Advanced Machine Learning

Symmetry

Inductive Bias, Symmetry, Invariance, Group theory

Outline

1. **Inductive Bias**
2. Invariance
3. Group Theory

Inductive Bias

- Learning machines differ in how they split up the space of inputs
- Perceptrons split the space using a hyperplane, RBFs split the space depending on some set of centres, MLPs successive split the world at different layers
- These differences are known as the **inductive bias** of the machine
- The different inductive bias lead to different performance
- How can we exploit the inductive bias to get good performance?

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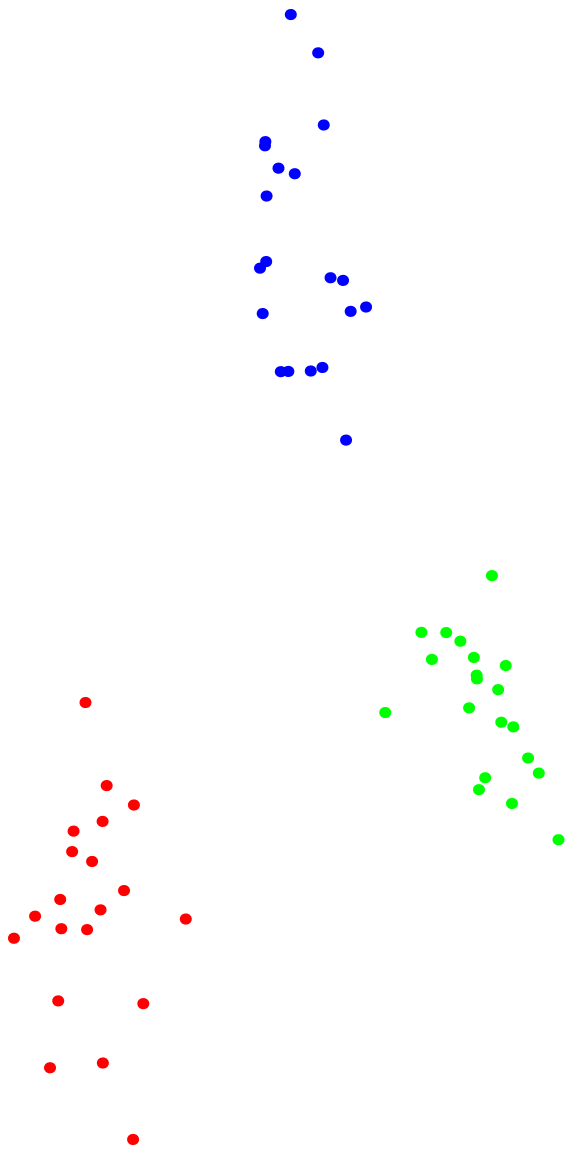
The Real World

- The problems that we care about come from a highly structured world where the solutions inherit some of the properties of that world
- Usually similar input have similar outputs (we don't expect to change one pixel in an image and that it should be classified differently)
- The classes are often quite well separated



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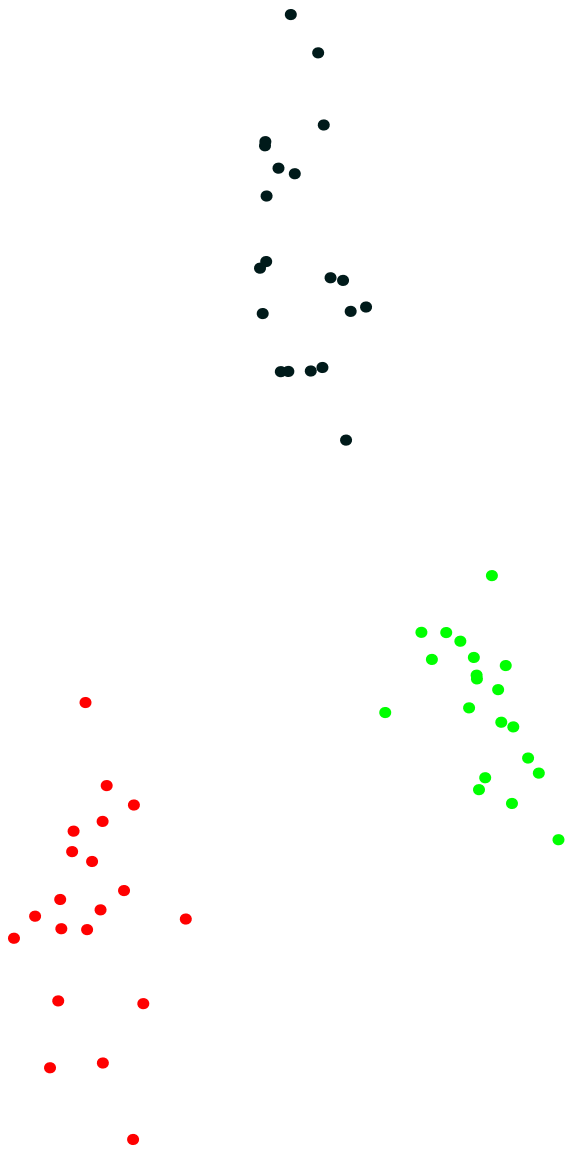

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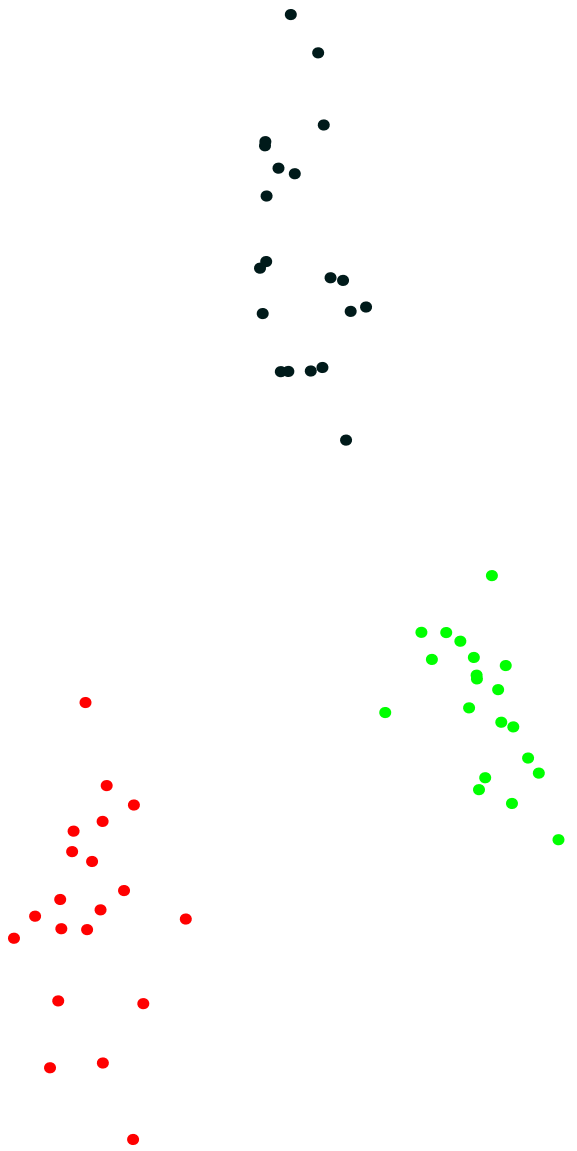

Smoothness

- A natural assumption is smoothness (the classification surface or regression surface changes slowly as we change the input)
- Often there is a hyperparameter that controls this
  - ⋆ The kernel parameter γ in SVMs (or ℓ in Gaussian Processes)
  - ⋆ k in k-nearest neighbours
  - ⋆ The size of the L_2 regulisation term in neural networks
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3. Group Theory

Symmetry

- There are sometimes symmetries in the world we can exploit
- In image classification we consider an object should be classified the same wherever it is in the image
- The classification should be invariant to translations (scaling and perhaps rotations)
- The classification function possesses a translational symmetry
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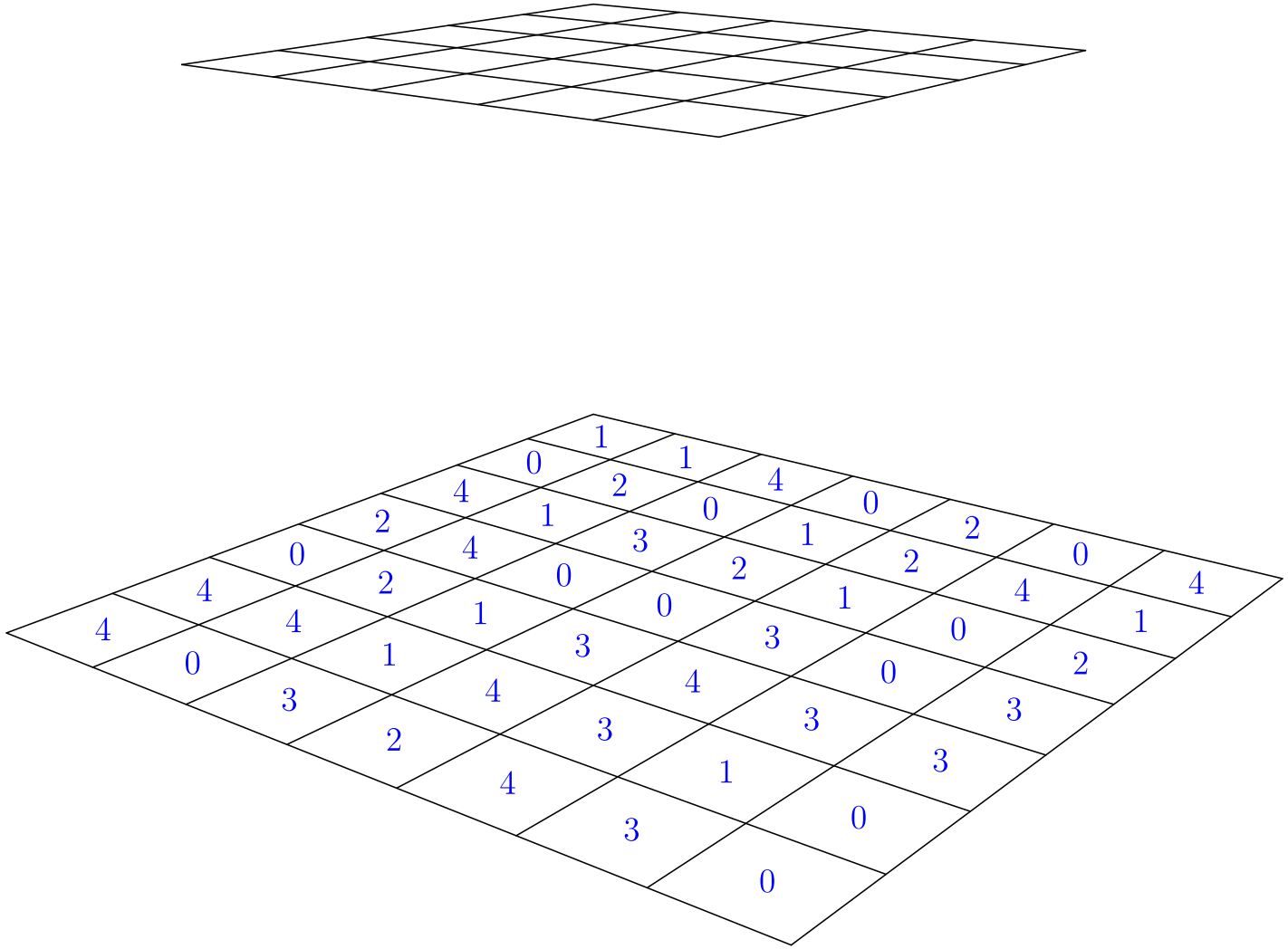
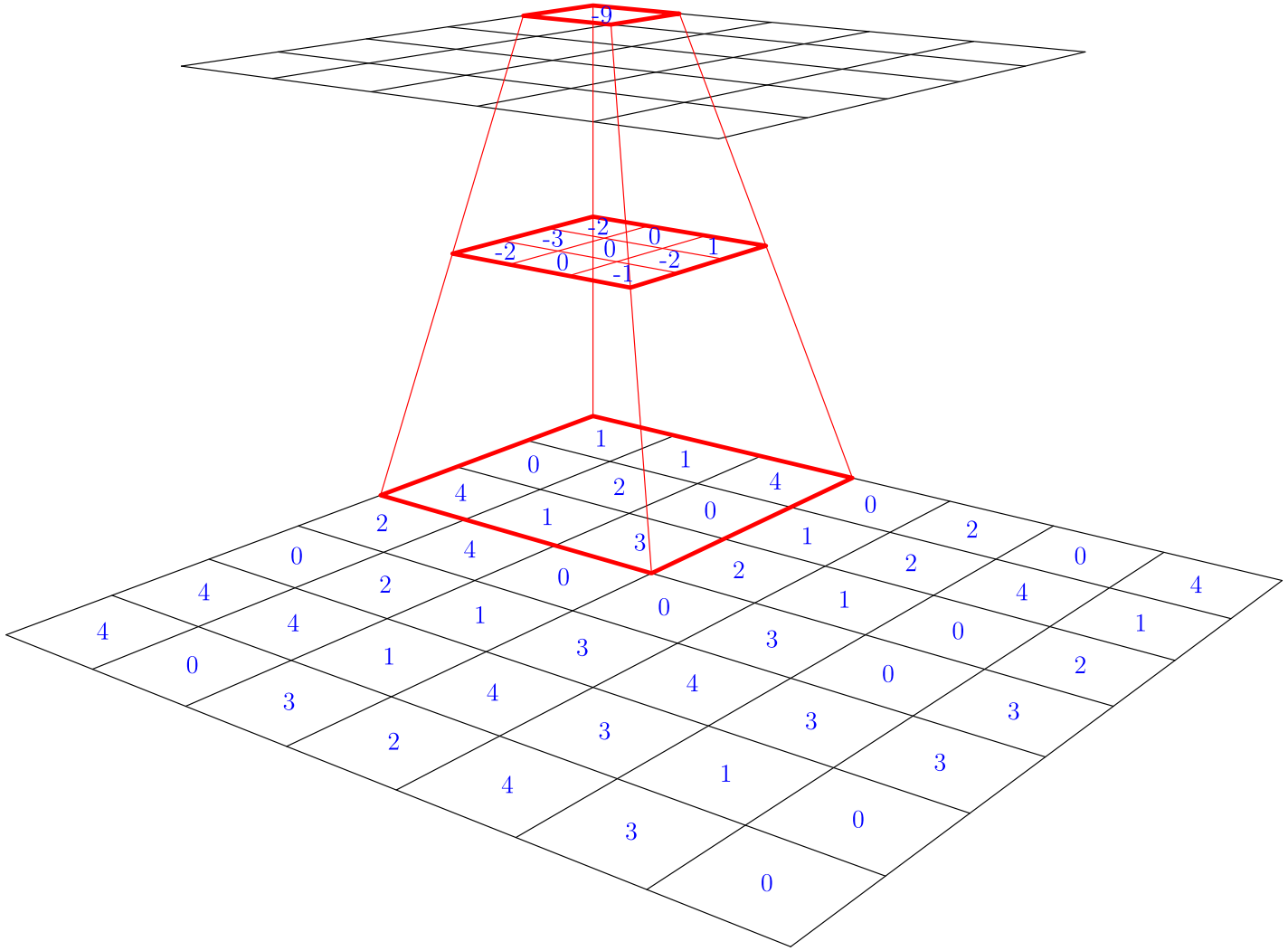
- The classification function possesses a translational symmetry
- Learning machines that respect translational invariance have far less propensity to overfit—they don't need to learn that the same object in a different part of the image is the same

