EE-559 – Deep learning

4a. DAG networks, autograd, convolution layers

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https://fleuret.org/dlc/

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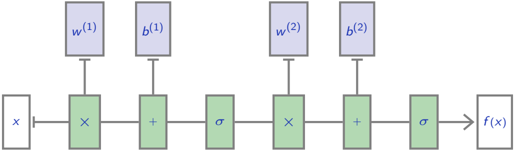
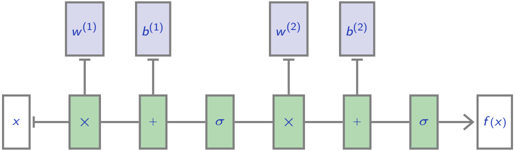
DAG networks

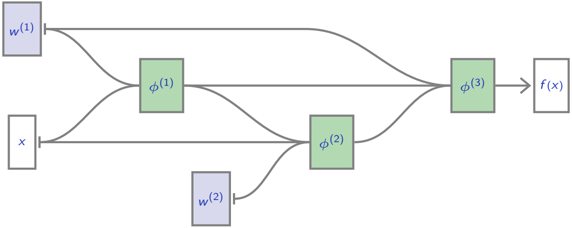
Everything we have seen for an MLP



Everything we have seen for an MLP



can be generalized to an arbitrary "Directed Acyclic Graph" (DAG) of operators



Remember that we use tensorial notation.

If $(a_1, \dots, a_Q) = \phi(b_1, \dots, b_R)$, we have

$$\left[\frac{\partial a}{\partial b}\right] = J_\phi = \begin{pmatrix} \frac{\partial a_1}{\partial b_1} & \dots & \frac{\partial a_1}{\partial b_R} \\ \vdots & \ddots & \vdots \\ \frac{\partial a_Q}{\partial b_1} & \dots & \frac{\partial a_Q}{\partial b_R} \end{pmatrix}.$$

This notation does not specify at which point this is computed. It will always be for the forward-pass activations.

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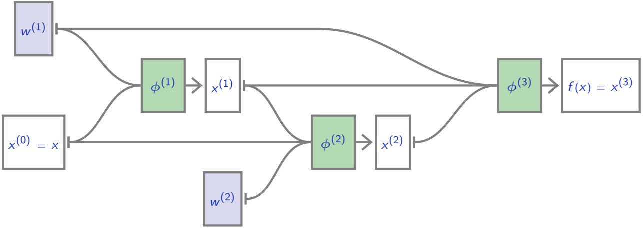
Also, if $(a_1, \dots, a_Q) = \phi(b_1, \dots, b_R, c_1, \dots, c_S)$, we use

$$\left[\frac{\partial a}{\partial c}\right] = J_{\phi|c} = \begin{pmatrix} \frac{\partial a_1}{\partial c_1} & \cdots & \frac{\partial a_1}{\partial c_S} \\ \vdots & \ddots & \vdots \\ \frac{\partial a_Q}{\partial c_1} & \cdots & \frac{\partial a_Q}{\partial c_S} \end{pmatrix}.$$

Forward pass



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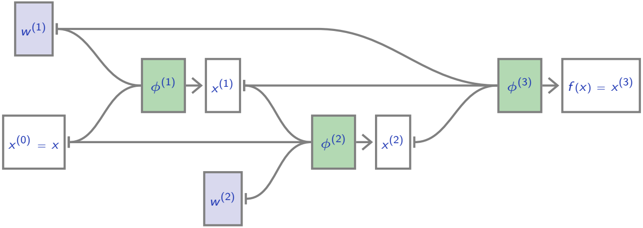
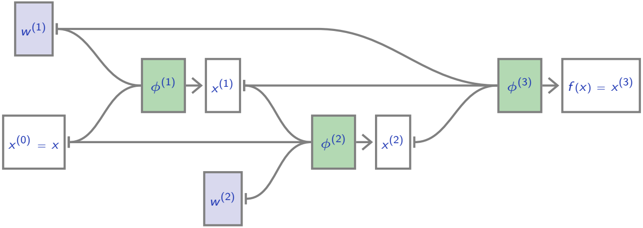


$$x^{(0)} = x$$

Forward pass



$$x^{(0)} = x$$
$$x^{(1)} = \phi^{(1)}(x^{(0)}; w^{(1)})$$

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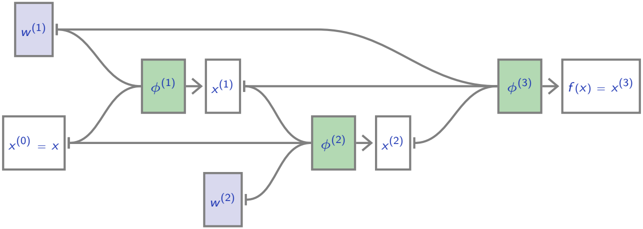

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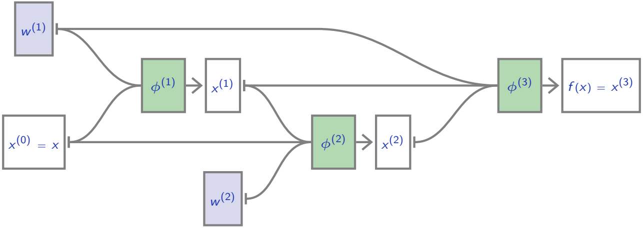

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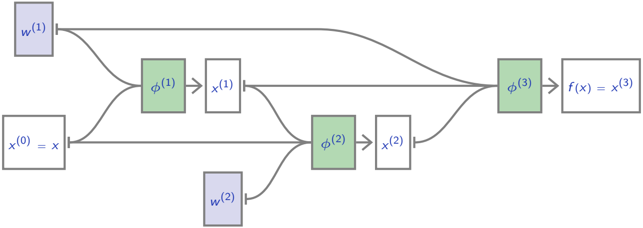
Backward pass, derivatives w.r.t activations



