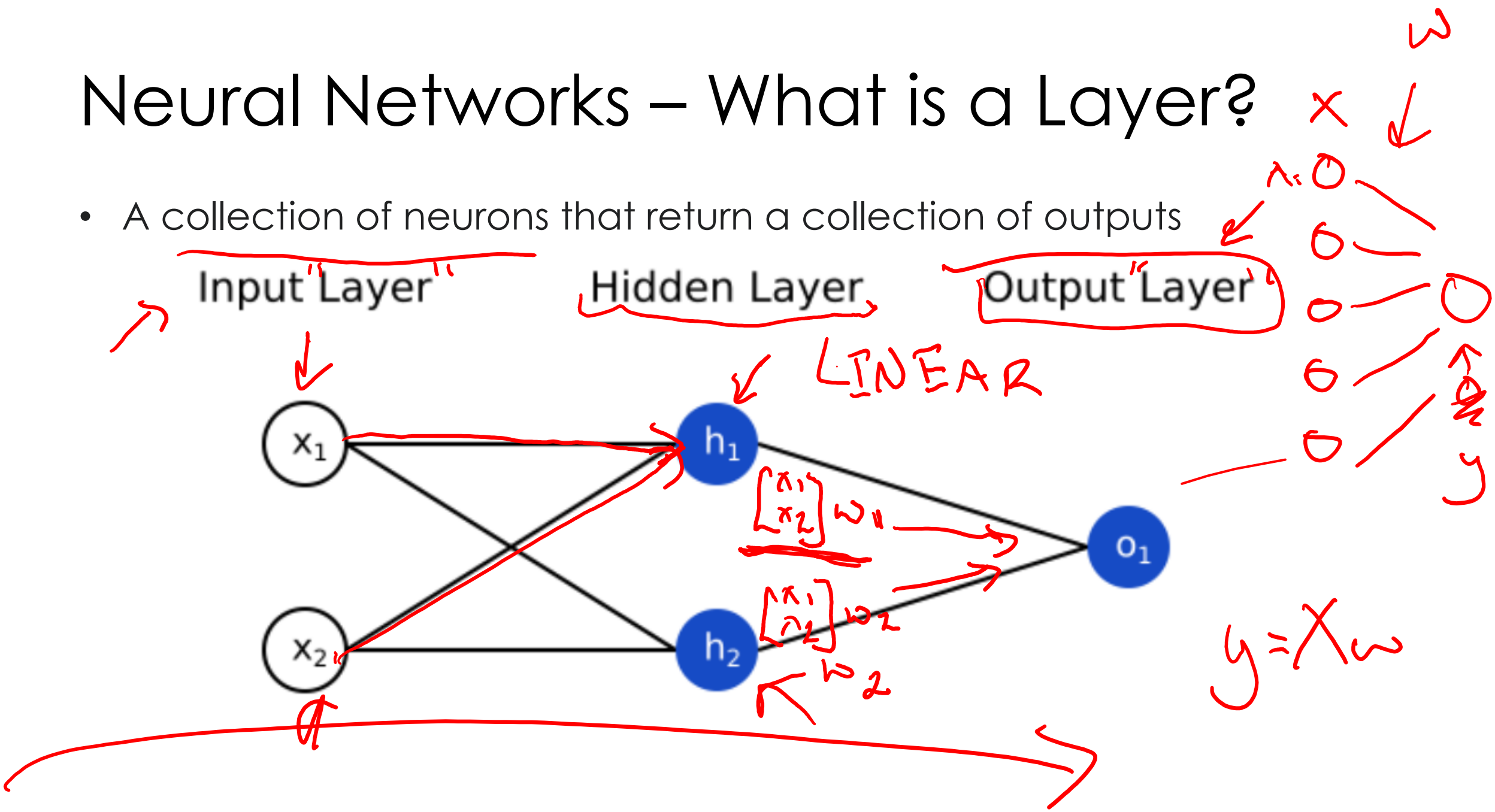
Neural Networks – What is a Neuron?