Convolutional Neural Networks

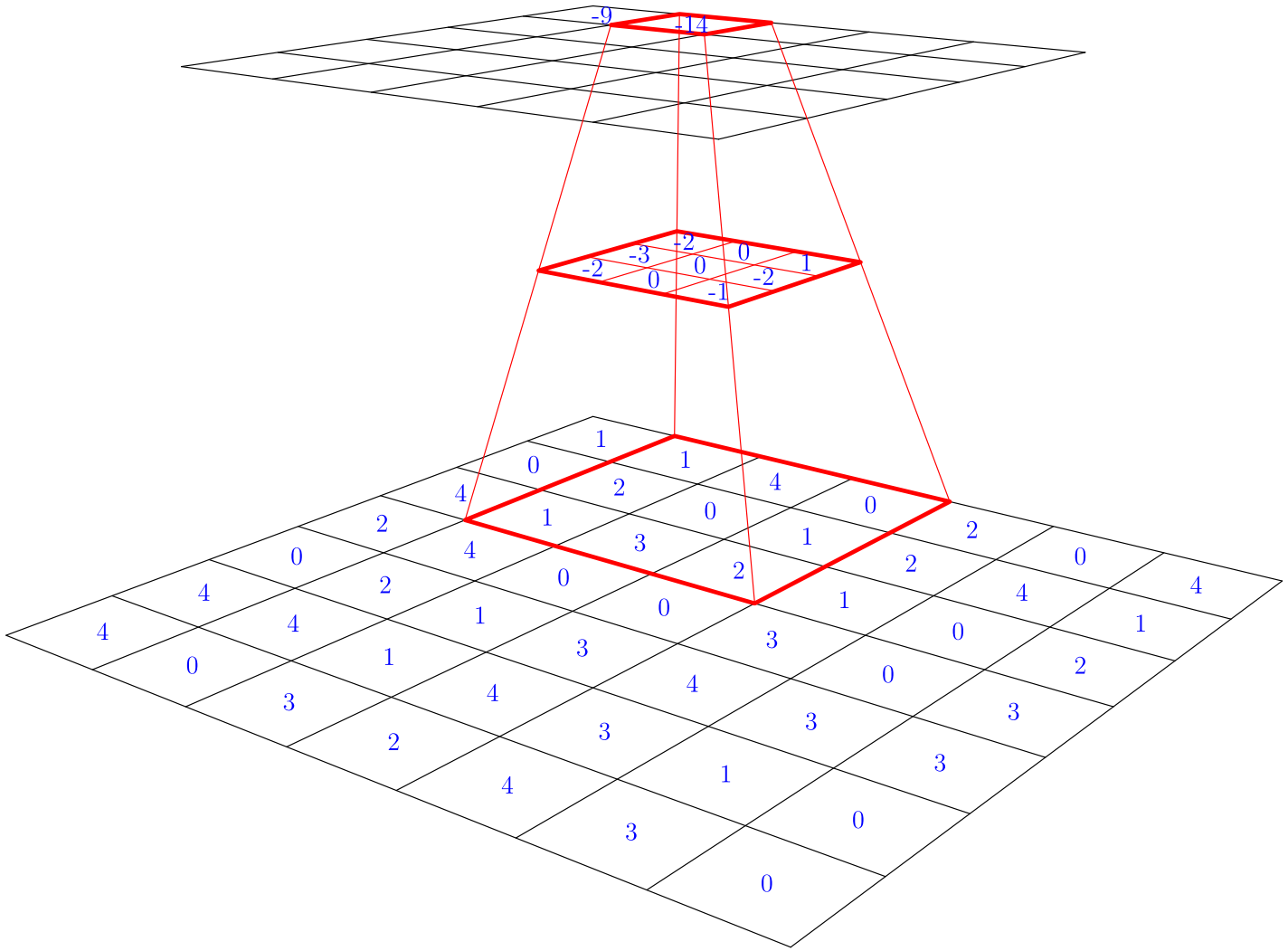


Convolutional Neural Networks



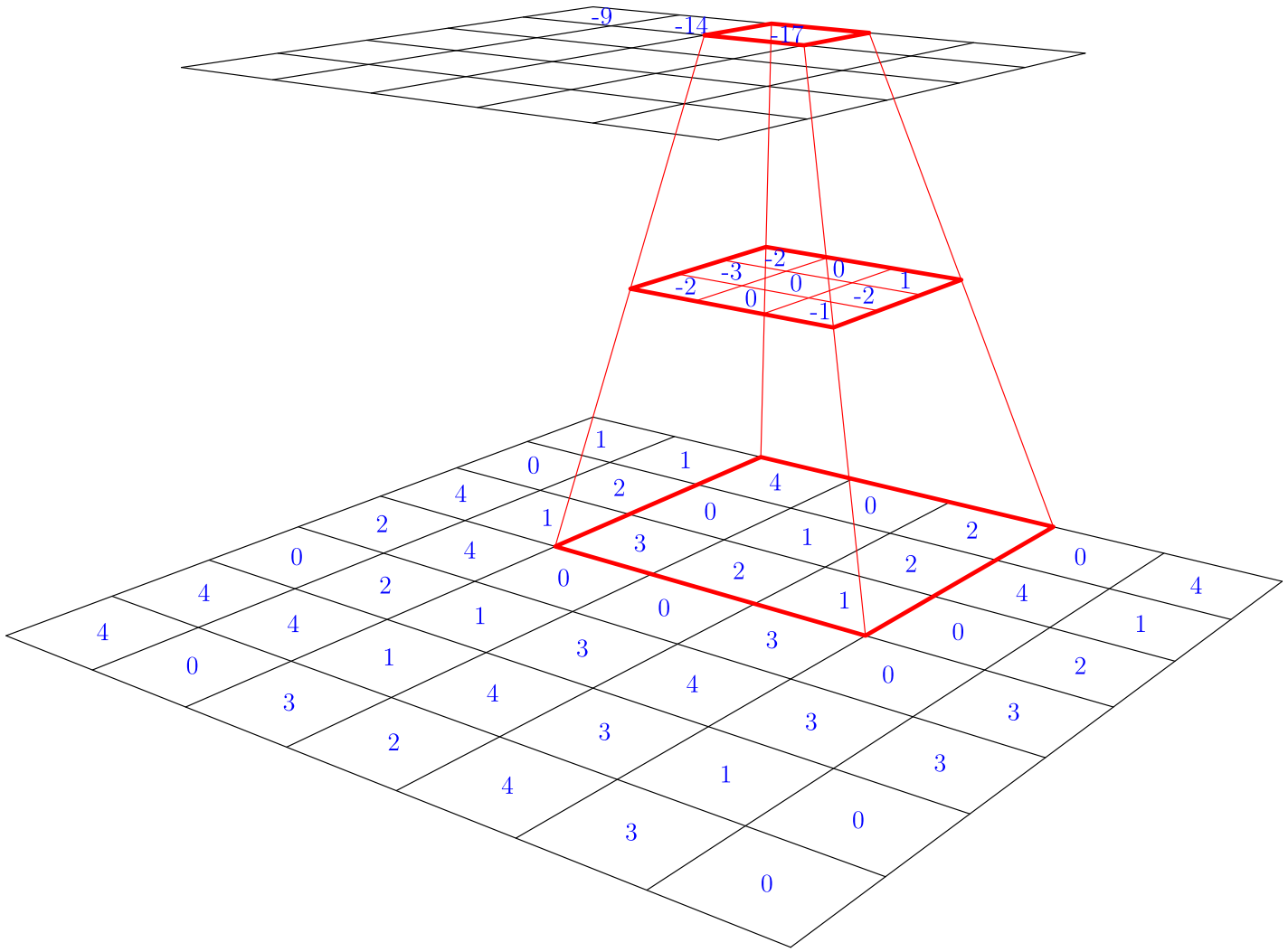
$$-2 \times 1 + 0 \times 1 + 1 \times 4$$
$$-3 \times 0 + 0 \times 2 - 2 \times 0$$
$$-2 \times 4 + 0 \times 1 - 1 \times 3 = -9$$

Convolutional Neural Networks



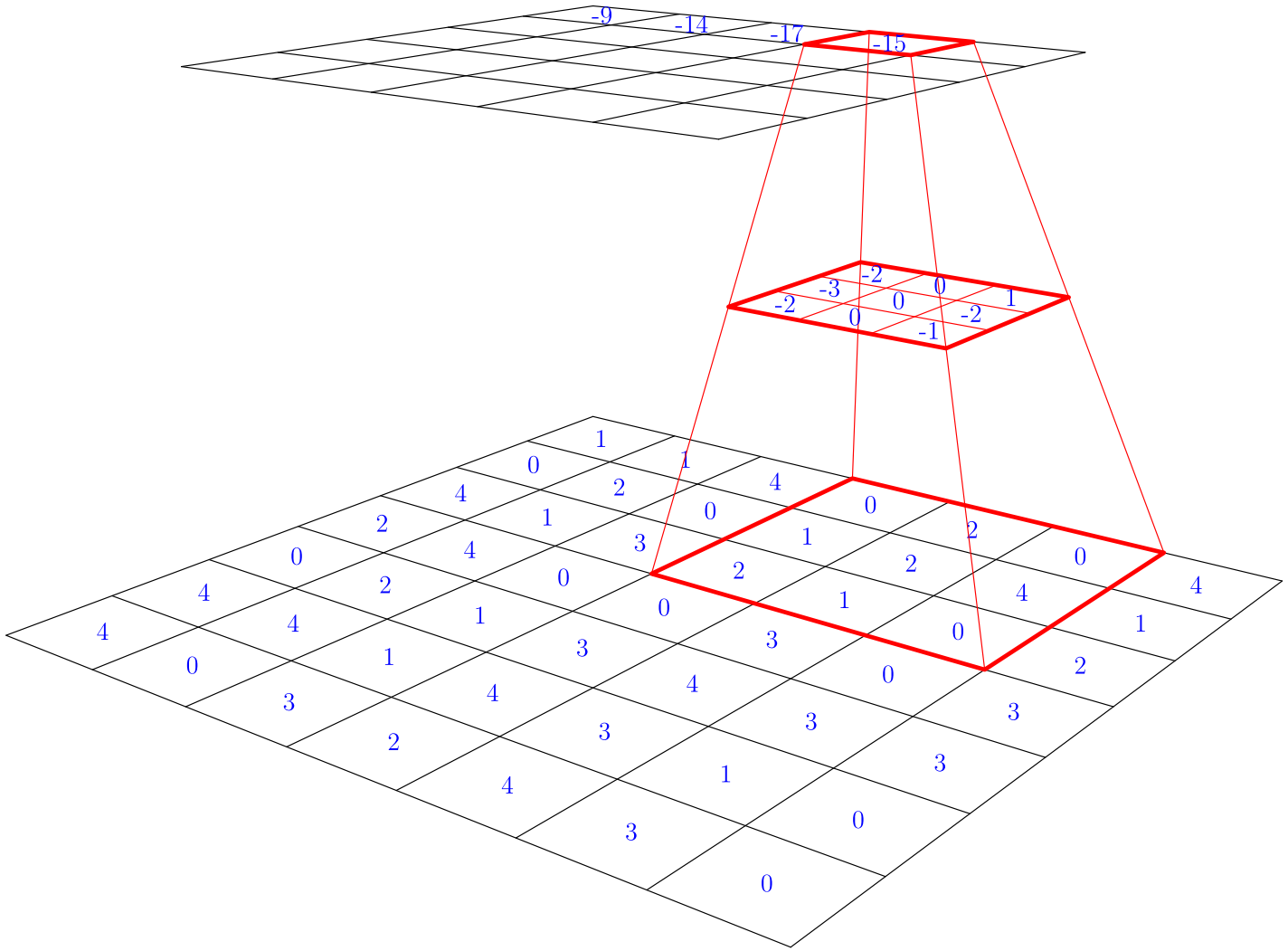
$-2 \times 1 + 0 \times 4 + 1 \times 0$
$-3 \times 2 + 0 \times 0 - 2 \times 1$
$-2 \times 1 + 0 \times 3 - 1 \times 2 = -14$

Convolutional Neural Networks



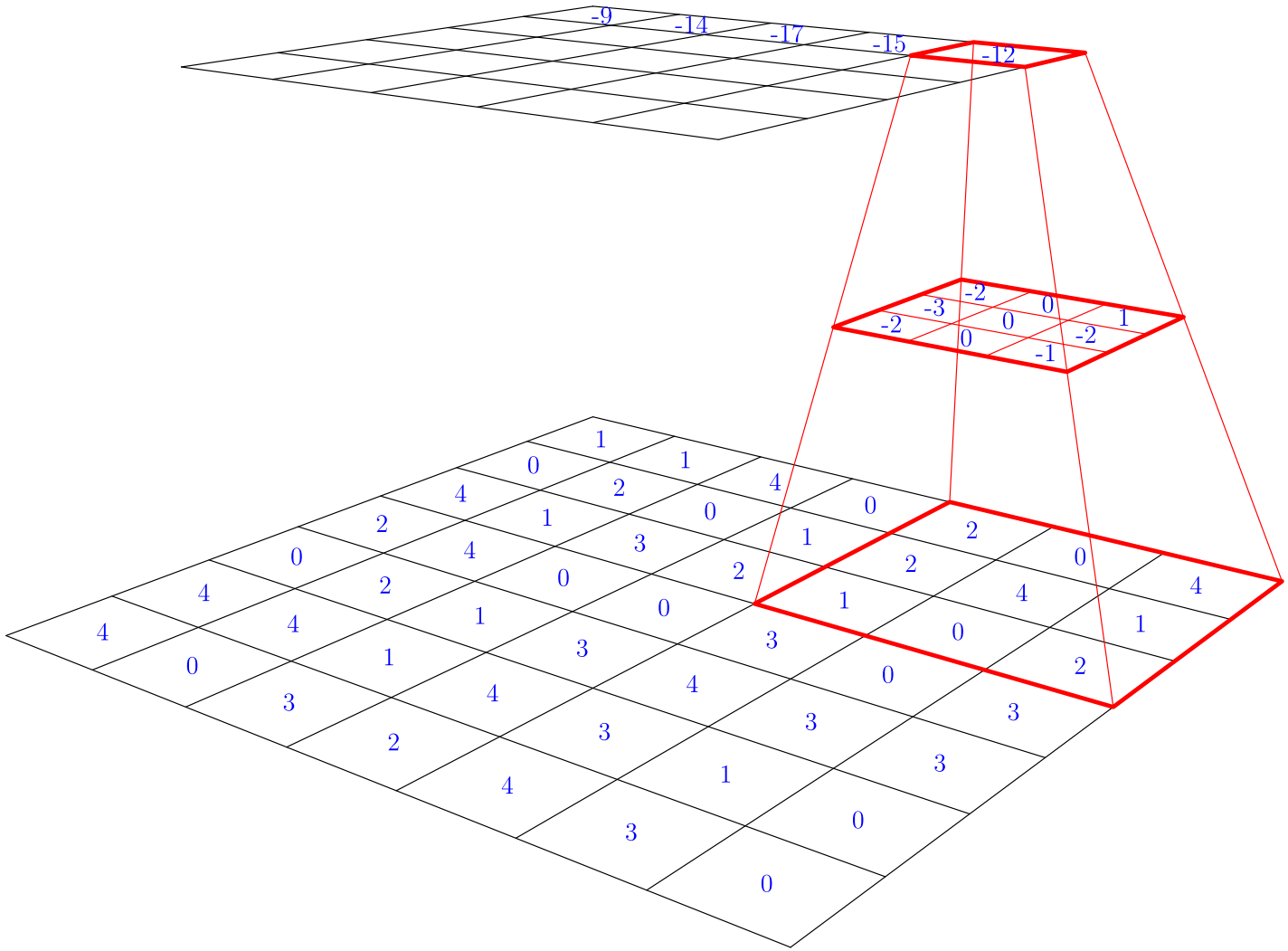
$$-2 \times 4 + 0 \times 0 + 1 \times 2$$
$$-3 \times 0 + 0 \times 1 - 2 \times 2$$
$$-2 \times 3 + 0 \times 2 - 1 \times 1 = -17$$

Convolutional Neural Networks



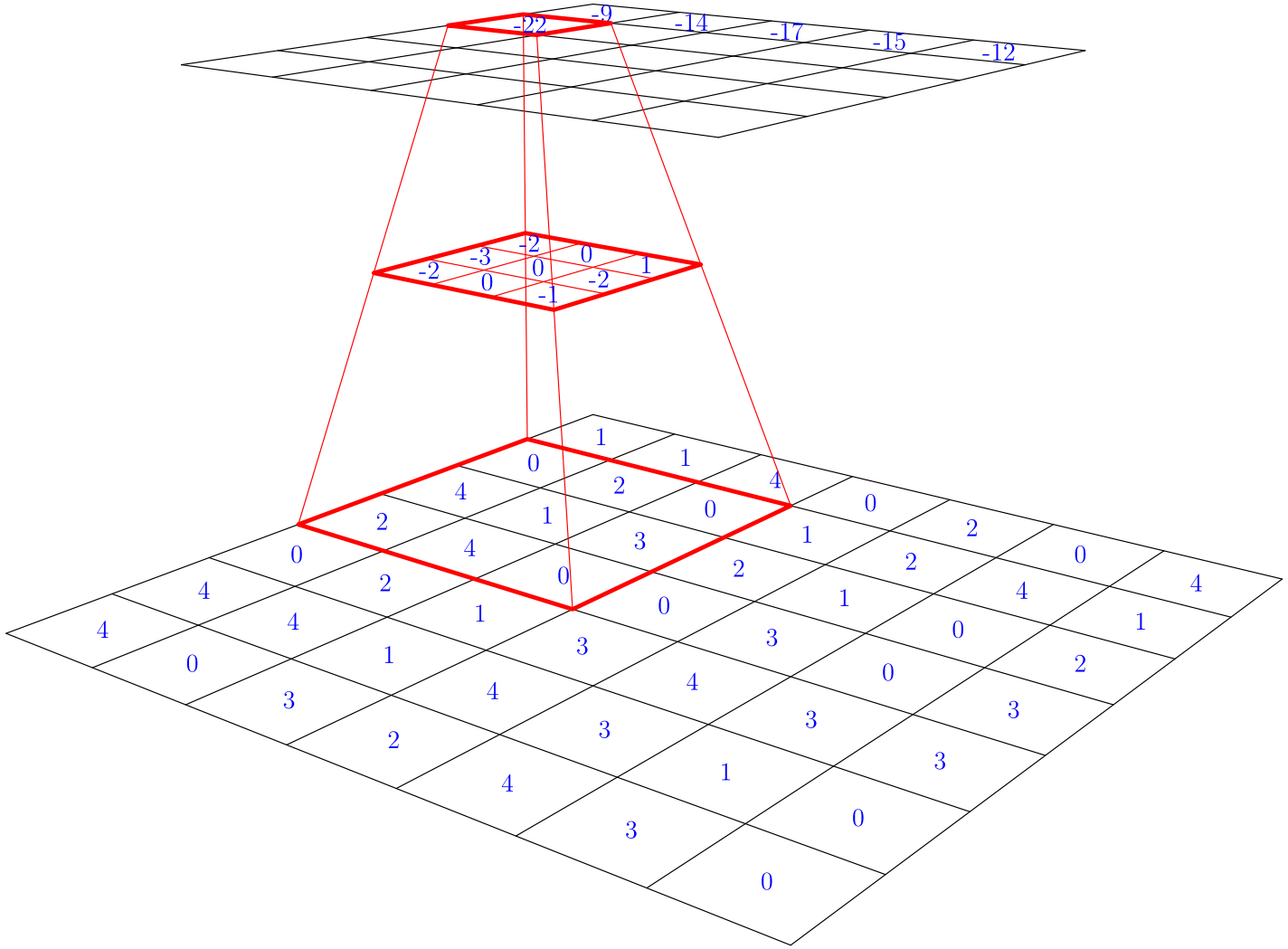
$$-2 \times 0 + 0 \times 2 + 1 \times 0$$
$$-3 \times 1 + 0 \times 2 - 2 \times 4$$
$$-2 \times 2 + 0 \times 1 - 1 \times 0 = -15$$