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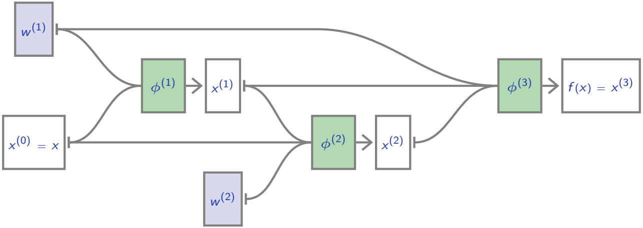

$$\left[\frac{\partial \ell}{\partial x^{(2)}}\right] = \left[\frac{\partial x^{(3)}}{\partial x^{(2)}}\right]\left[\frac{\partial \ell}{\partial x^{(3)}}\right] = J_{\phi^{(3)}|x^{(2)}}\left[\frac{\partial \ell}{\partial x^{(3)}}\right]$$

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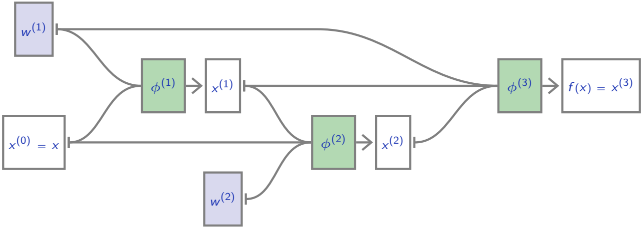

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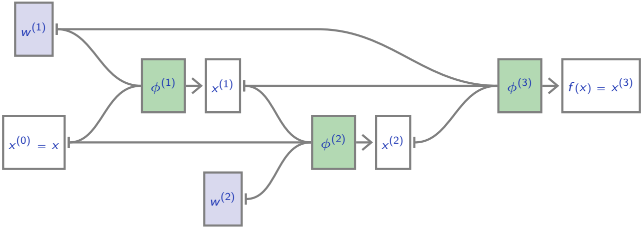

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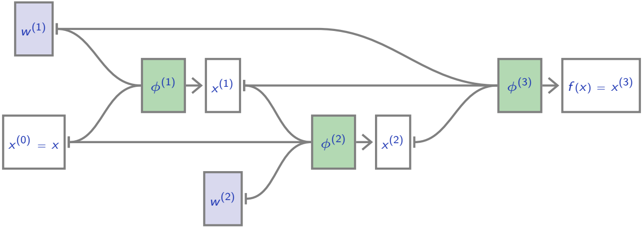

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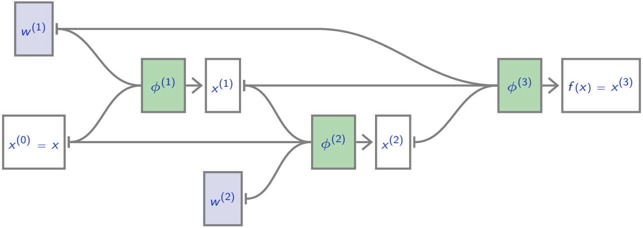

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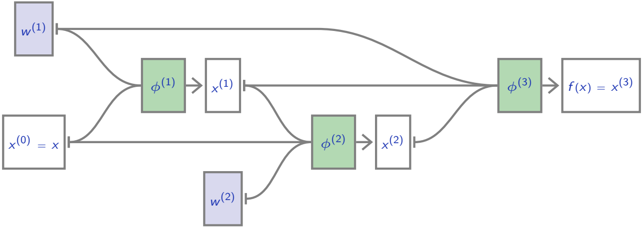

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So if we have a library of "tensor operators", and implementations of

$$
\begin{aligned}
&(x_1, \dots, x_d, w) \mapsto \phi(x_1, \dots, x_d; w) \\
\forall c,\ &(x_1, \dots, x_d, w) \mapsto J_{\phi|x_c}(x_1, \dots, x_d; w) \\
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we can build an arbitrary directed acyclic graph with these operators at the nodes, compute the response of the resulting mapping, and compute its gradient with back-prop.

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Multiple frameworks provide libraries of tensor operators and mechanisms to combine them into DAGs and automatically differentiate them.

	Language(s)	**License**	**Main backer**
PyTorch	**Python**	BSD	Facebook
Caffe2	C++, Python	Apache	Facebook
TensorFlow	Python, C++	Apache	Google
MXNet	Python, C++, R, Scala	Apache	Amazon
CNTK	Python, C++	MIT	Microsoft
Torch	Lua	BSD	Facebook
Theano	Python	BSD	U. of Montreal
Caffe	C++	BSD 2 clauses	U. of CA, Berkeley

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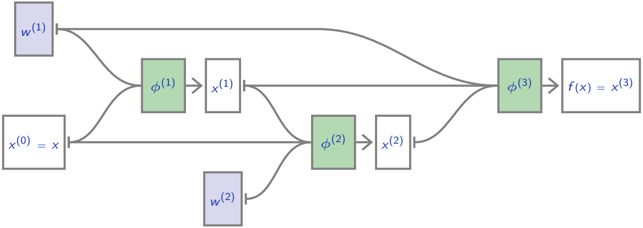
One approach is to define the nodes and edges of such a DAG statically (Torch, TensorFlow, Caffe, Theano, etc.)

For instance, in TensorFlow, to run a forward/backward pass on



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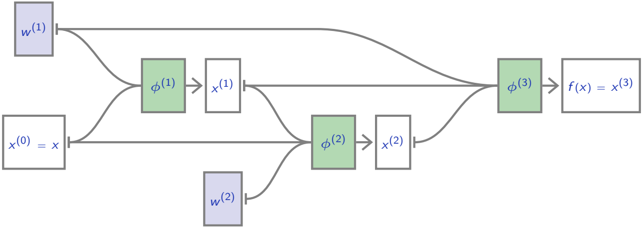

with

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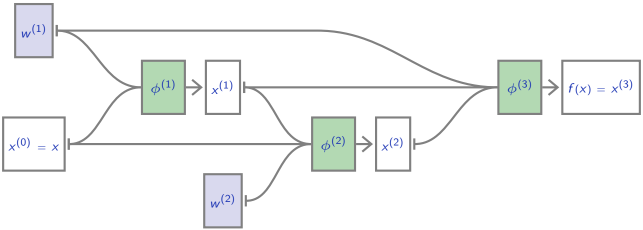

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we can do

```
w1 = tf.Variable(tf.random_normal([5, 5]))
w2 = tf.Variable(tf.random_normal([5, 5]))
x = tf.Variable(tf.random_normal([5, 1]))
x0 = x
x1 = tf.matmul(w1, x0)
x2 = x0 + tf.matmul(w2, x1)
x3 = tf.matmul(w1, x1 + x2)
q = tf.norm(x3)

gw1, gw2 = tf.gradients(q, [w1, w2])

with tf.Session() as sess:
    sess.run(tf.global_variables_initializer())
    _gw1, _gw2 = sess.run([gw1, gw2])
```

Autograd

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This "autograd" mechanism has two main benefits:

- Simpler syntax: one just need to write the forward pass as a standard sequence of Python operations,
- greater flexibility: Since the graph is not static, the forward pass can be dynamically modulated.