- Basic unit of a neural network
- Takes an input, does some math, creates a single output



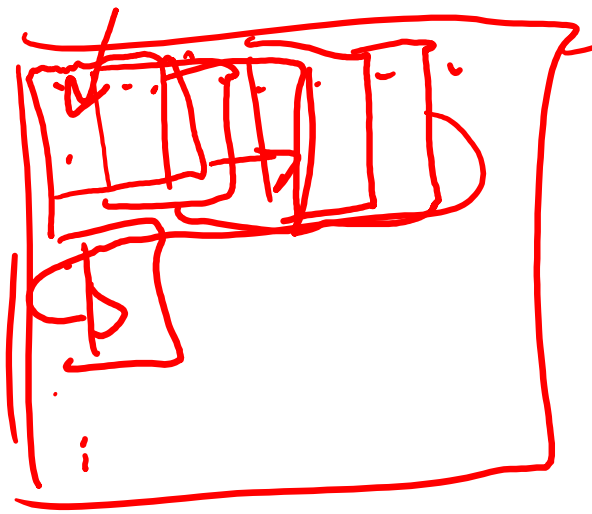
Neural Networks – What is a Layer?

- A collection of neurons that return a collection of outputs



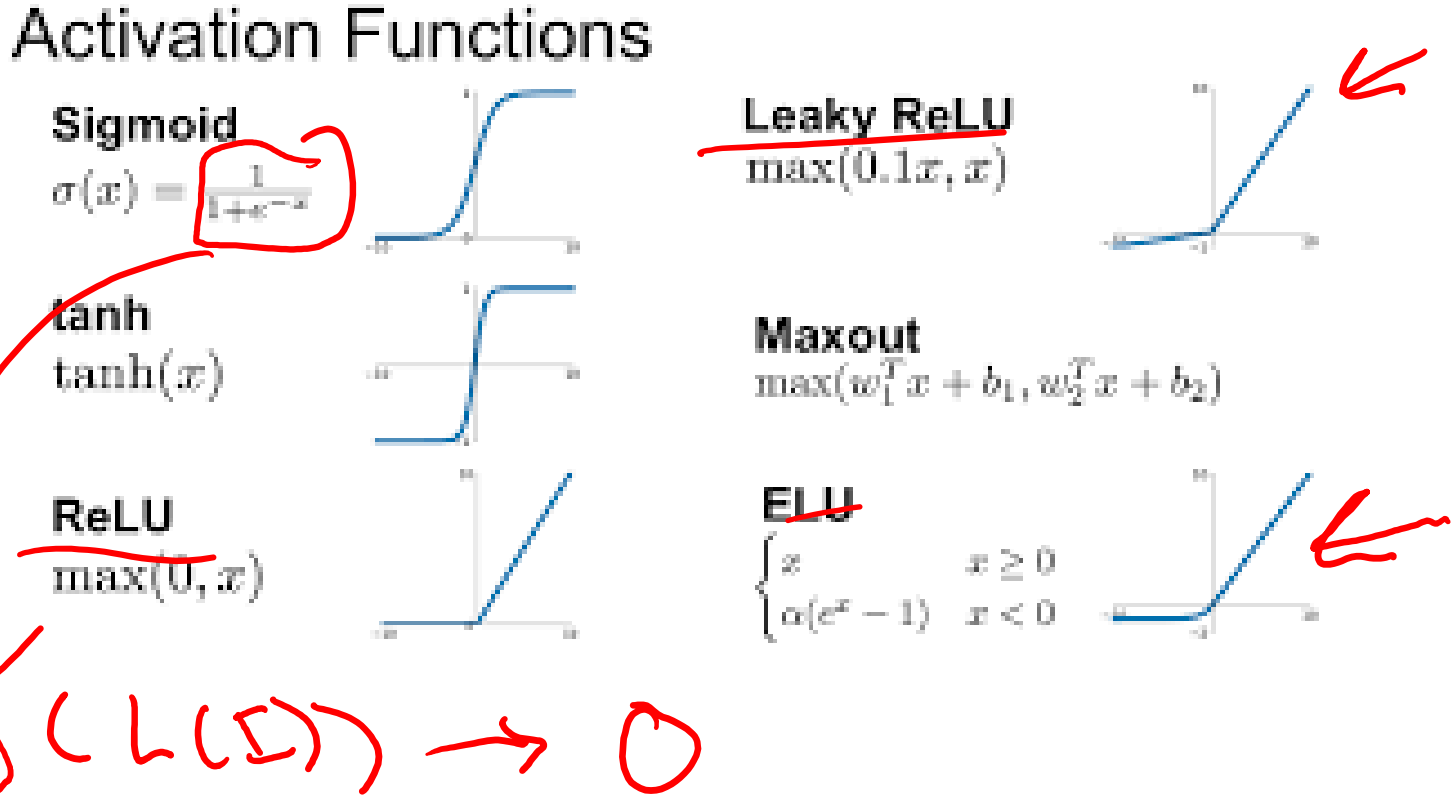
Neural Networks – Types of Layers

- Fully-Connected
- Convolutional