Convolutional Neural Networks



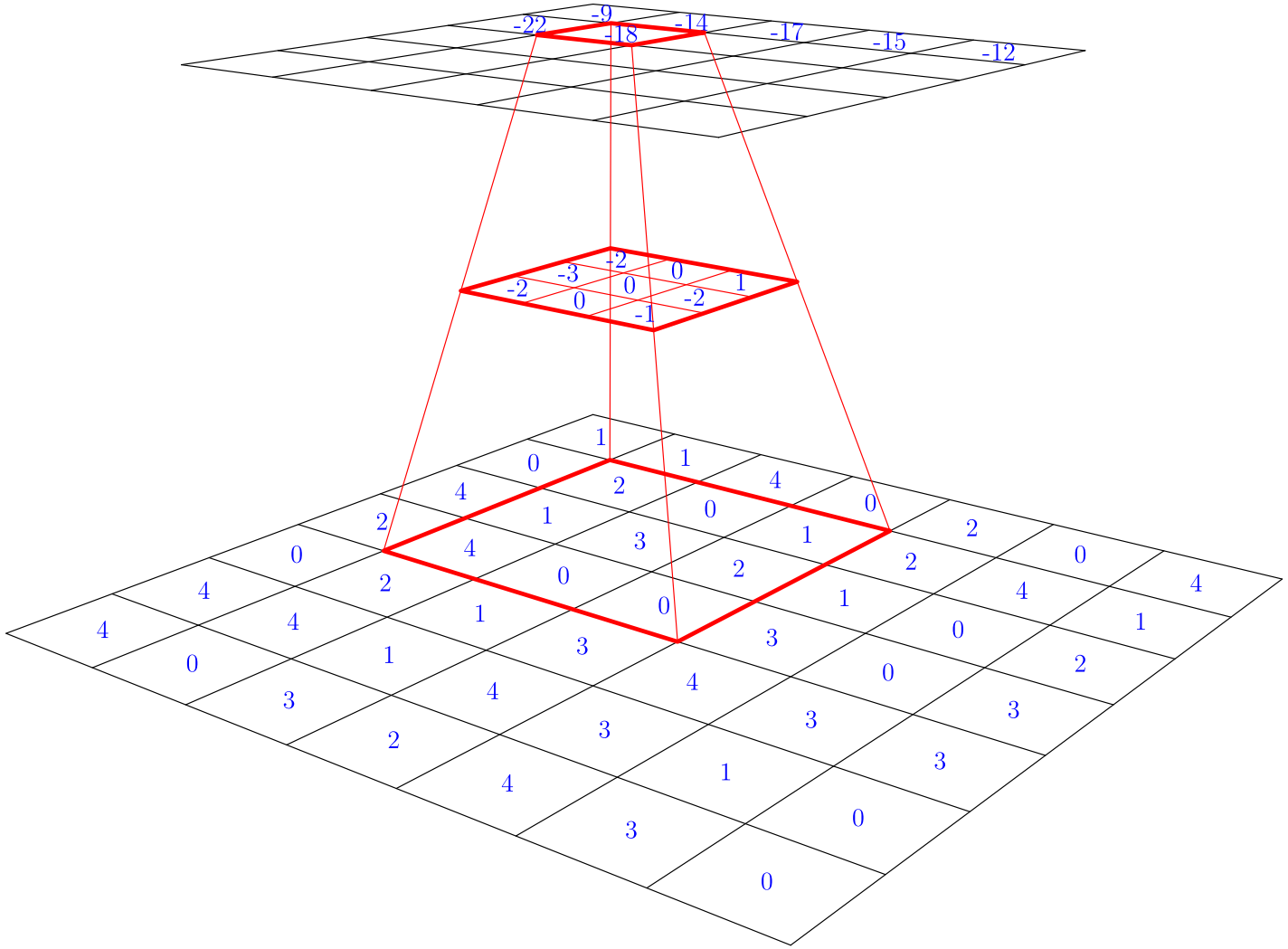
$$-2 \times 2 + 0 \times 0 + 1 \times 4$$
$$-3 \times 2 + 0 \times 4 - 2 \times 1$$
$$-2 \times 1 + 0 \times 0 - 1 \times 2 = -12$$

Convolutional Neural Networks



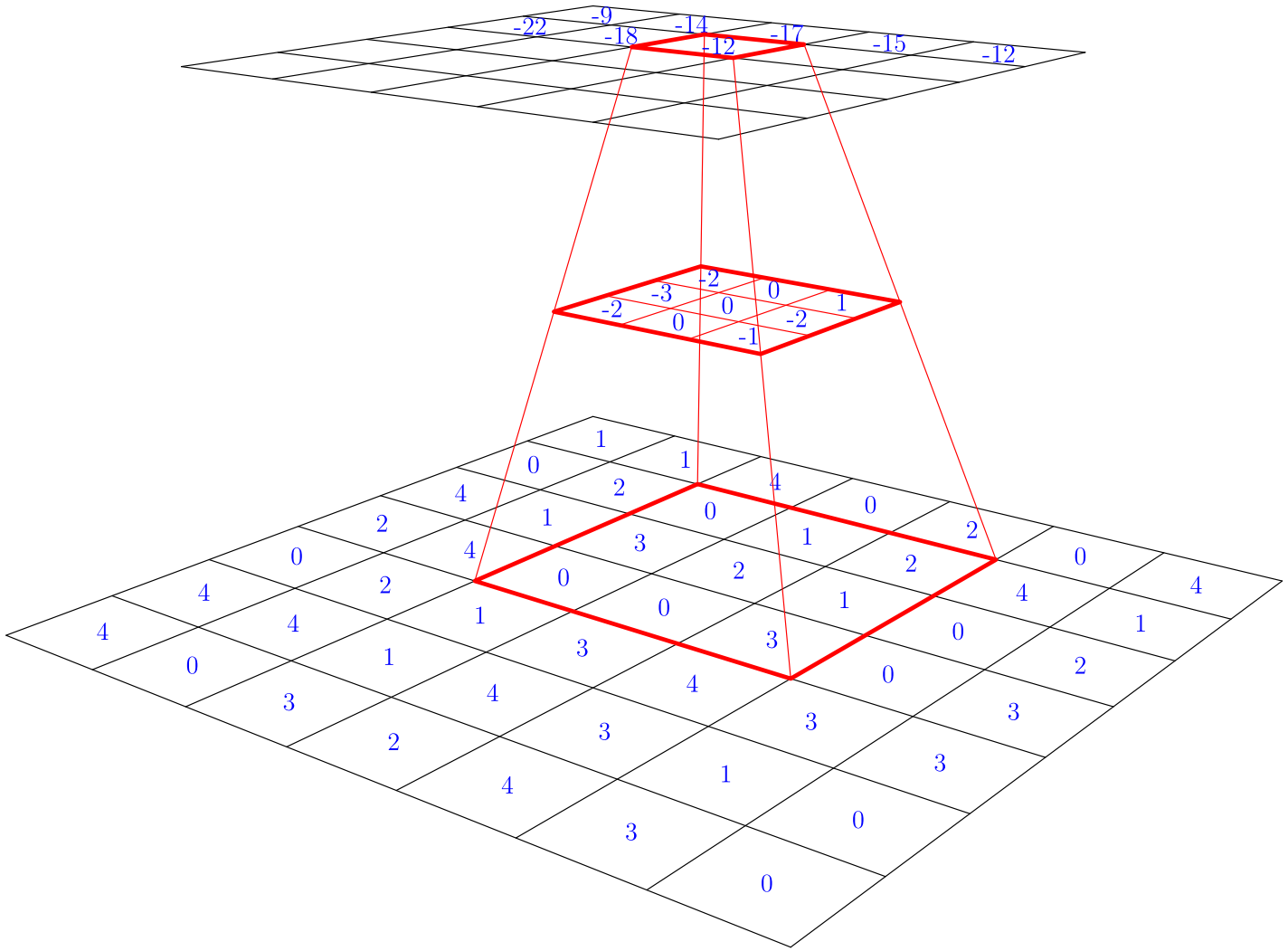
$$-2 \times 0 + 0 \times 2 + 1 \times 0$$
$$-3 \times 4 + 0 \times 1 - 2 \times 3$$
$$-2 \times 2 + 0 \times 4 - 1 \times 0 = -22$$

Convolutional Neural Networks



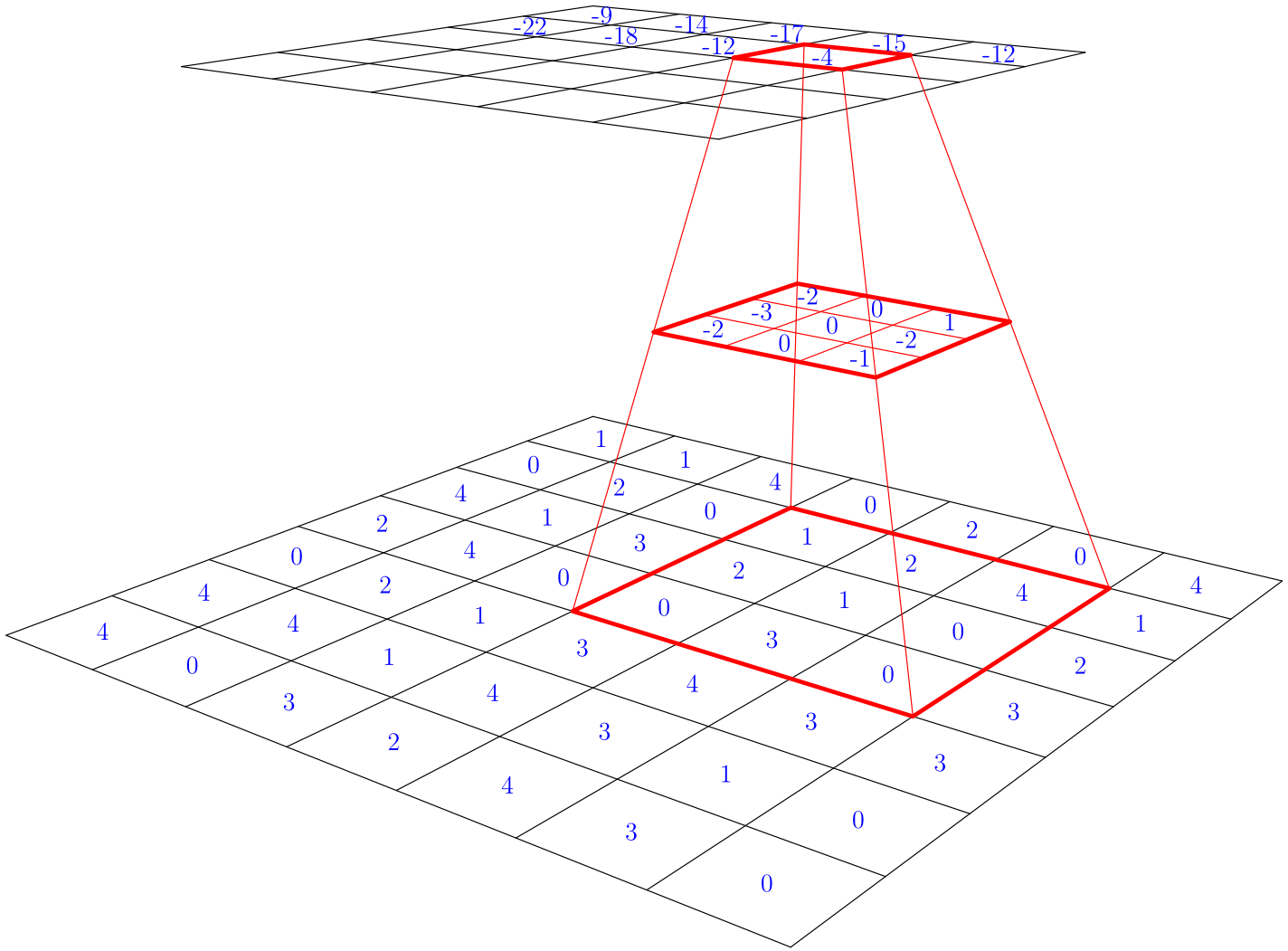
$$-2 \times 2 + 0 \times 0 + 1 \times 1$$
$$-3 \times 1 + 0 \times 3 - 2 \times 2$$
$$-2 \times 4 + 0 \times 0 - 1 \times 0 = -18$$

Convolutional Neural Networks



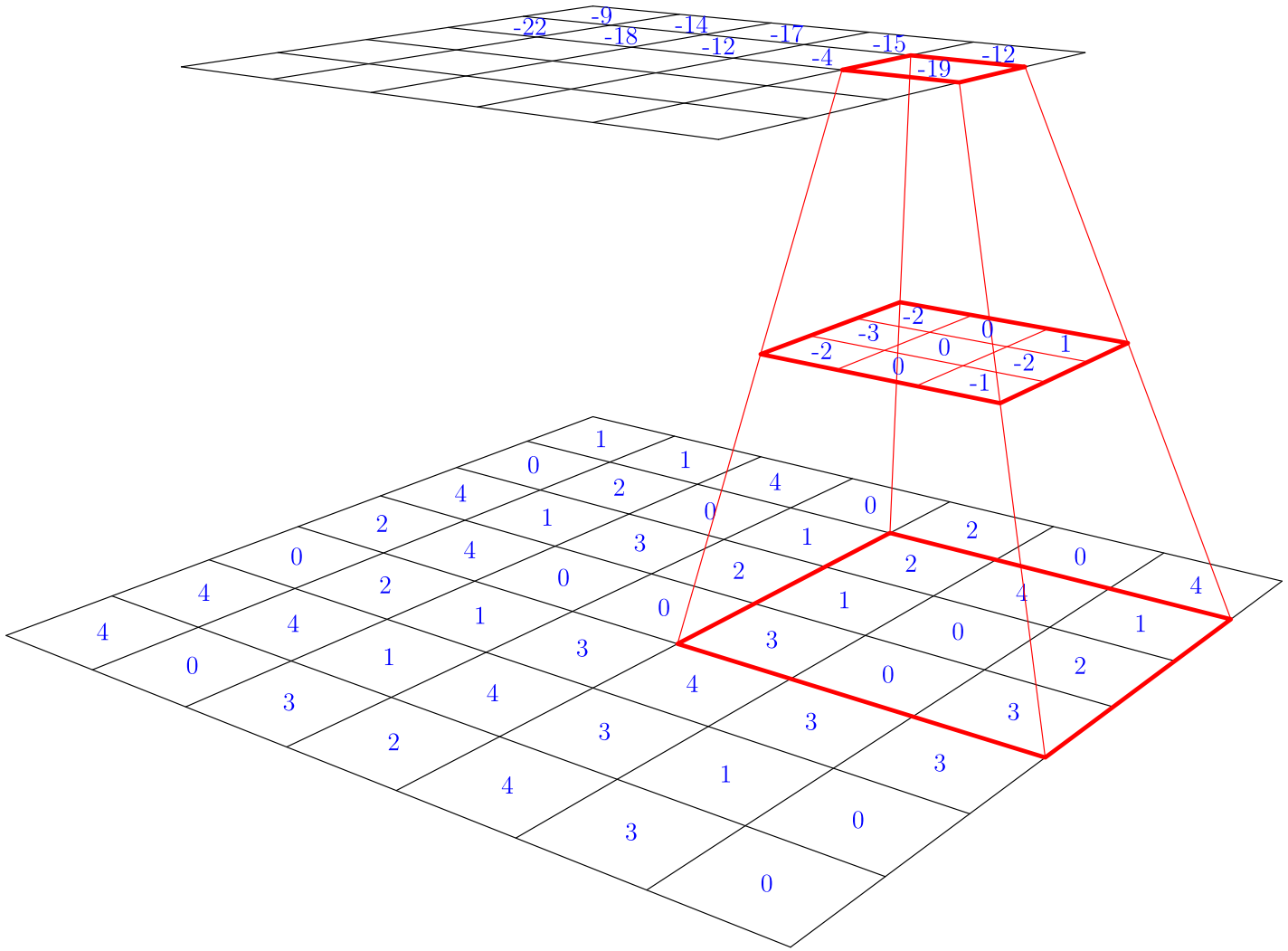
$$-2 \times 0 + 0 \times 1 + 1 \times 2$$
$$-3 \times 3 + 0 \times 2 - 2 \times 1$$
$$-2 \times 0 + 0 \times 0 - 1 \times 3 = -12$$