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A `Variable` is first a wrapper around a `Tensor`. It has the following fields

- `data` is the `Tensor` containing the data itself,
- `grad` is a `Variable` of same dimension to sum the gradient,
- `requires_grad` is a `Boolean` stating if we need the gradient w.r.t this `Variable` (default is `False`).

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A `Parameter` is a `Variable` with `requires_grad` to `True` by default, and known to be a parameter by various utility functions.

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⚠ A `Variable` can only embed a `Tensor`, so functions returning a scalar (*e.g.* a loss) now return a 1d `Variable` with a single value.

`torch.autograd.grad(outputs, inputs)` computes and returns the sum of gradients of outputs wrt the specified inputs. This is always a `tuple` of `Variable`.

An alternative is to use `torch.autograd.backward(variables)` or `Variable.backward()`, which accumulates the gradients in the `grad` fields of the leaf `Variable`s.

Consider a simple example $(x_1, x_2, x_3) = (1, 2, 2)$, and

$$\ell = \|x\| = \sqrt{x_1^2 + x_2^2 + x_3^2}.$$

We have $\ell = 3$ and

$$\frac{\partial \ell}{\partial x_i} = \frac{x_i}{\|x\|}.$$

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```
>>> from torch import Tensor
>>> from torch.autograd import Variable
>>> x = Variable(Tensor([1, 2, 2]), requires_grad = True)
>>> l = x.norm()
>>> l
Variable containing:
 3
[torch.FloatTensor of size 1]

>>> g = torch.autograd.grad(l, x)
>>> g
(Variable containing:
 0.3333
 0.6667
 0.6667
[torch.FloatTensor of size 3]
,)
```

Alternatively, `Variable.backward()` accumulates the gradient in the variable's `grad` fields.

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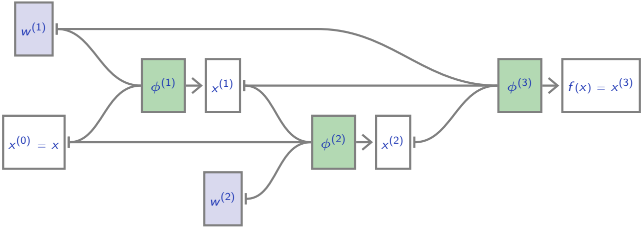

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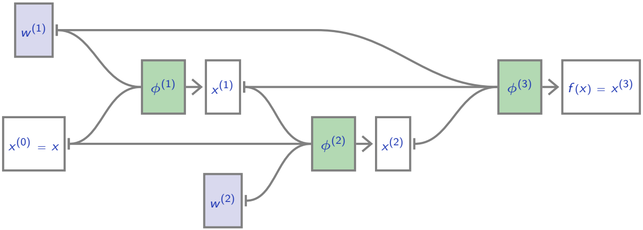

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we can do

```
w1 = Parameter(Tensor(5, 5).normal_())
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x = Variable(Tensor(5).normal_())

x0 = x
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x2 = x0 + w2.mv(x1)
x3 = w1.mv(x1 + x2)

q = x3.norm()

q.backward()
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We can look precisely at the graph built during a computation.

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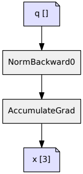

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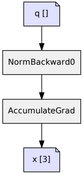
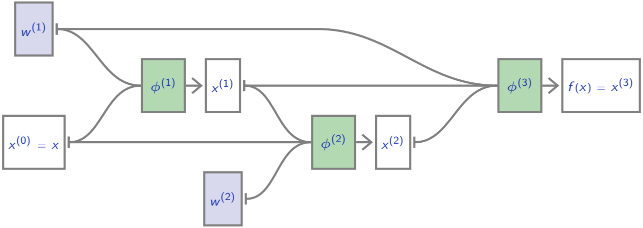


This graph was generated with

https://fleuret.org/git/agtree2dot

and Graphviz.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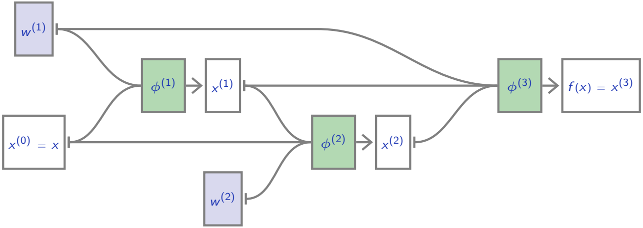


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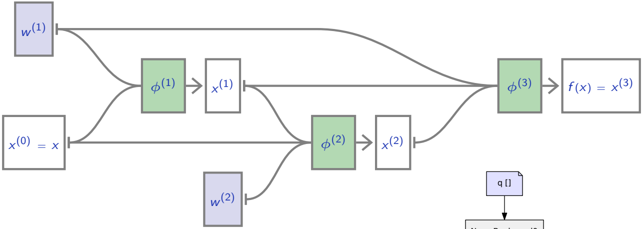


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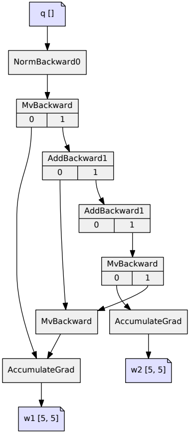