- Attention
- … and many more!



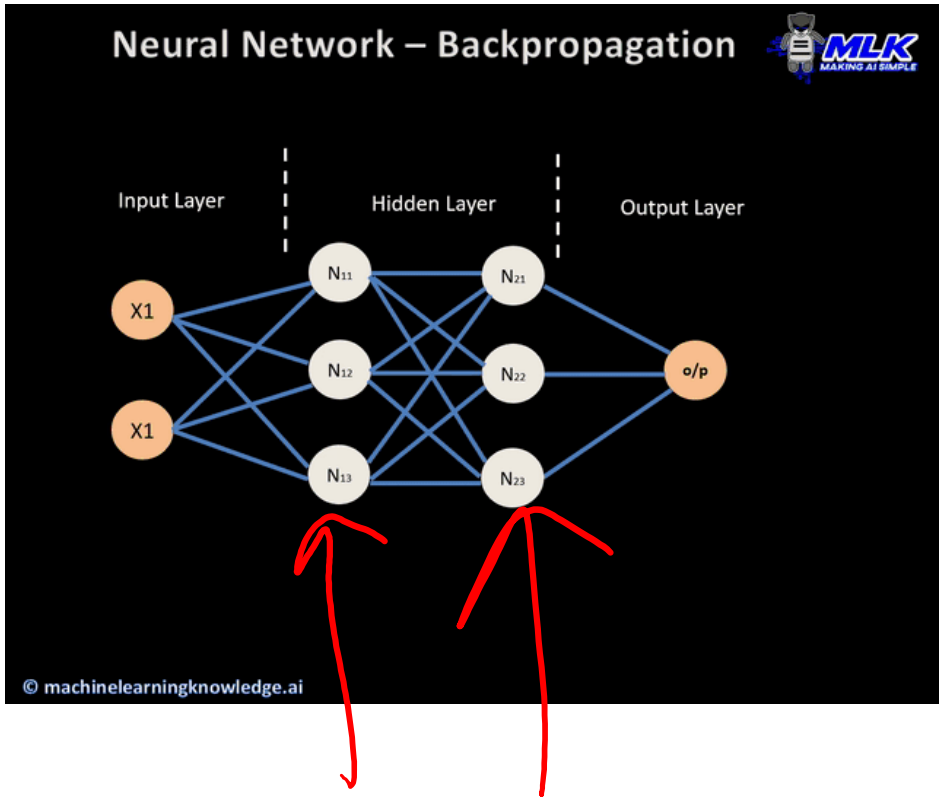
Neural Networks – What is activation?

- A function to apply to the output of the layer
- Has important geometric results that we will discuss in class



Neural Networks – How do we train?

- An algorithm called backpropagation! **More in class.**



PyTorch Notebook