Convolutional Neural Networks



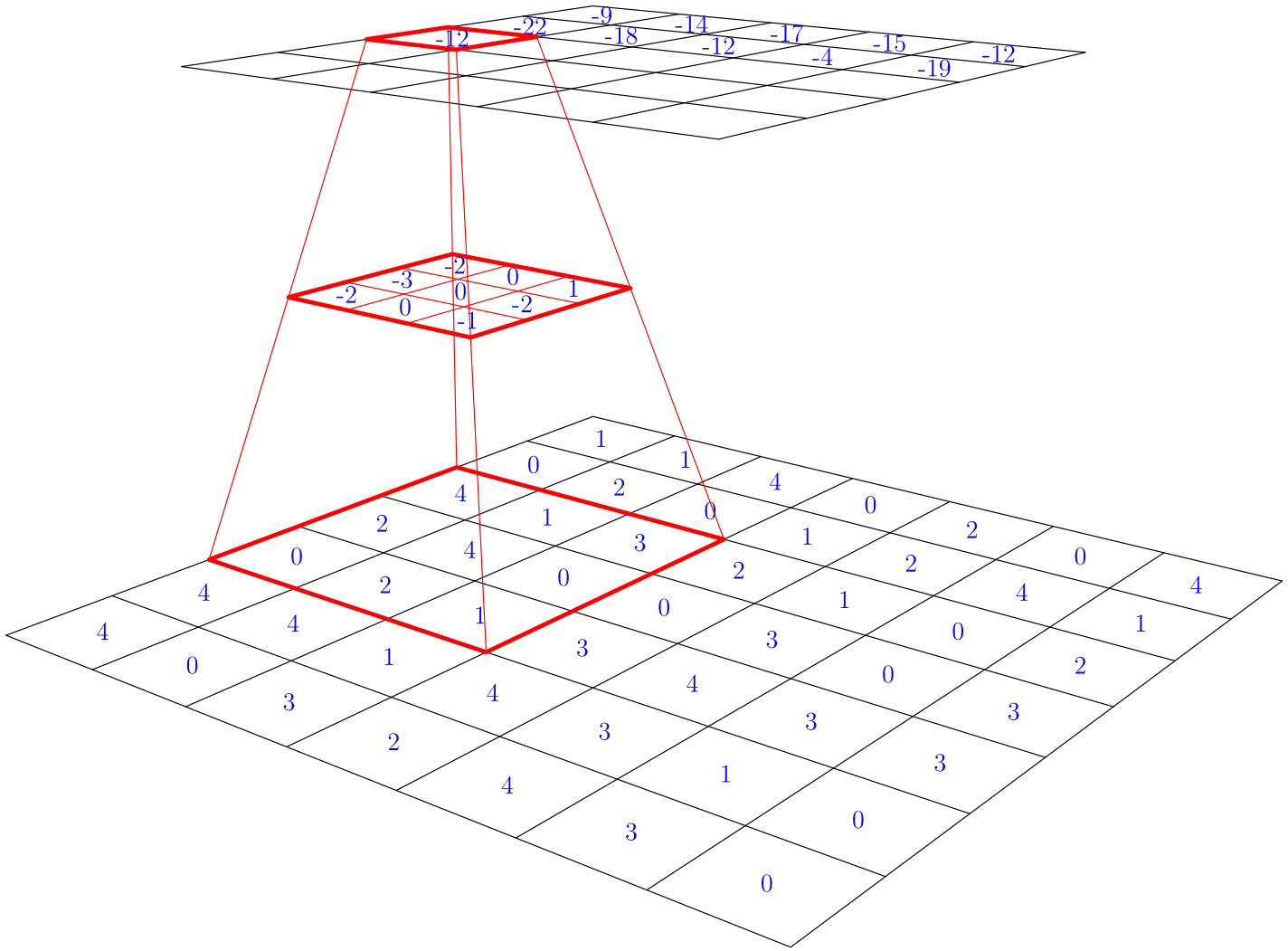
$$-2 \times 1 + 0 \times 2 + 1 \times 4$$
$$-3 \times 2 + 0 \times 1 - 2 \times 0$$
$$-2 \times 0 + 0 \times 3 - 1 \times 0 = -4$$

Convolutional Neural Networks



$$-2 \times 2 + 0 \times 4 + 1 \times 1$$
$$-3 \times 1 + 0 \times 0 - 2 \times 2$$
$$-2 \times 3 + 0 \times 0 - 1 \times 3 = -19$$

Convolutional Neural Networks



$$-2 \times 4 + 0 \times 1 + 1 \times 3$$
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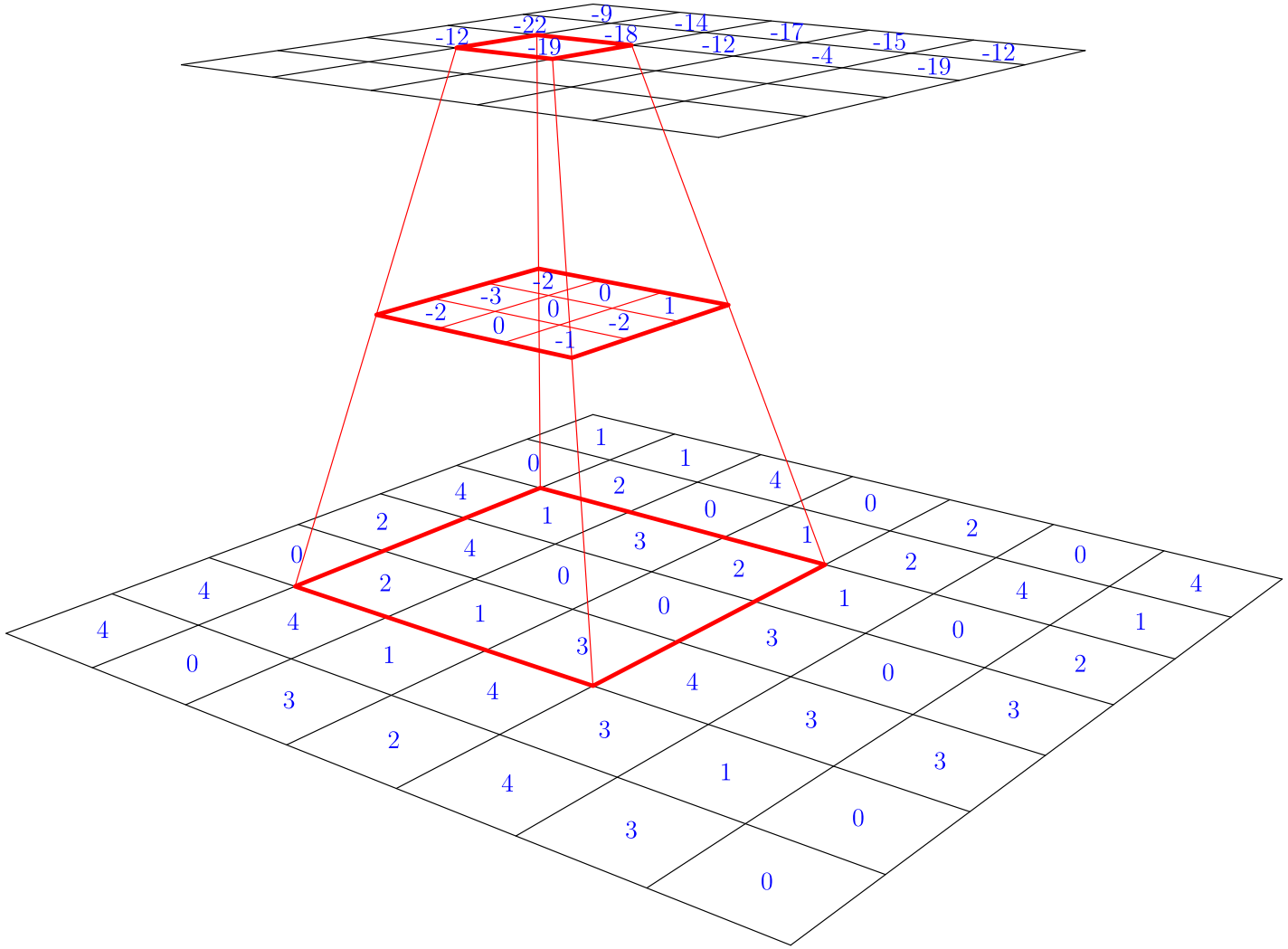
Convolutional Neural Networks



$$-2 \times 1 + 0 \times 3 + 1 \times 2$$
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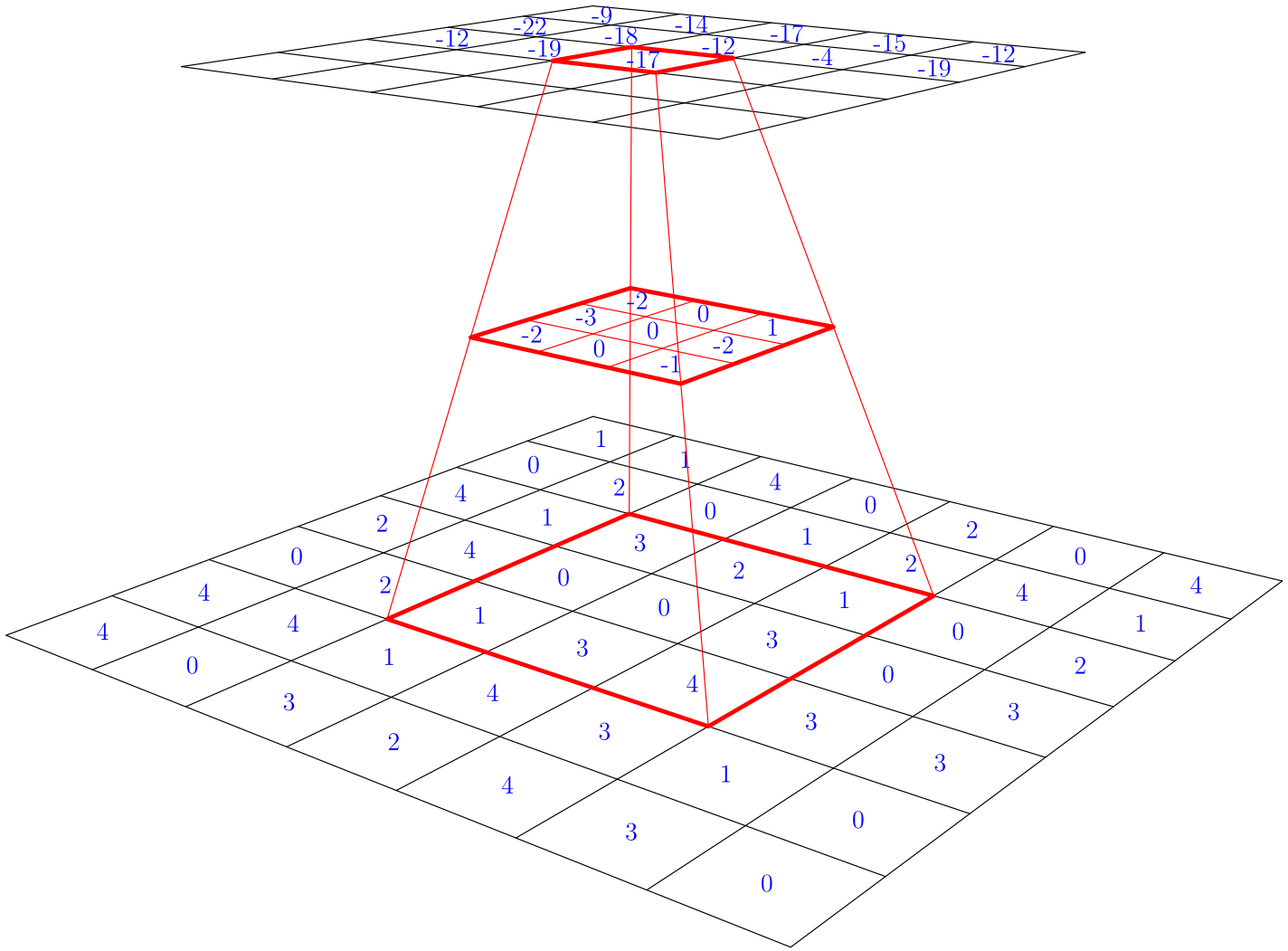
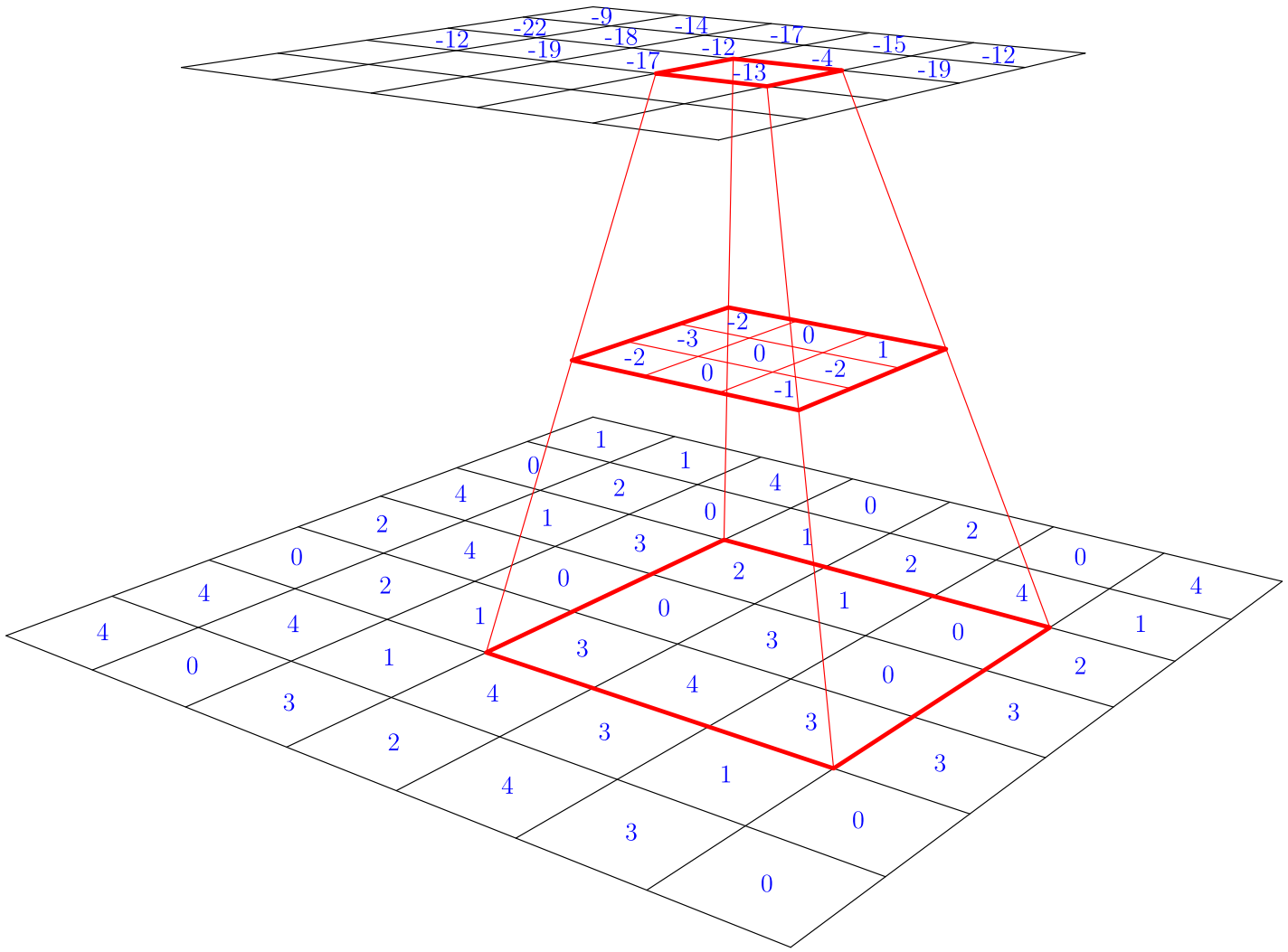
Convolutional Neural Networks