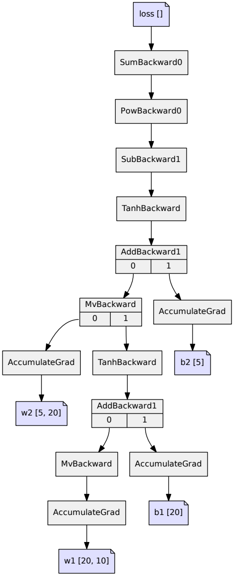
```
w1 = Parameter(Tensor(20, 10))
b1 = Parameter(Tensor(20))
w2 = Parameter(Tensor(5, 20))
b2 = Parameter(Tensor(5))

x = Variable(Tensor(10).normal_())
h = torch.tanh(w1.mv(x) + b1)
y = torch.tanh(w2.mv(h) + b2)

target = Variable(Tensor(5).normal_())

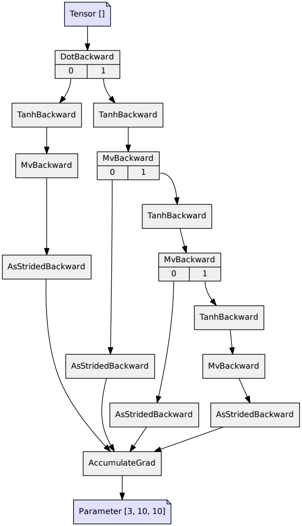
loss = (y - target).pow(2).sum()
```

```python
w1 = Parameter(Tensor(20, 10))
b1 = Parameter(Tensor(20))
w2 = Parameter(Tensor(5, 20))
b2 = Parameter(Tensor(5))

x = Variable(Tensor(10).normal_())
h = torch.tanh(w1.mv(x) + b1)
y = torch.tanh(w2.mv(h) + b2)

target = Variable(Tensor(5).normal_())

loss = (y - target).pow(2).sum()
```



```
w = Parameter(Tensor(3, 10, 10))

def blah(k, x):
    for i in range(k):
        x = torch.tanh(w[i].mv(x))
    return x

u = blah(1, Variable(Tensor(10)))
v = blah(3, Variable(Tensor(10)))
q = u.dot(v)
```

```
w = Parameter(Tensor(3, 10, 10))

def blah(k, x):
    for i in range(k):
        x = torch.tanh(w[i].mv(x))
    return x

u = blah(1, Variable(Tensor(10)))
v = blah(3, Variable(Tensor(10)))
q = u.dot(v)
```



⚠ `Variable.backward()` **accumulates** the gradients in the different `Variable`s, so one may have to zero them before.

This accumulating behavior is desirable in particular to compute the gradient of a loss summed over several "mini-batches," or the gradient of a sum of losses.

```
>>> x = Variable(Tensor([3, 4]), requires_grad = True)
>>> a = x.norm()
>>> a.backward()
>>> b = x.dot(Variable(Tensor([-10, 10])))
>>> b.backward()
>>> x.grad
Variable containing:
 -9.4000
 10.8000
[torch.FloatTensor of size 2]
```

```
>>> x = Variable(Tensor([3, 4]), requires_grad = True)
>>> q = x.norm() + x.dot(Variable(Tensor([-10, 10])))
>>> q.backward()
>>> x.grad
Variable containing:
 -9.4000
 10.8000
[torch.FloatTensor of size 2]
```

⚠ Although they are related, **the autograd graph is not the network's structure**, but the graph of operations to compute the gradient. It can be data-dependent and miss or replicate sub-parts of the network.

Finally, since the gradient itself is a `Variable`, autograd can generate the computational graph for computing **higher-order derivatives**.

This is done by passing `create_graph=True` to `torch.autograd.grad(...)`

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```
>>> x = Variable(Tensor([ 1, 2, 3 ]), requires_grad = True)
>>> s1 = x.pow(2).sum()
>>> g1, = torch.autograd.grad(s1, x, create_graph = True)
>>> g1
Variable containing:
 2
 4
 6
[torch.FloatTensor of size 3]
```

Finally, since the gradient itself is a `Variable`, autograd can generate the computational graph for computing **higher-order derivatives**.

This is done by passing `create_graph=True` to `torch.autograd.grad(...)`

```
>>> x = Variable(Tensor([ 1, 2, 3 ]), requires_grad = True)
>>> s1 = x.pow(2).sum()
>>> g1, = torch.autograd.grad(s1, x, create_graph = True)
>>> g1
Variable containing:
 2
 4
 6
[torch.FloatTensor of size 3]
```

```
>>> s2 = g1[0].exp() - g1[2].exp()
>>> g2, = torch.autograd.grad(s2, x)
>>> g2
Variable containing:
  14.7781
   0.0000
-806.8576
[torch.FloatTensor of size 3]
```

Weight sharing

In our generalized DAG formulation, we have in particular implicitly allowed the same parameters to modulate different parts of the processing.

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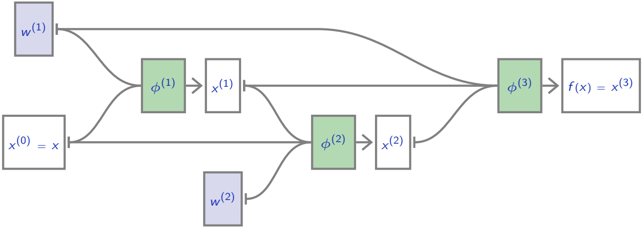
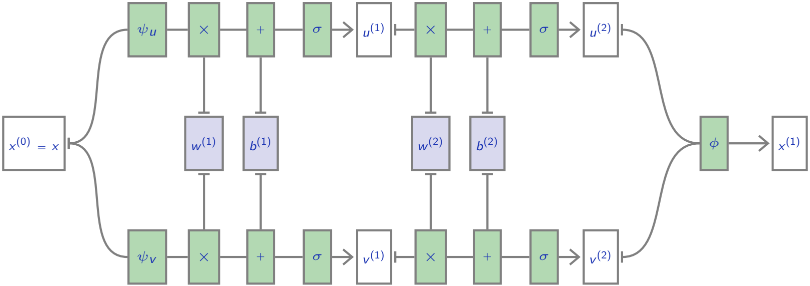
For instance $w^{(1)}$ in our example parametrizes both $\phi^{(1)}$ and $\phi^{(3)}$.



This is called **weight sharing**.

Weight sharing allows in particular to build **siamese networks** where a full sub-network is replicated several times.



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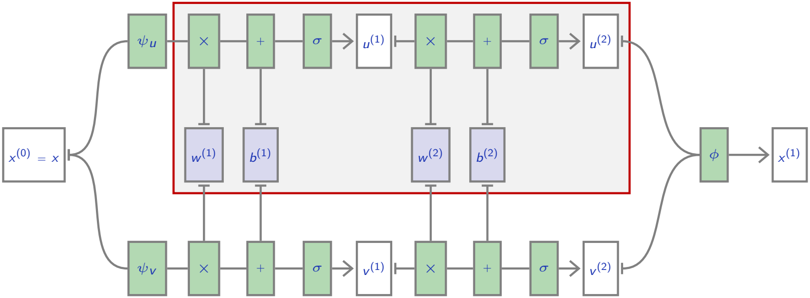

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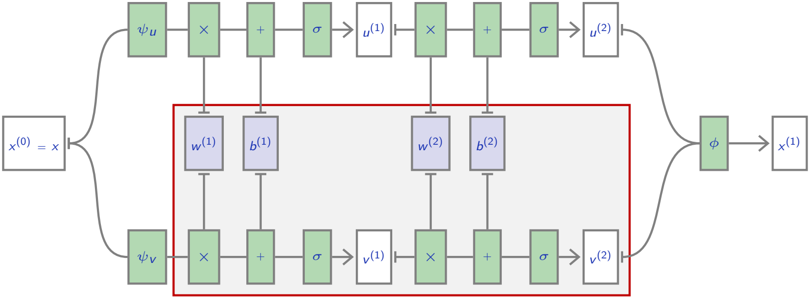

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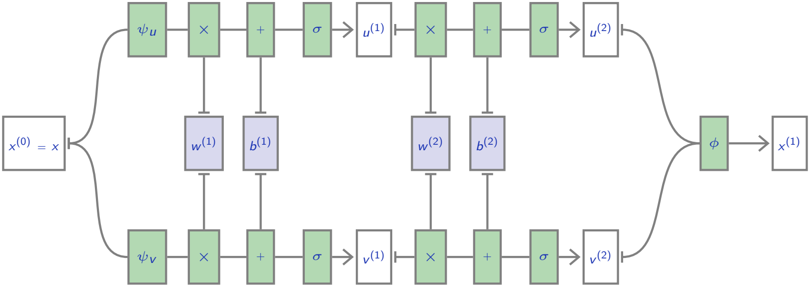

Convolutional layers

If they were handled as normal "unstructured" vectors, large-dimension signals such as sound samples or images would require models of intractable size.

For instance a linear layer taking a 256×256 RGB image as input, and producing an image of same size would require

$$(256 \times 256 \times 3)^2 \simeq 3.87e{+}10$$

parameters, with the corresponding memory footprint ($\simeq$150Gb !), and excess of capacity.