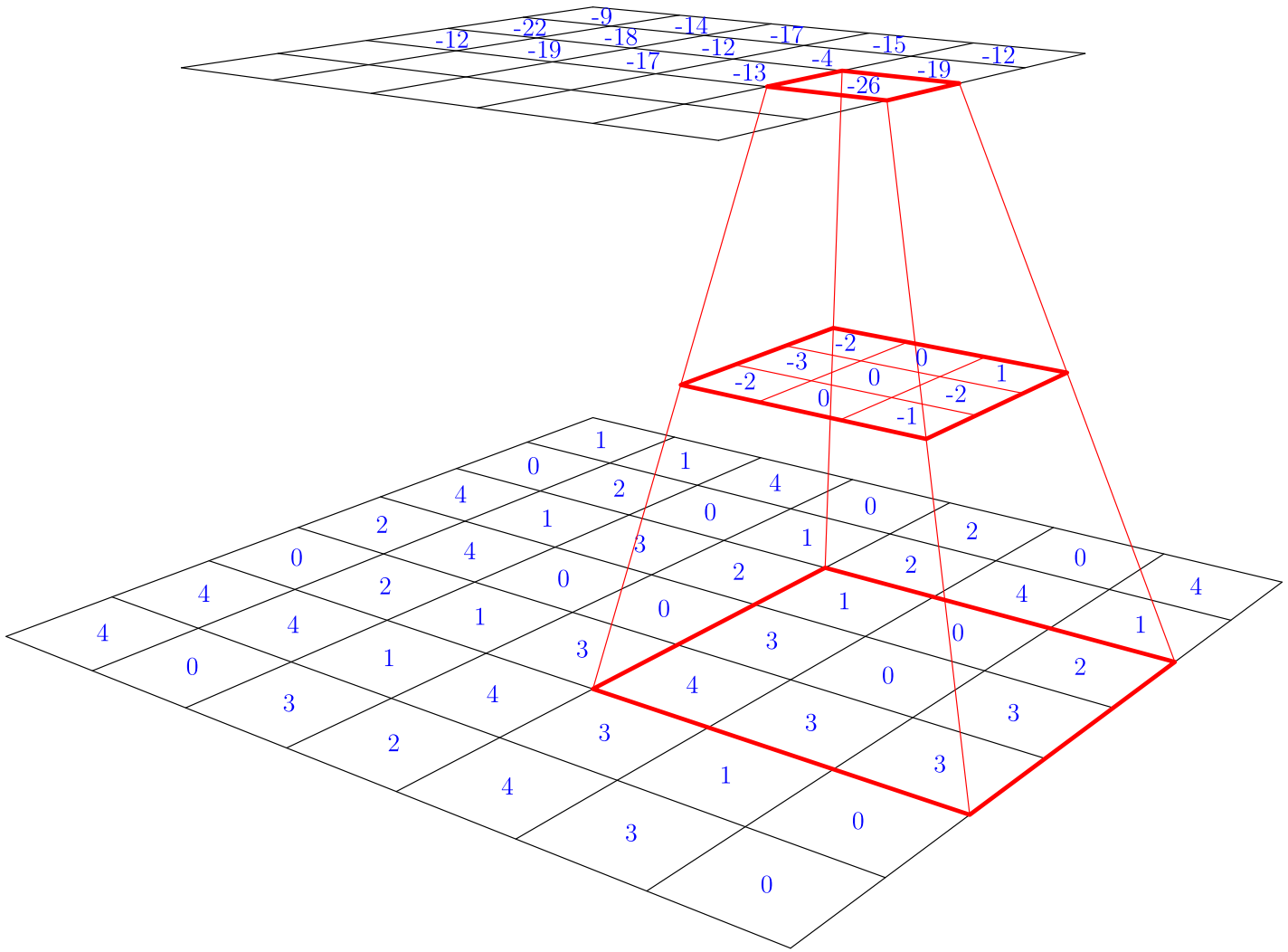
$$-2 \times 3 + 0 \times 2 + 1 \times 1$$
$$-3 \times 0 + 0 \times 0 - 2 \times 3$$
$$-2 \times 1 + 0 \times 3 - 1 \times 4 = -17$$

Convolutional Neural Networks



$$-2 \times 2 + 0 \times 1 + 1 \times 0$$
$$-3 \times 0 + 0 \times 3 - 2 \times 0$$
$$-2 \times 3 + 0 \times 4 - 1 \times 3 = -13$$

Convolutional Neural Networks



$$-2 \times 1 + 0 \times 0 + 1 \times 2$$
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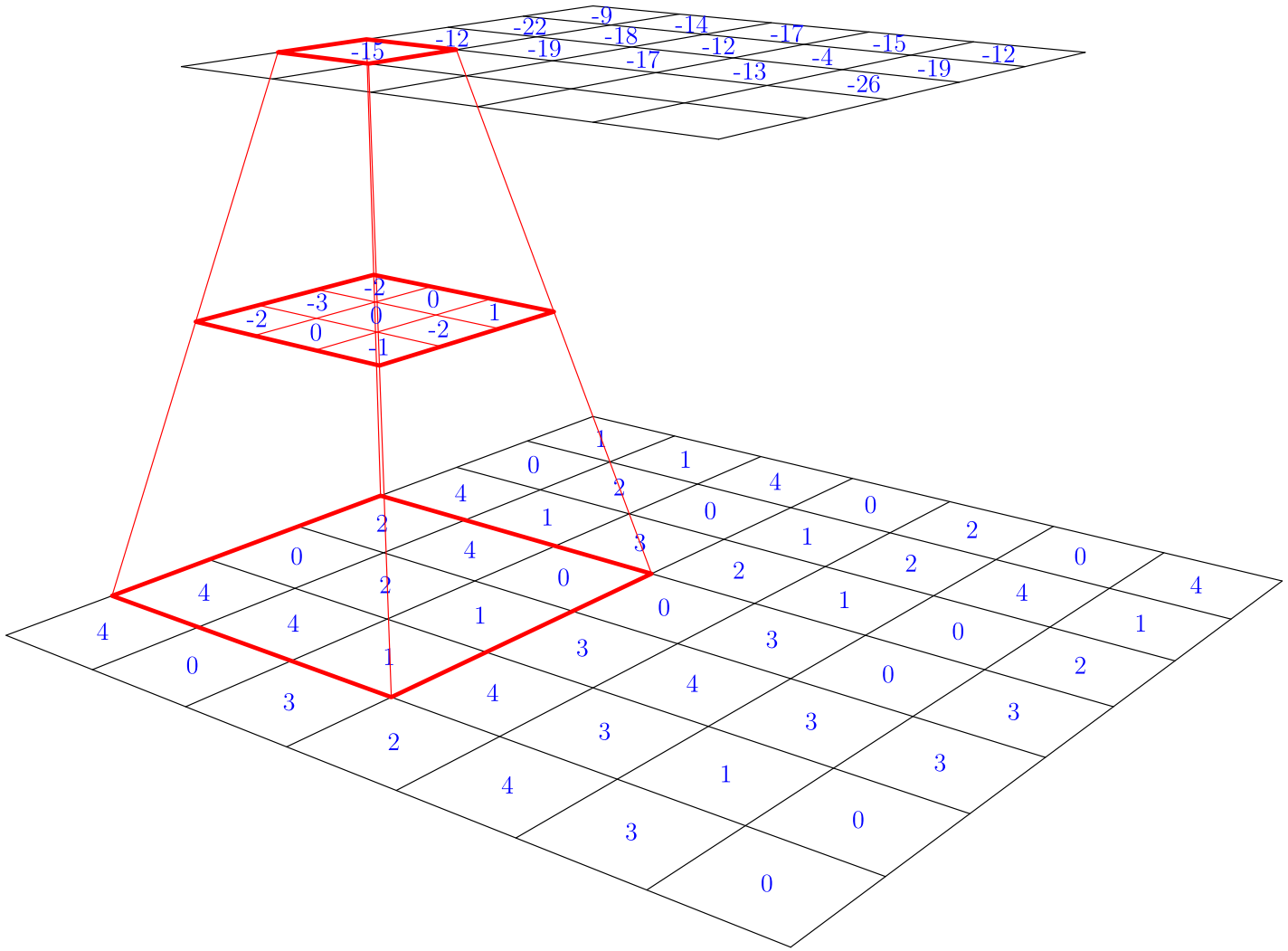
$$-2 \times 4 + 0 \times 3 - 1 \times 3 = -26$$

Convolutional Neural Networks



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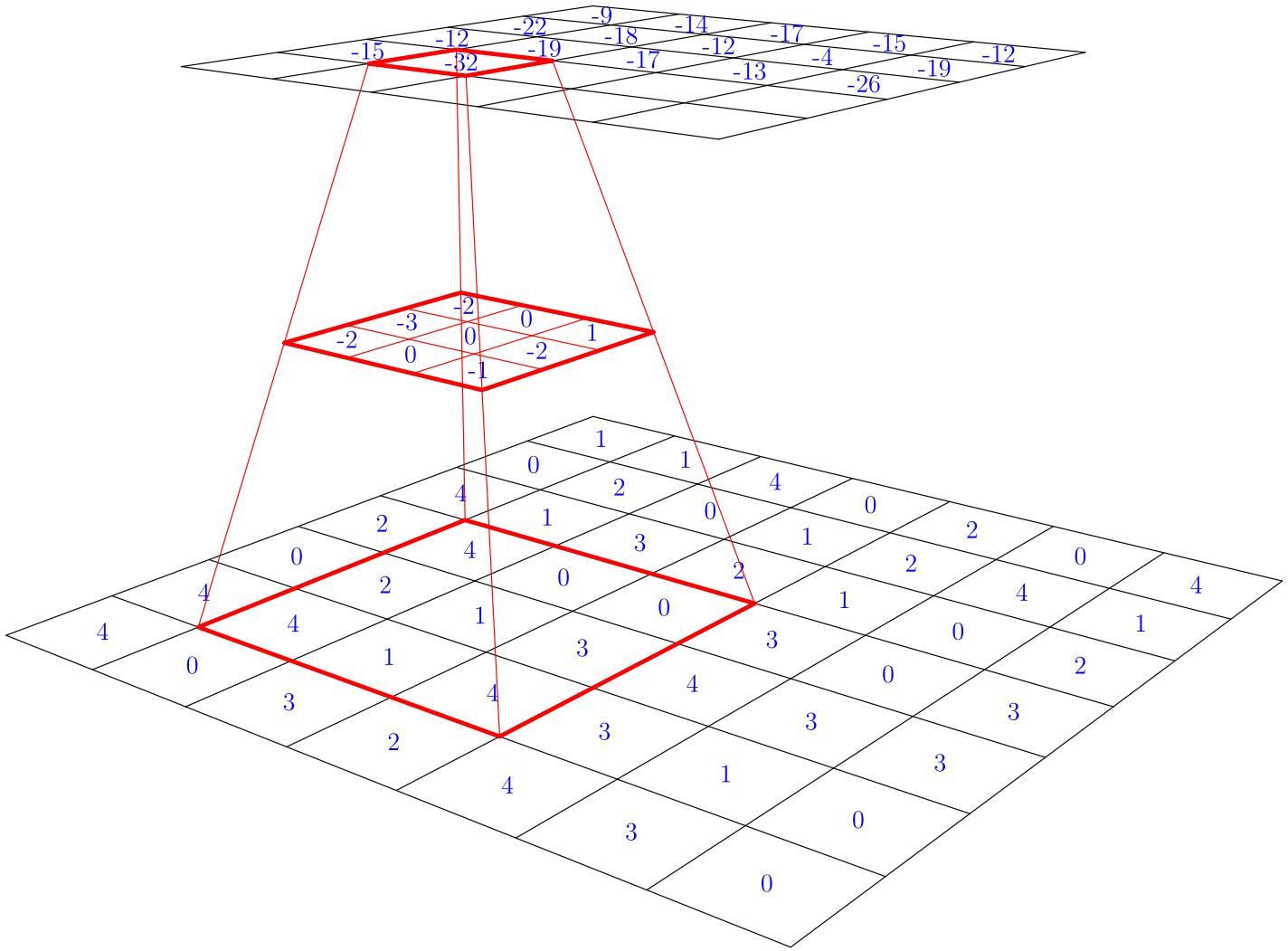
Convolutional Neural Networks



$$-2 \times 4 + 0 \times 0 + 1 \times 0$$
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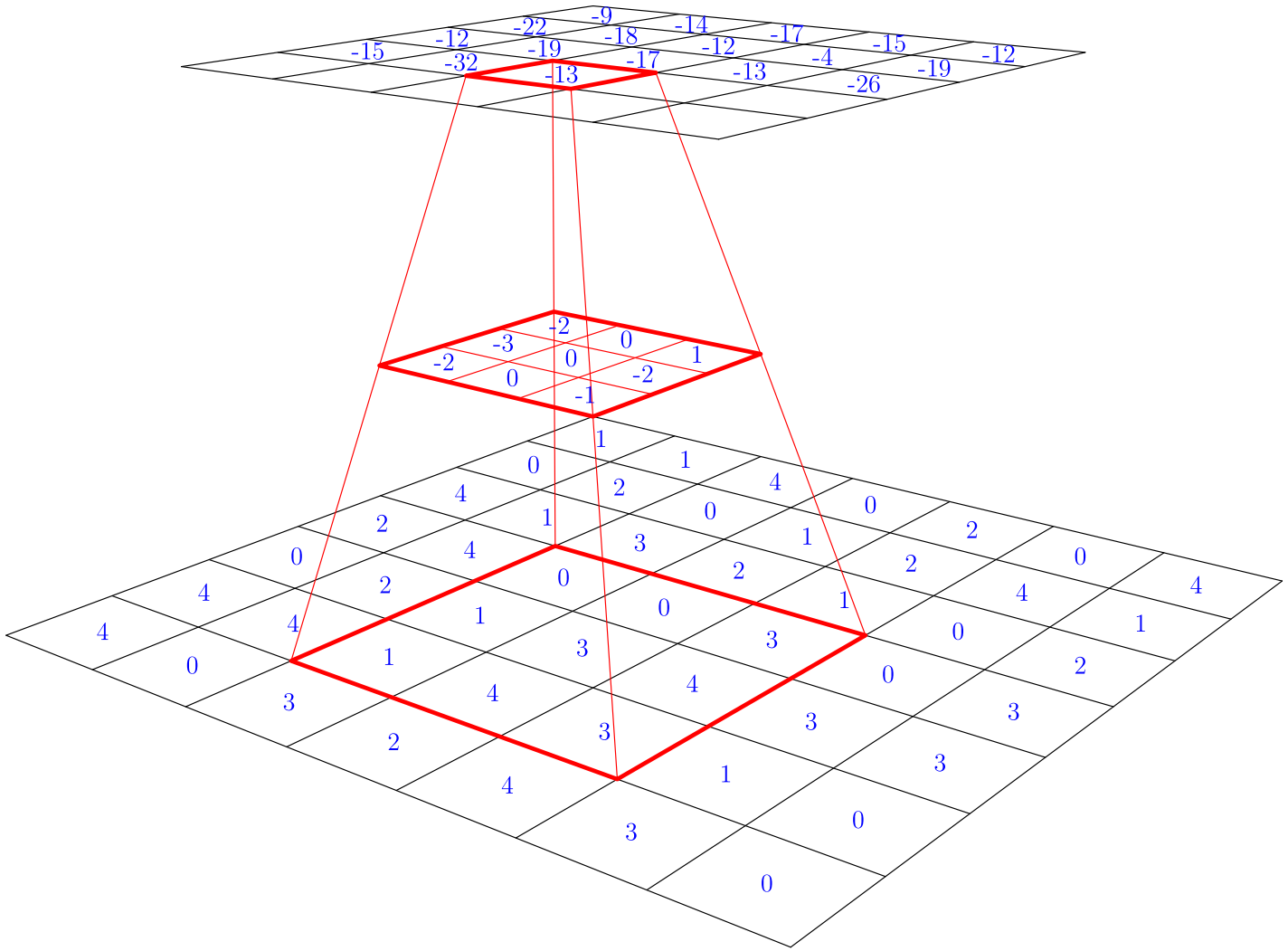
$$-2 \times 4 + 0 \times 1 - 1 \times 4 = -32$$