Moreover, this requirement is inconsistent with the intuition that such large signals have some “invariance in translation”. **A representation meaningful at a certain location can / should be used everywhere.**

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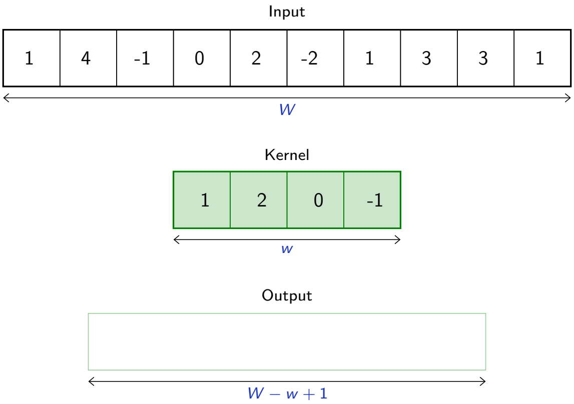
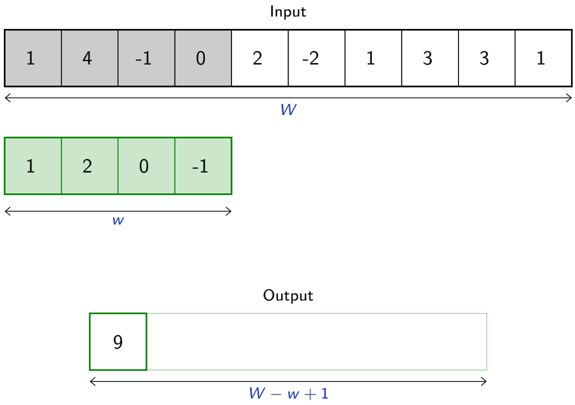
A convolutional layer embodies this idea. It applies the same linear transformation locally, everywhere, and preserves the signal structure.

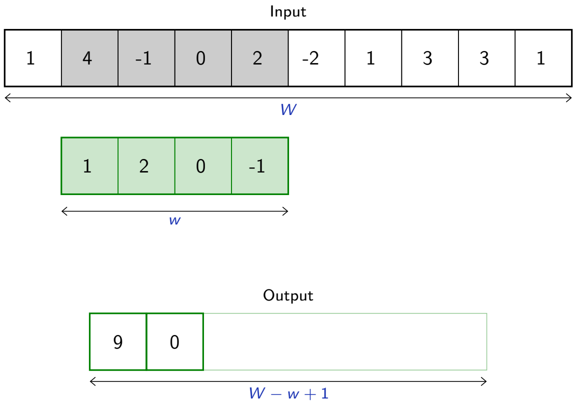
Input

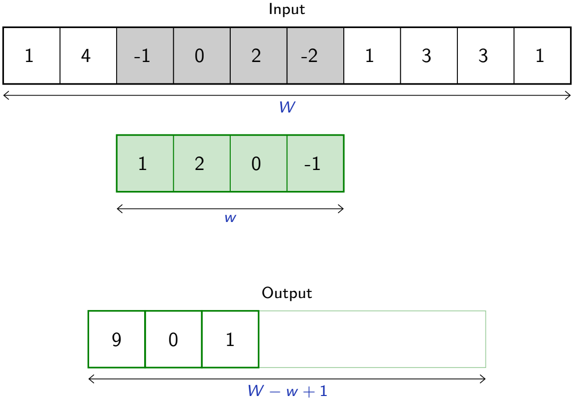
1	4	-1	0	2	-2	1	3	3	1

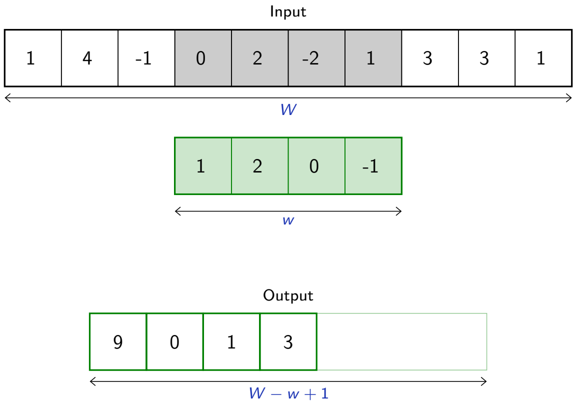
W


Input
1 4 -1 0 2 -2 1 3 3 1
W
Kernel
1 2 0 -1
w
Output
W − w + 1

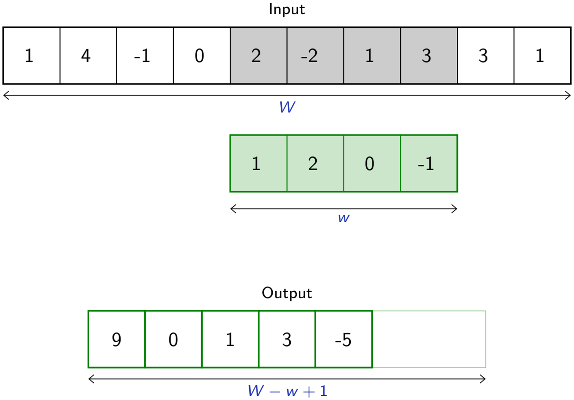

Input
1
4
-1
0
2
-2
1
3
3
1
W
1
2
0
-1
w
Output
9
$W - w + 1$

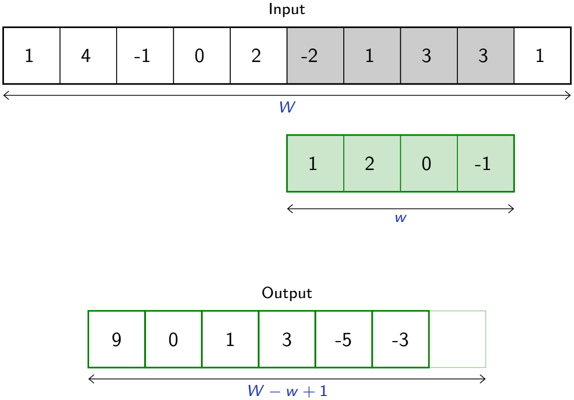

Input
1
4
-1
0
2
-2
1
3
3
1
W
1
2
0
-1
w
Output
9
0
W − w + 1

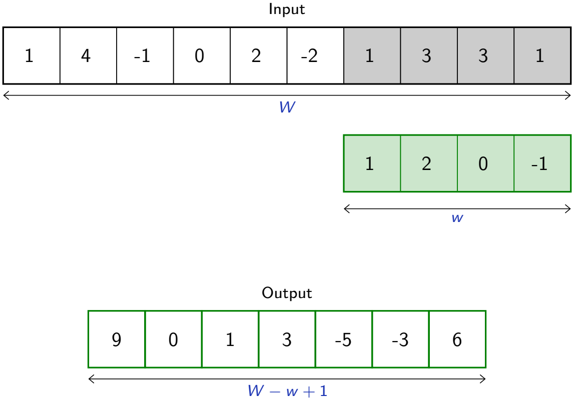

Input
1
4
-1
0
2
-2
1
3
3
1
W
1
2
0
-1
w
Output
9
0
1
W − w + 1

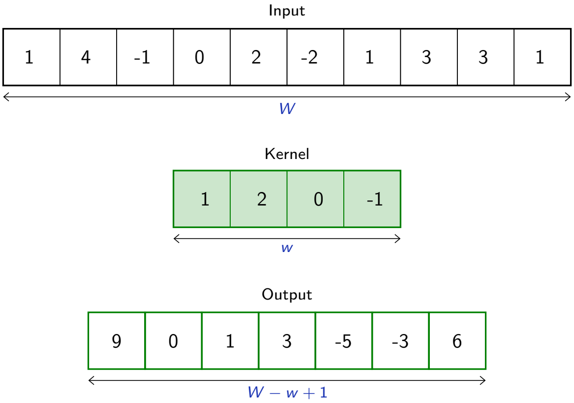


Input
1
4
-1
0
2
-2
1
3
3
1
W
1
2
0
-1
w
Output
9
0
1
3
$W - w + 1$


Input
1
4
-1
0
2
-2
1
3
3
1
W
1
2
0
-1
w
Output
9
0
1
3
-5
W − w + 1


Input
1 4 -1 0 2 -2 1 3 3 1
W
1 2 0 -1
w
Output
9 0 1 3 -5 -3
W − w + 1


Input
1 4 -1 0 2 -2 1 3 3 1
W
1 2 0 -1
w
Output
9 0 1 3 -5 -3 6
$W - w + 1$


Input
1 4 -1 0 2 -2 1 3 3 1
W
Kernel
1 2 0 -1
w
Output
9 0 1 3 -5 -3 6
$W - w + 1$

Formally, in 1d, given

$$x = (x_1, \dots, x_W)$$

and a "convolutional kernel" (or "filter") of width w

$$u = (u_1, \dots, u_w)$$

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the convolution $x \circledast u$ is a vector of size $W - w + 1$, with

$$\begin{aligned}(x \circledast u)_i &= \sum_{j=1}^{w} x_{i-1+j}\, u_j \\ &= (x_i, \dots, x_{i+w-1}) \cdot u\end{aligned}$$

for instance

$$(1, 2, 3, 4) \circledast (3, 2) = (3 + 4, 6 + 6, 9 + 8) = (7, 12, 17).$$

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for instance

$$(1, 2, 3, 4) \circledast (3, 2) = (3 + 4, 6 + 6, 9 + 8) = (7, 12, 17).$$

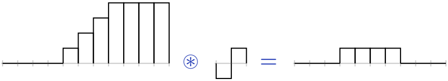
This differs from the usual convolution since the kernel and the signal are both visited in increasing index order.

Convolution can implement a differential operator

$$(0,0,0,0,1,2,3,4,4,4,4) \circledast (-1,1) = (0,0,0,1,1,1,1,0,0,0).$$

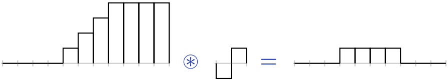
Convolution can implement a differential operator

$$(0, 0, 0, 0, 1, 2, 3, 4, 4, 4, 4) \circledast (-1, 1) = (0, 0, 0, 1, 1, 1, 1, 0, 0, 0).$$

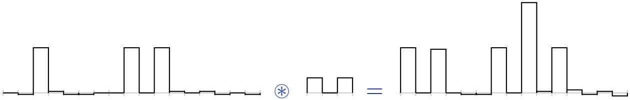


Convolution can implement a differential operator

$$(0, 0, 0, 0, 1, 2, 3, 4, 4, 4, 4) \circledast (-1, 1) = (0, 0, 0, 1, 1, 1, 1, 0, 0, 0).$$

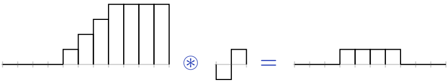


or a crude "template matcher"

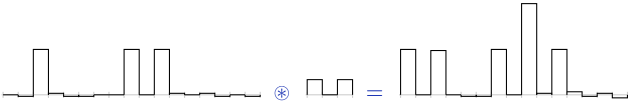


Convolution can implement a differential operator

$$(0,0,0,0,1,2,3,4,4,4,4) \circledast (-1,1) = (0,0,0,1,1,1,1,0,0,0).$$



or a crude "template matcher"



Both of these computation examples are indeed "invariant by translation".