Convolutional Neural Networks



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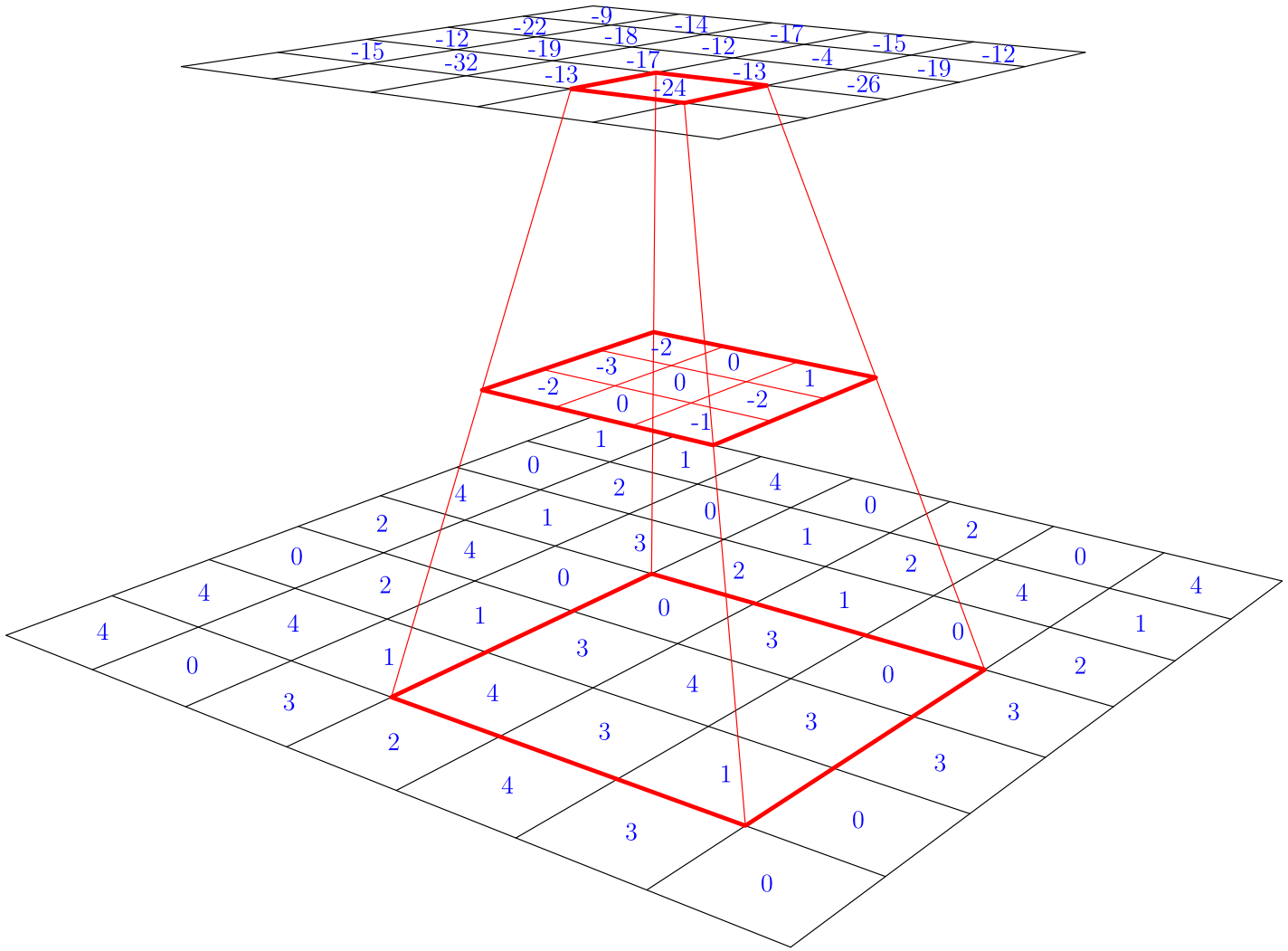
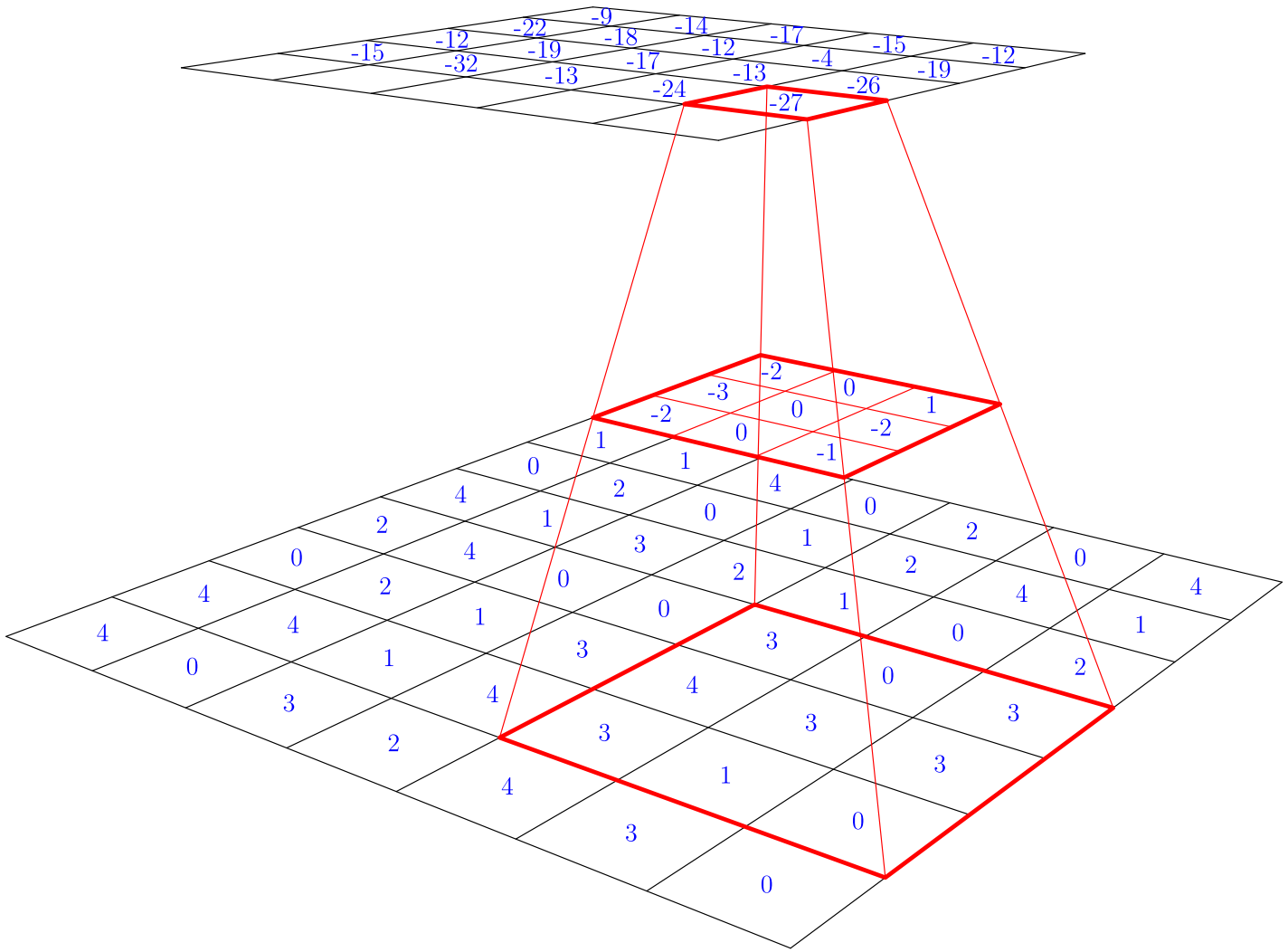
Convolutional Neural Networks



$-2 \times 0 + 0 \times 3 + 1 \times 0$
$-3 \times 3 + 0 \times 4 - 2 \times 3$
$-2 \times 4 + 0 \times 3 - 1 \times 1 = -24$

Convolutional Neural Networks



$$-2 \times 3 + 0 \times 0 + 1 \times 3$$
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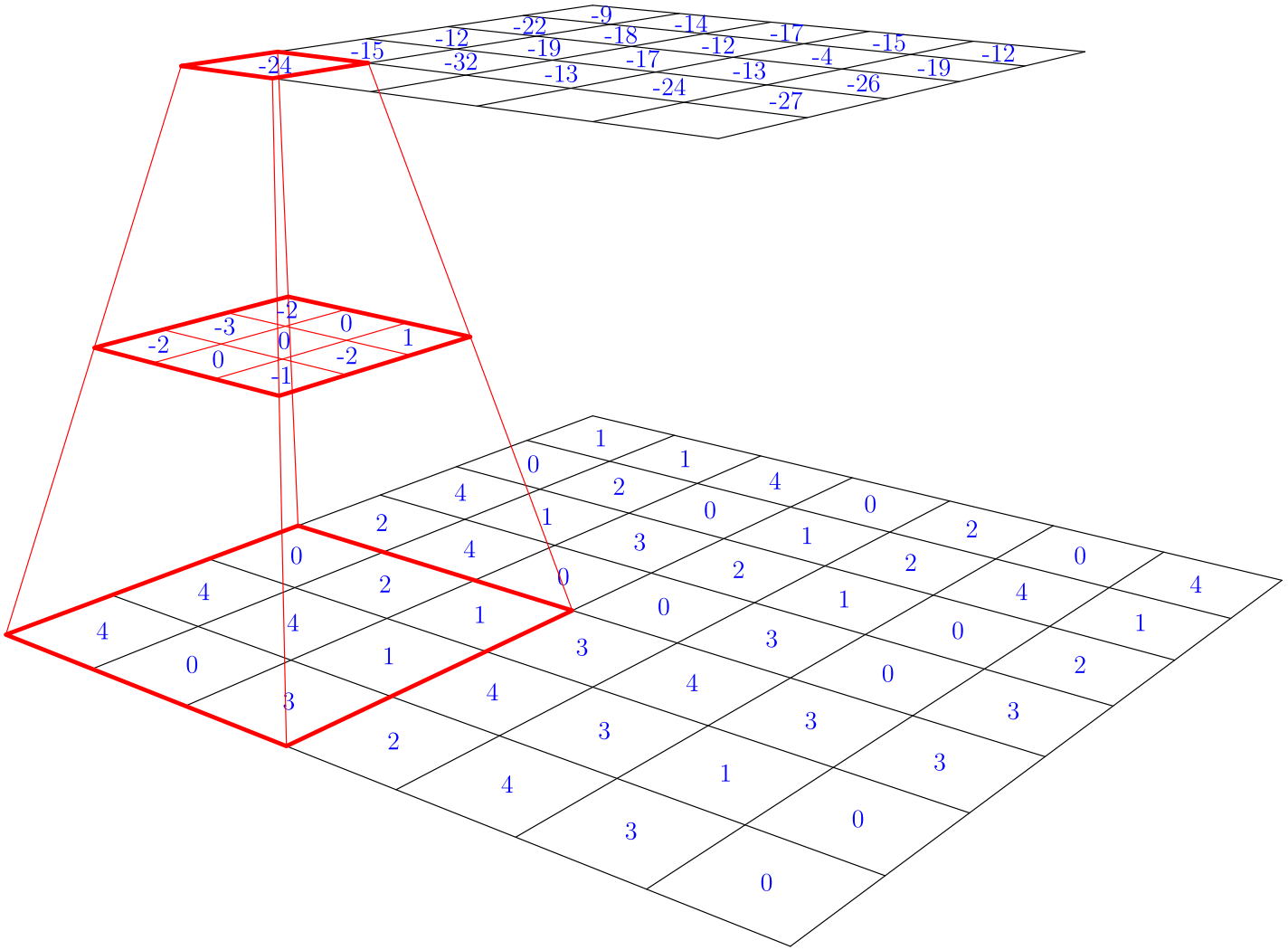
Convolutional Neural Networks



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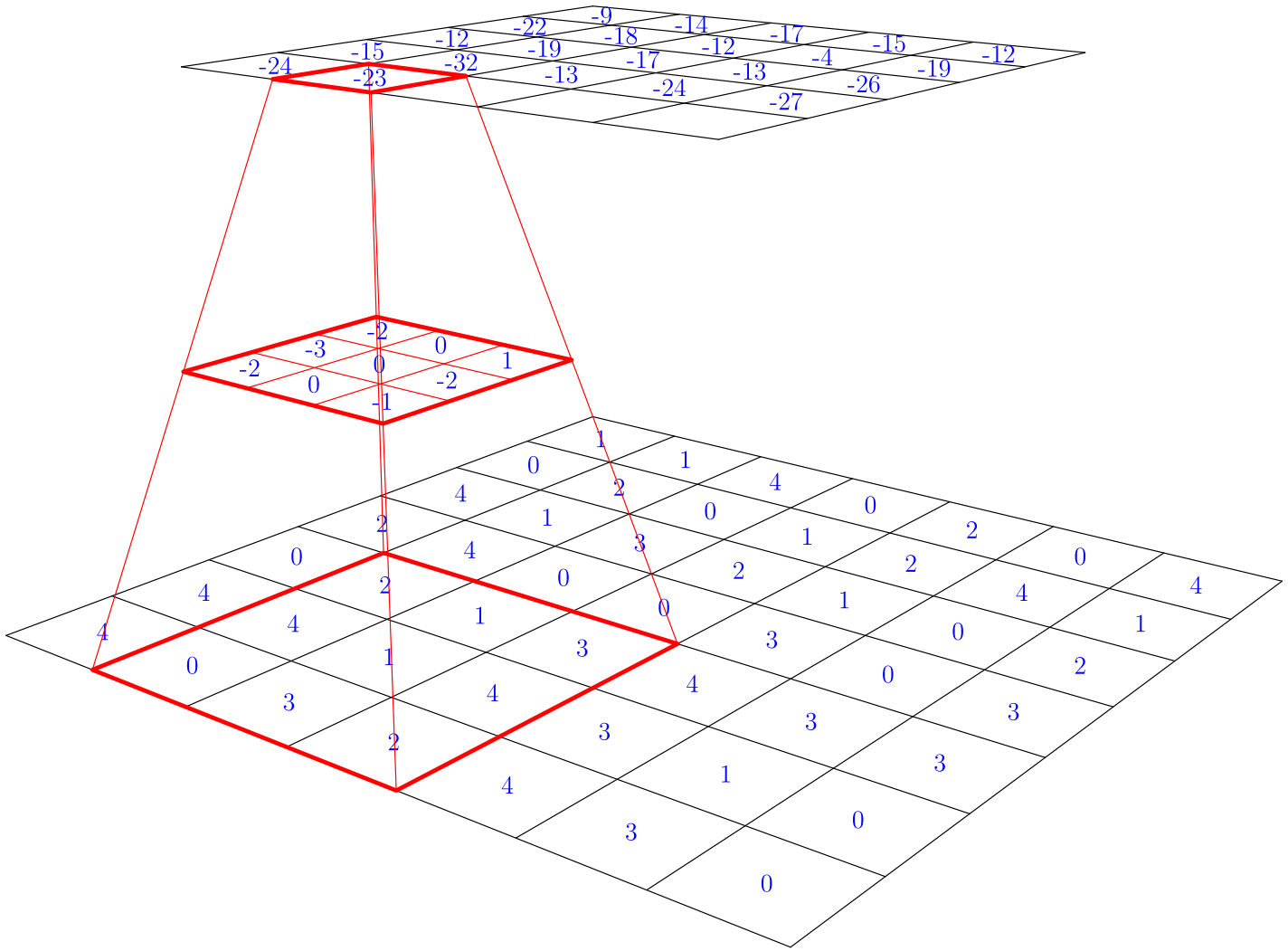
Convolutional Neural Networks



$-2 \times 2 + 0 \times 1 + 1 \times 3$
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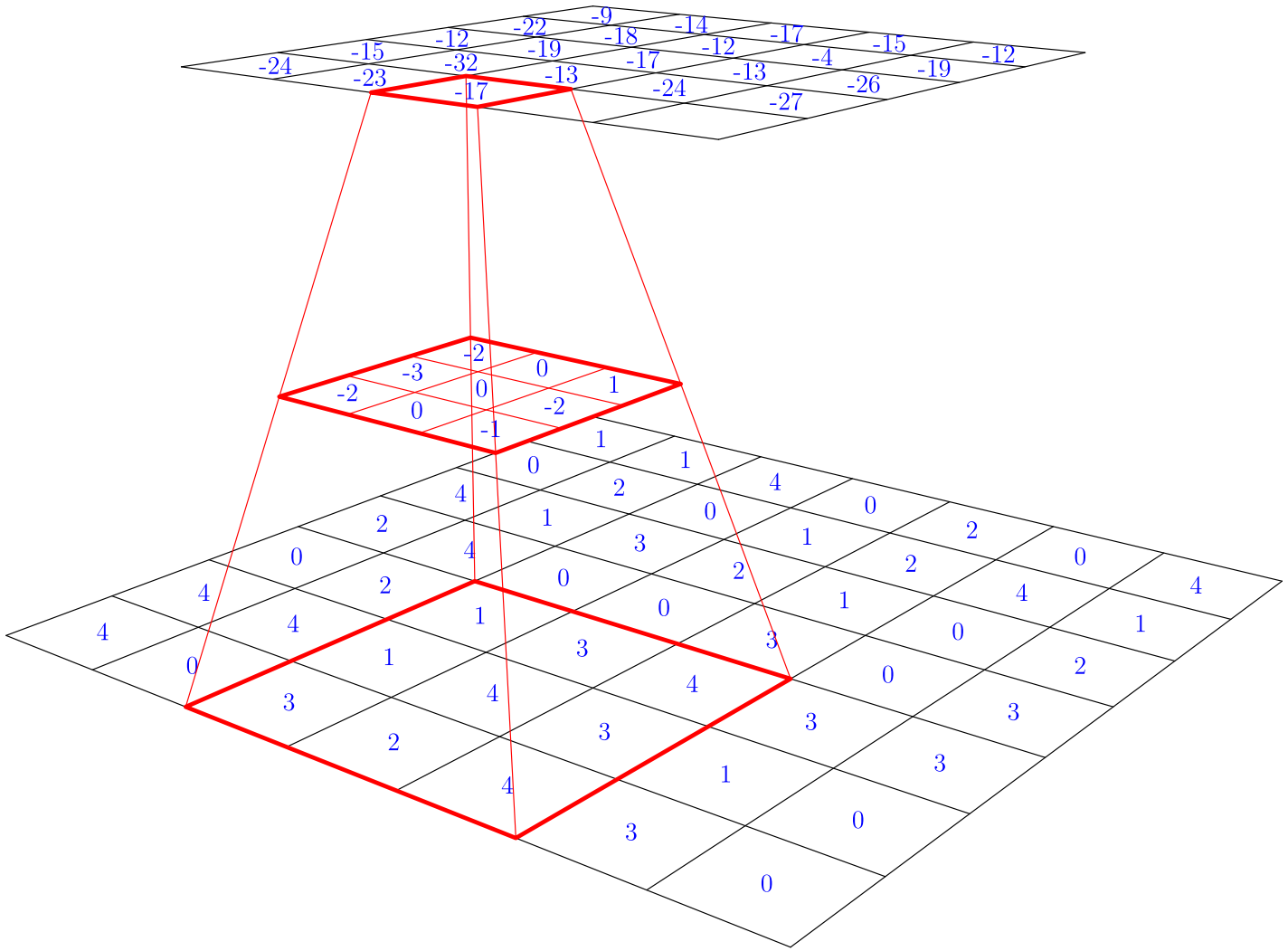
Convolutional Neural Networks



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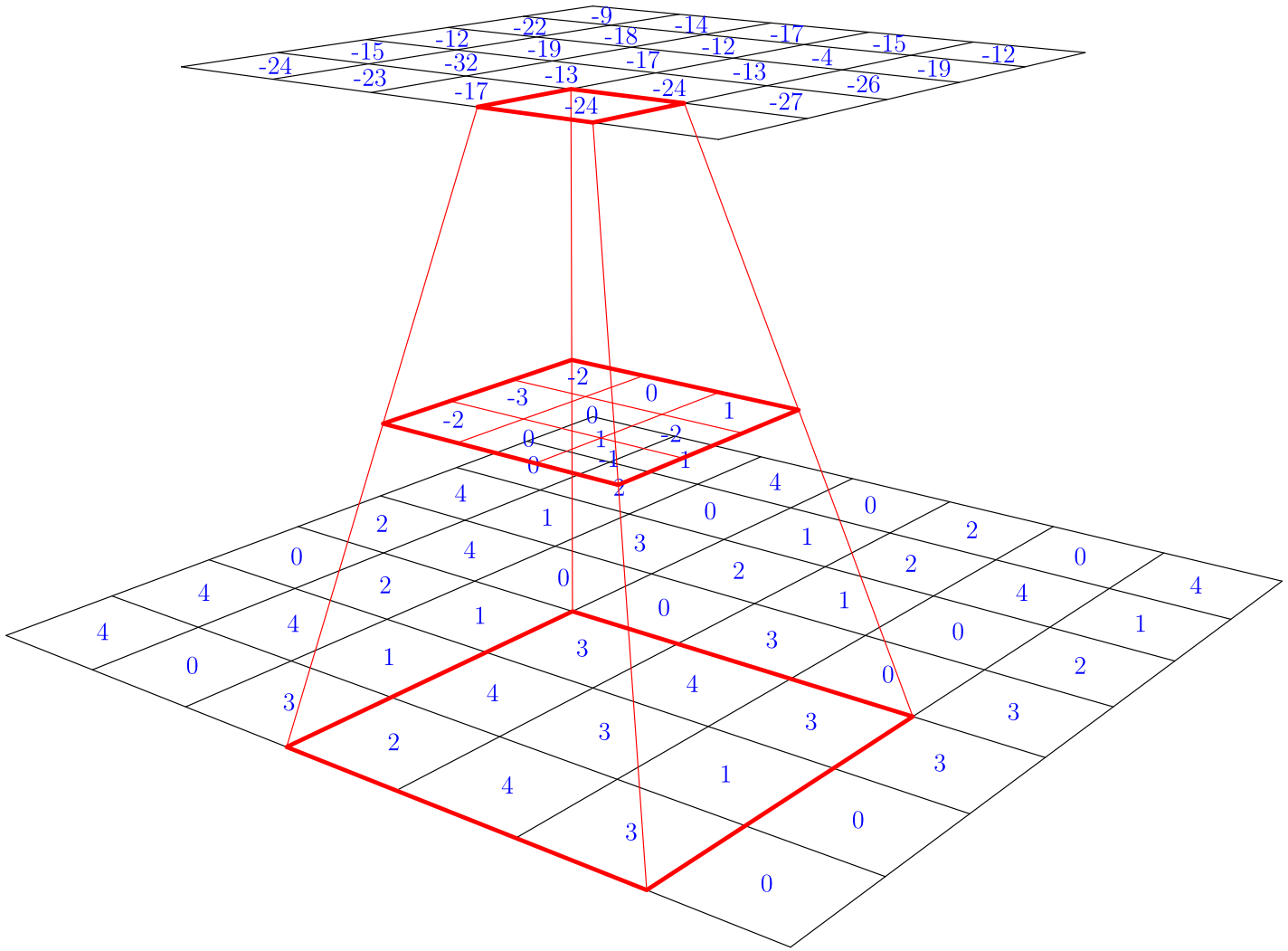
Convolutional Neural Networks



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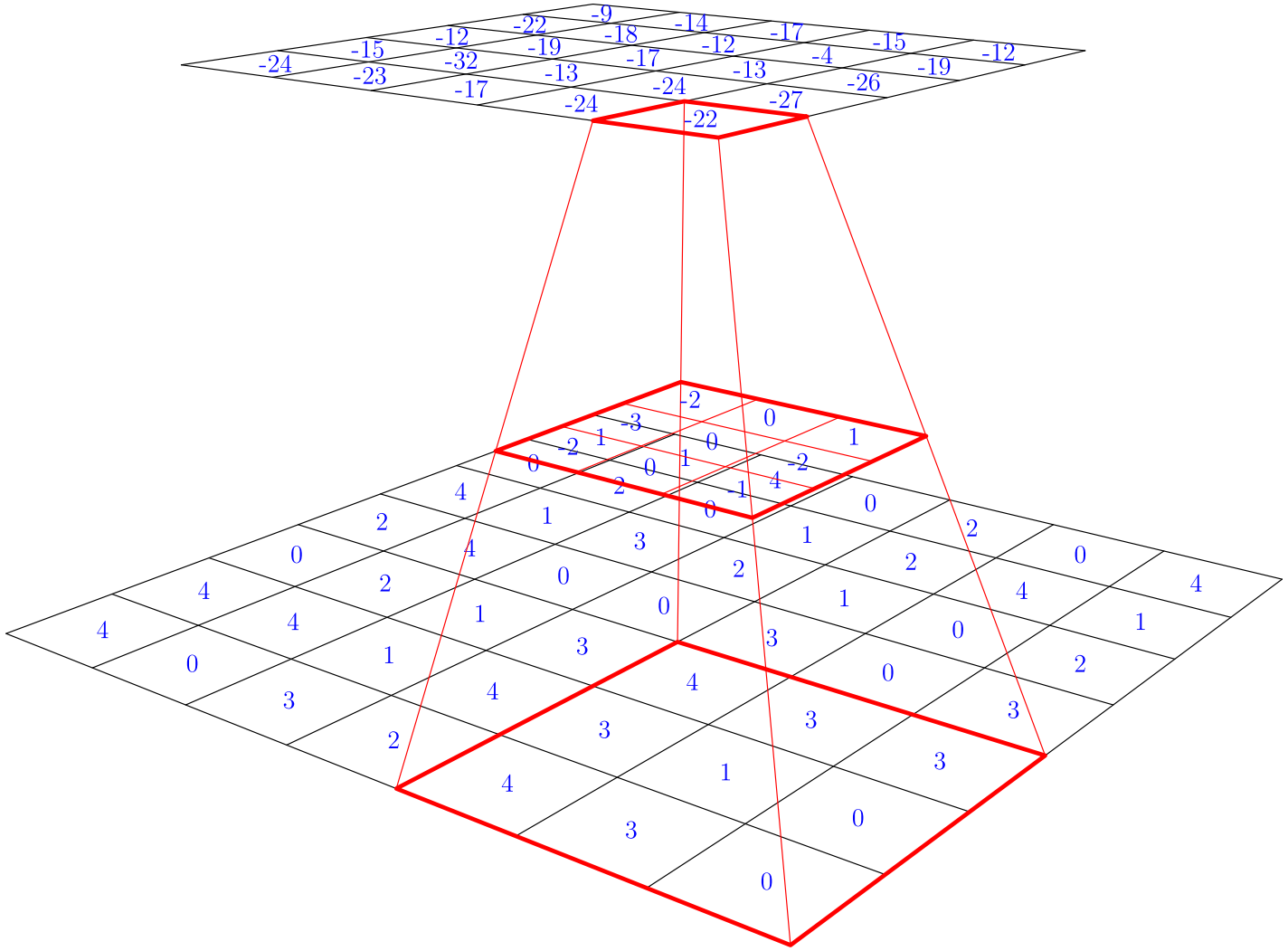
Convolutional Neural Networks



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Equivariance

- CNNs are not translationally invariant
- The output will be different if we shift the input
- They are (up to edge effects) **equivariant** in that we would get the same result if we shifted both the input and the output in the same way
- They are not perfectly equivariant (they break at the pixel level and at the full image level—due to edges)
- But they are sufficient good that CNNs have dominated computer vision for years

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Equivariance

- CNNs are not translationally invariant
- The output will be different if we shift the input
- They are (up to edge effects) **equivariant** in that we would get the same result if we shifted both the input and the output in the same way
- They are not perfectly equivariant (they break at the pixel level and at the full image level—due to edges)
- But they are sufficient good that CNNs have dominated computer vision for years (ignoring visual transformers)

Other Symmetries

- The identity of an object should not change if we move the camera further away or rotate the camera
- CNNs are not naturally scale or rotationally invariant
- Rotation invariance doesn't always reflect "the world"—people usually stand on their feet not on their heads
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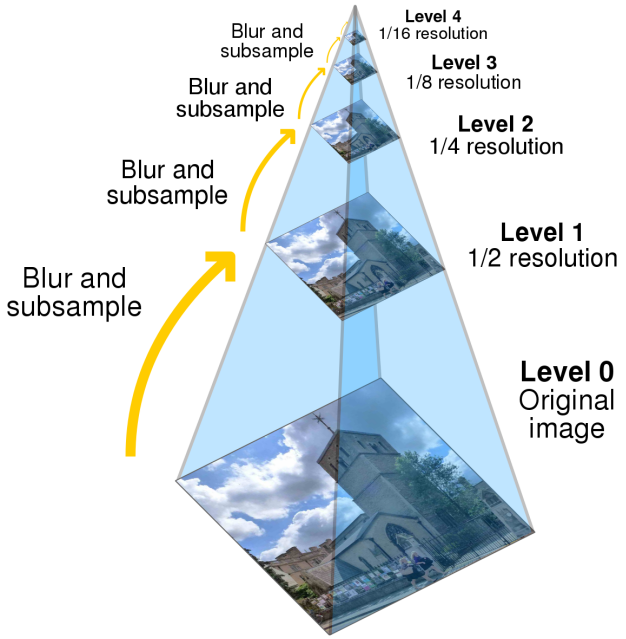
Scale Symmetry

- CNNs are not scale invariant
- There are various pyramid image processing techniques to try and build in approximate scale invariance



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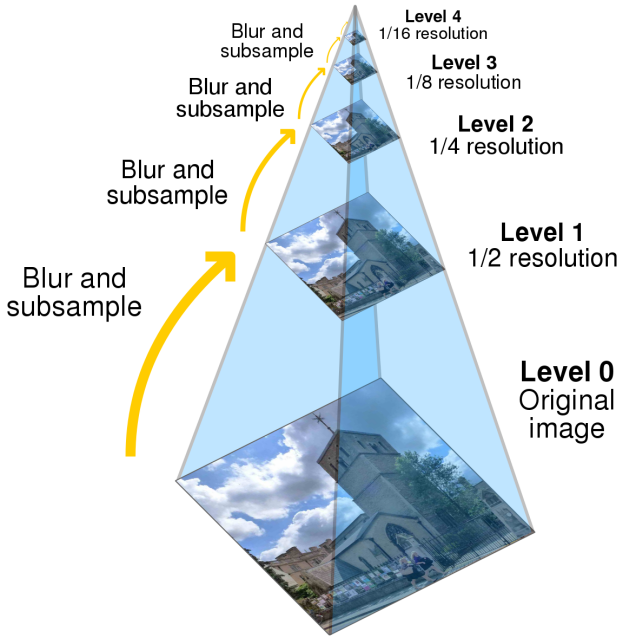

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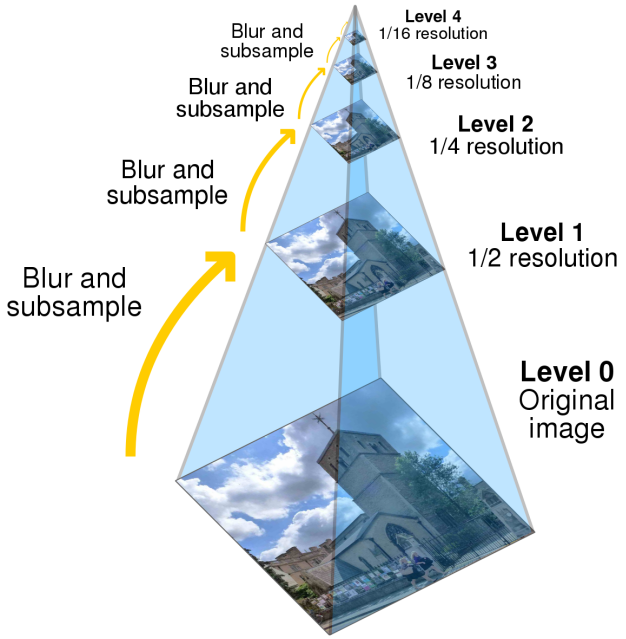

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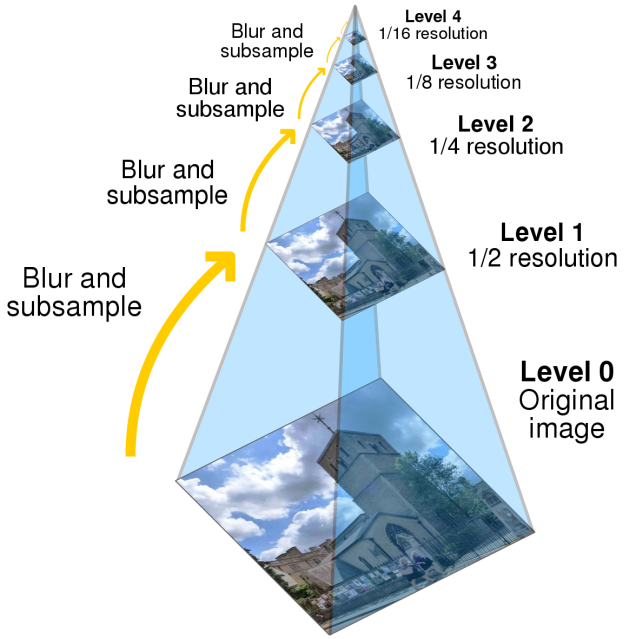

Learning Invariance

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- We therefore hope that our networks learns this by training on objects of different sizes, orientations, lighting conditions, etc.

- Knowing this is an invariance we want, it is now common practice to do data augmentation where we perform transformations that replicate physical plausible changes in the data

- We are removing spurious rules by (artificially) increasing our dataset size

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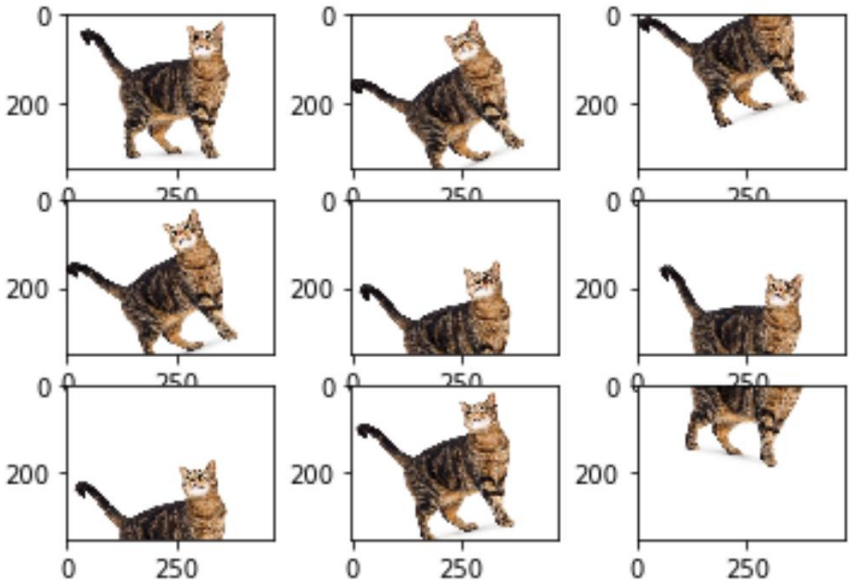

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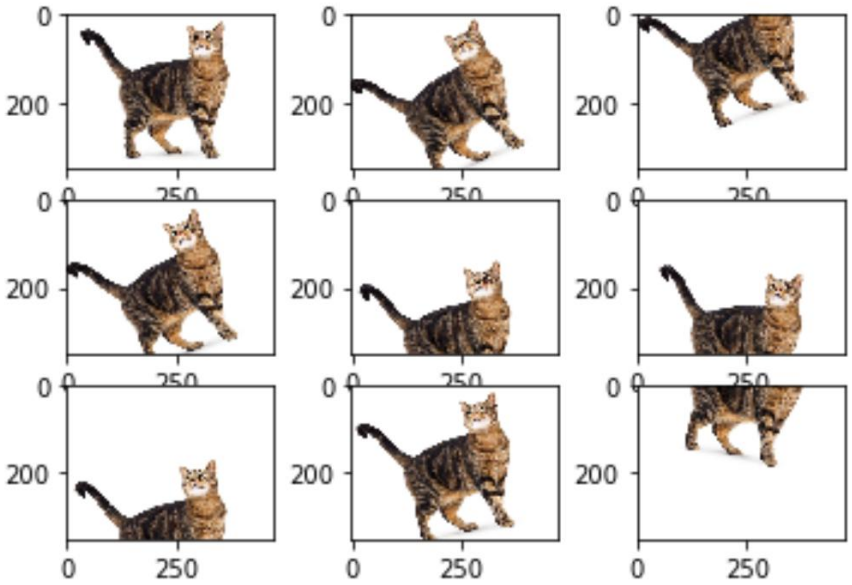

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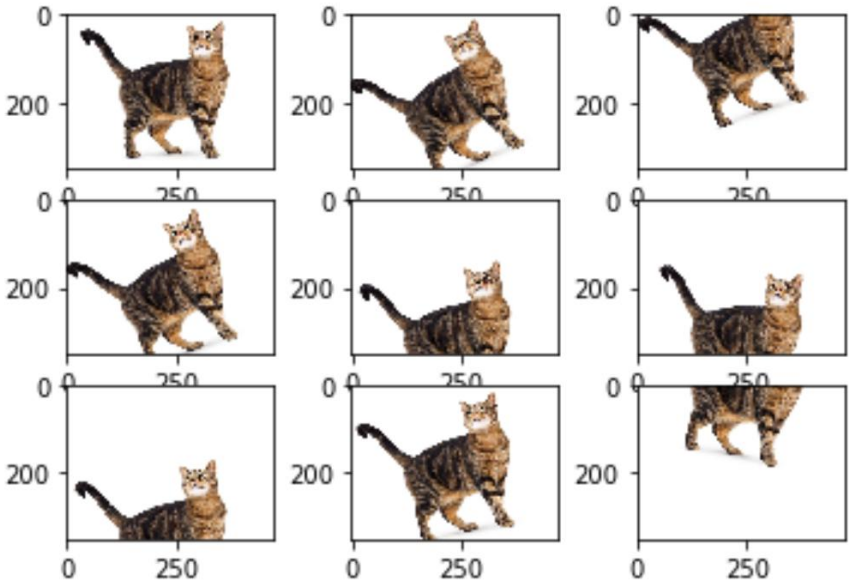

- Data augmentation is standard practice in deep learning for images and makes a very considerable difference

Other Symmetries Exist

- In NLP it is now common to translate sentences to a foreign language and back to the original language to learn invariance to minor changes in the words used
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- An example might be sets of objects in an image or vertices in a graph
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- These make the results invariant to the distance of the camera or the length of $\boldsymbol{a}$ and $\boldsymbol{b}$

Outline

1. Inductive Bias
2. Invariance
3. **Group Theory**

Group Theory

- Symmetries are very well studied in mathematics
- The language of symmetries are **groups**
- These capture the structure of transformations that represent some symmetry
- Group theory is highly abstract and it is easy to lose sight of its connection to symmetry, but it has proved itself extraordinarily powerful in revealing structures

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Groups

- Groups consists of a set (we can think of the elements as transformations), $\mathcal{G} = \{a,b,\cdots\}$
- And an operator "$\cdot$" (which we can often think of as composition)
- That is, $a \cdot b$ we can interpret as apply transformation b and then apply transformation a
- The set and transform form a group if they satisfy four axioms
  - ⋆ closure: for all $a,b \in \mathcal{G}$ then $a \cdot b \in \mathcal{G}$
  - ⋆ associativity: $a \cdot (b \cdot c) = (a \cdot b) \cdot c$
  - ⋆ existence of an identity e such that $a \cdot e = a$ for all a
  - ⋆ Every element, a, has an inverse a^{-1} such that $a^{-1} \cdot a = e$

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Tossing a coin

- We consider a coin with two actions
  - ⋆ flip the coin: f
  - ⋆ leave the coin alone: e
- These form a group (the cyclic group C_2)
  - ⋆ Closure is obvious $f \cdot e = f$, $f \cdot f = e$, $e \cdot e = e$ and $e \cdot f = f$
  - ⋆ Associativity: e.g. $(e \cdot f) \cdot f = e \cdot (f \cdot f)$
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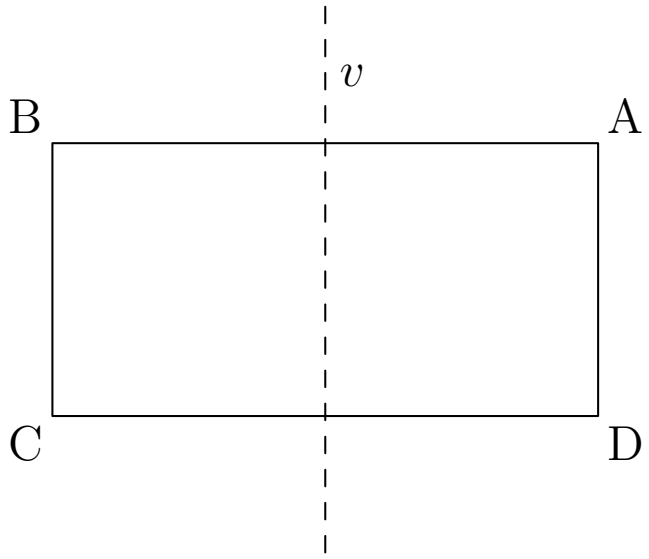

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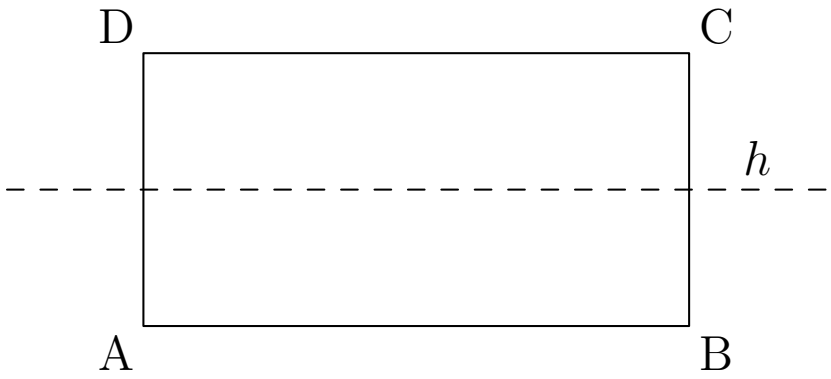

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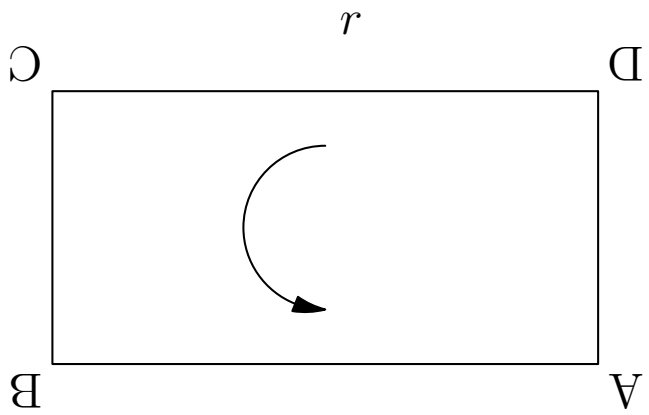

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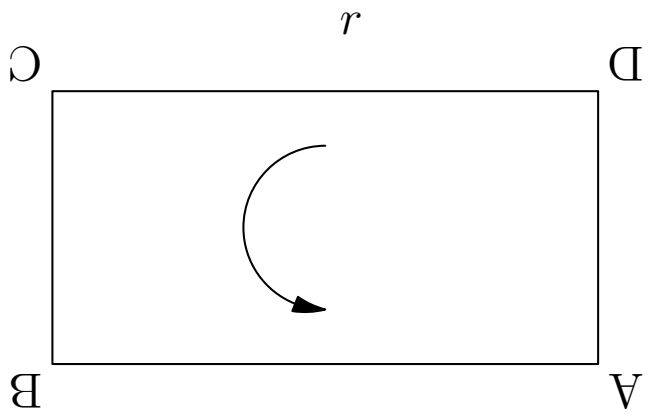

	e	v	h	r
e	e	v	h	r
v	v	e	r	h
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Non-commutativity

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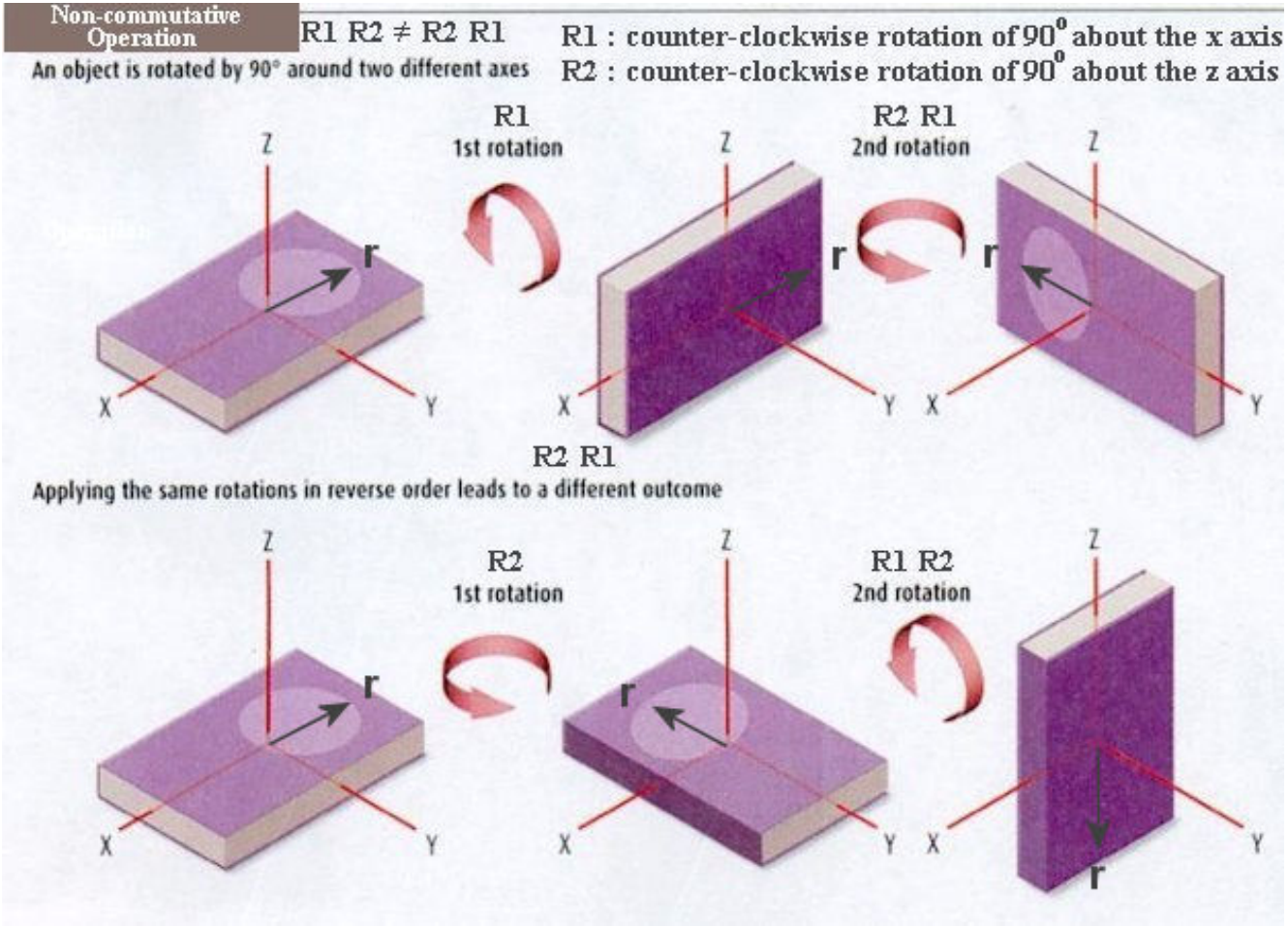

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- We consider $\cdot$ to denote composition so $a \cdot b$ denotes apply action b then action a
- When we say $c = a \cdot b$ we mean that action c is equivalent to apply action b followed by action a
- Suppose $g = a \cdot b$ and $h = b \cdot c$ then

$$g \cdot c = a \cdot h$$

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- These correspond to an equivalent set of actions

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Permutations

- The set of permutations of n objects form a group (known as the symmetric group S_n)
- The composition of a permutation is a permutation
- There is an identity (do nothing)
- For every permutation there is an inverse permutation
- Obviously S_n has $n!$ elements

- Permutations have a lot of structure (in terms of elements cycling, subgroups, etc.)

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- The group describes the set of discrete shifts
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- The set of rational number under addition also forms a group
- Nothing new here, you've known about these since you were a toddler

Continuous Groups

- The set of reals under addition form a group and describes translations in one dimension
- The set of reals excluding 0 form a group under multiplication with an identity 1 and inverse of x being $1/x$
- These describe scale transformation
- These are not terrifically interesting groups

Continuous Groups

- The set of reals under addition form a group and describes translations in one dimension
- The set of reals excluding 0 form a group under multiplication with an identity 1 and inverse of x being $1/x$
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- Things get more interesting in high dimensional space

Lie Groups

- Continuous groups are known as Lie Groups
- They describe things like general translational invariance, rotational invariance, relativistic invariance
- The transformations can be represented by a set of matrices
- To study these one looks at infintesimal transformations and the algebra between these infintesimal transformations (Lie algebras)
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Rotations $SO(n)$

- The set of $n \times n$ orthogonal matrices (matrices, $\mathbf{M}$, such that $\mathbf{M}^\mathsf{T}\mathbf{M} = \mathbf{M}\mathbf{M}^\mathsf{T} = \mathbf{I}$) form a group $O(n)$
- Note that $\det(\mathbf{M}) = \pm 1$
- These correspond to rotations and reflections
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- Invariances are important as if a machine properly captures a true invariance it can massively limit the space of functions being approximated
- Often it is hard to build-in invariances into the machine learning model and practitioners will often resort to data augmentation in the hope that these invariances can be learned
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- I'm not going to expect you to know any details about group theory