It generalizes naturally to a multi-dimensional input, although specification can become complicated.

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Its most usual form for "convolutional networks" processes a 3d tensor as input (*i.e.* a multi-channel 2d signal) to output a 2d tensor. The kernel is not swiped across channels, just across rows and columns.

In this case, if the input tensor is of size $C \times H \times W$, and the kernel is $C \times h \times w$, the output is $(H - h + 1) \times (W - w + 1)$.

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⚠ We say "2d signal" even though it has C channels, since it is a feature vector indexed by a 2d location without structure on the feature indexes.

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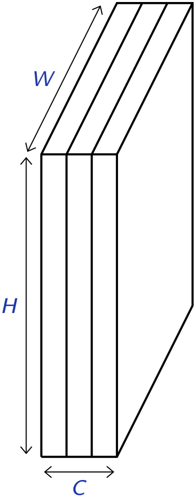
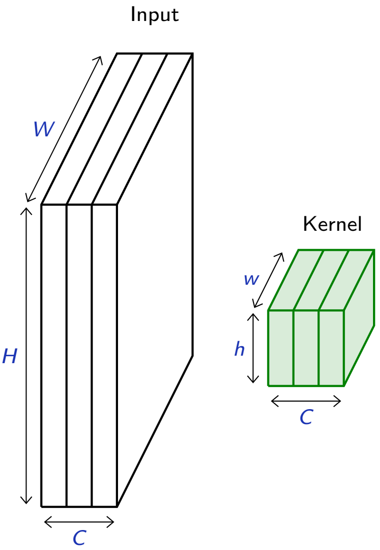
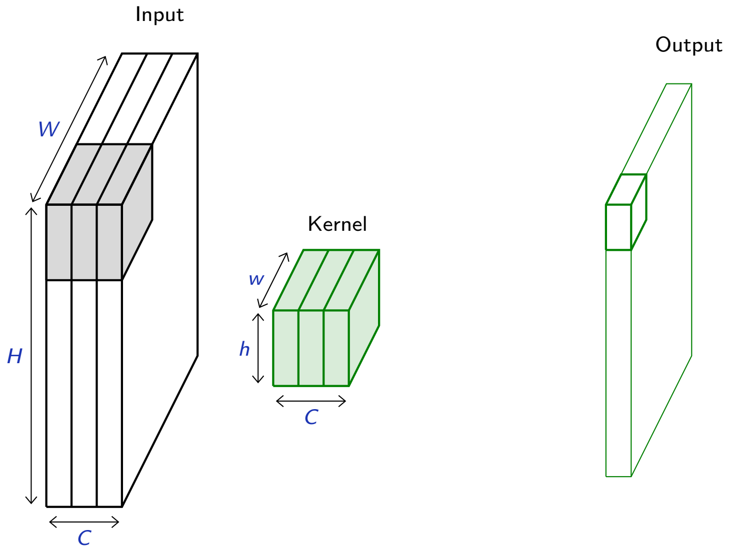
⚠ We say "2d signal" even though it has C channels, since it is a feature vector indexed by a 2d location without structure on the feature indexes.

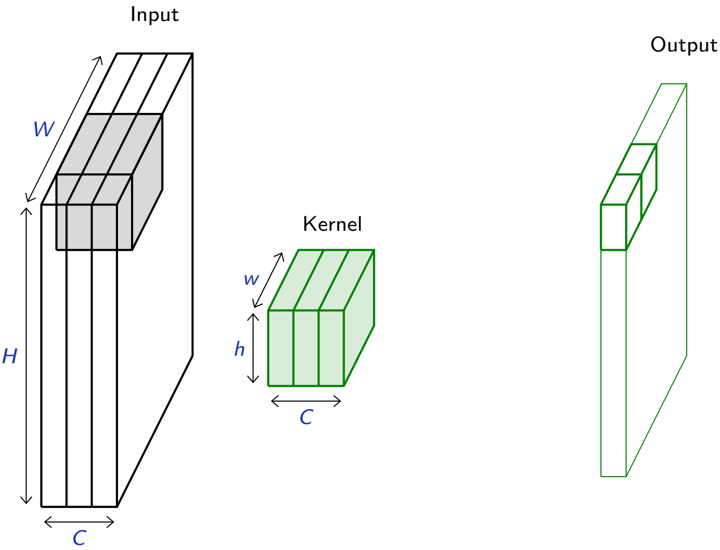
In a standard convolutional layer, D such convolutions are combined to generate a $D \times (H - h + 1) \times (W - w + 1)$ output.

Input

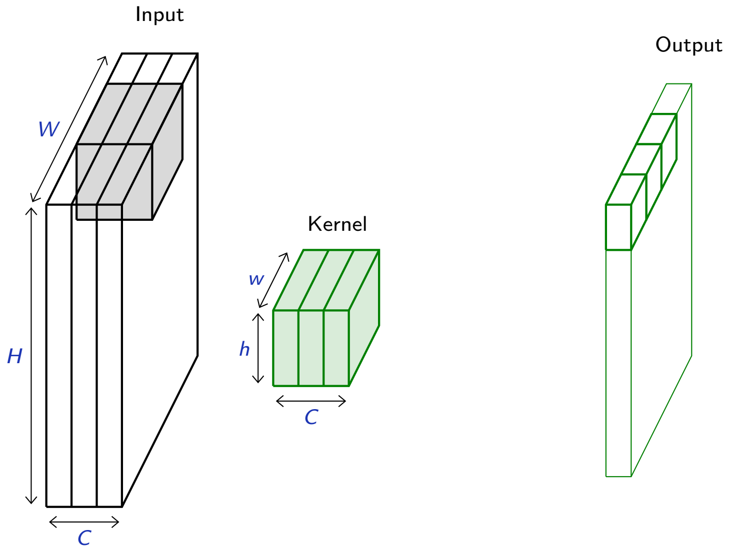


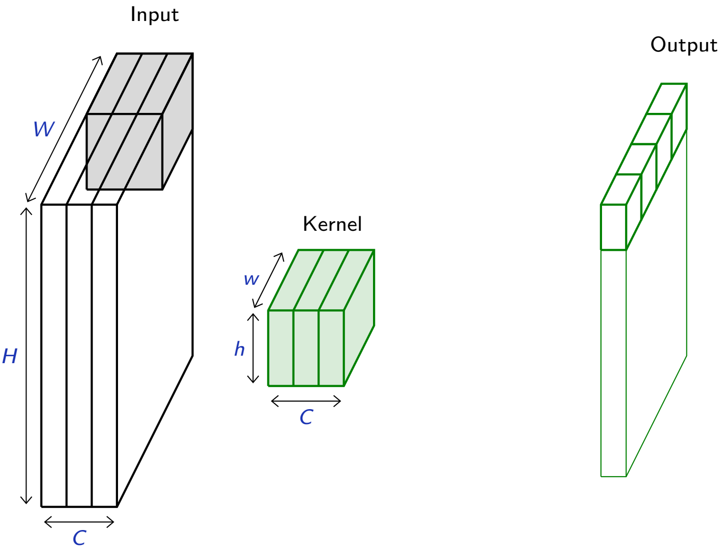

Input
W
H
C
Kernel
w
h
C

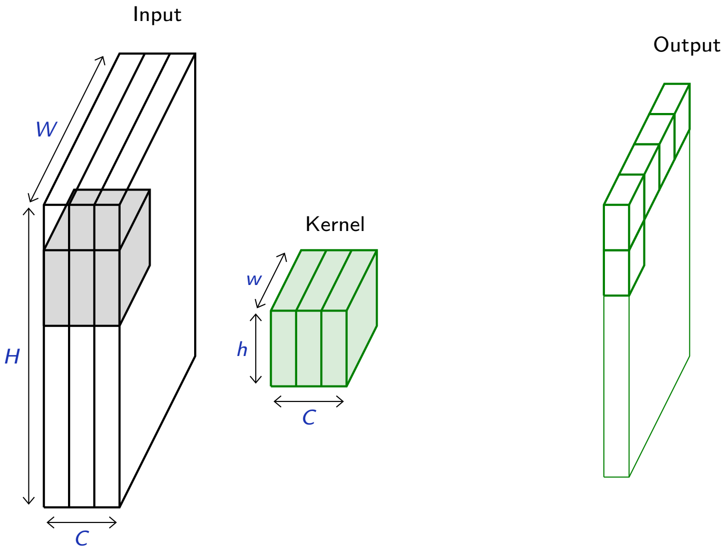

Input
W
H
C
Kernel
w
h
C
Output

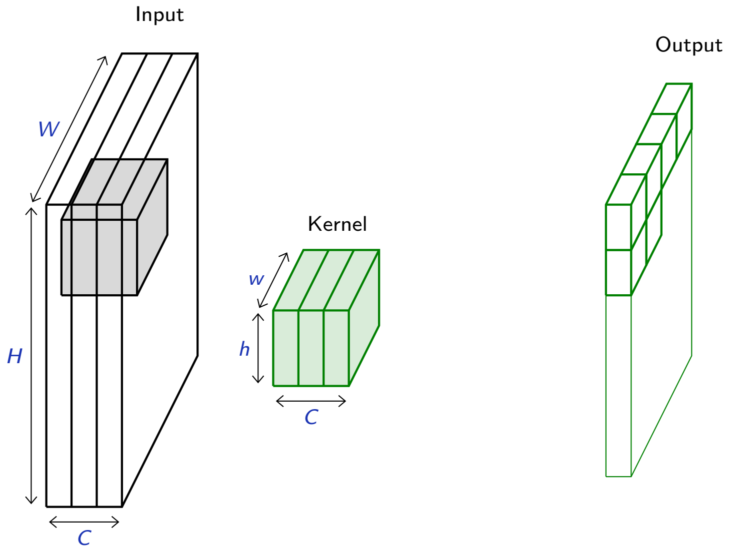


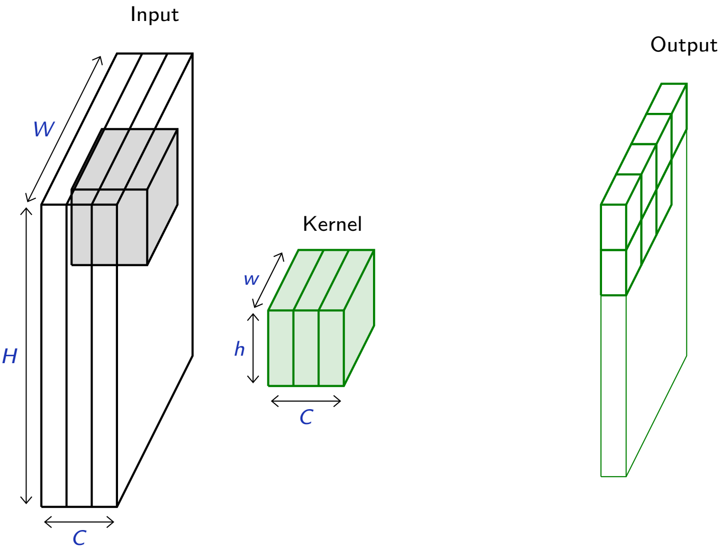
Input
Output
W
Kernel
w
H
h
C
C

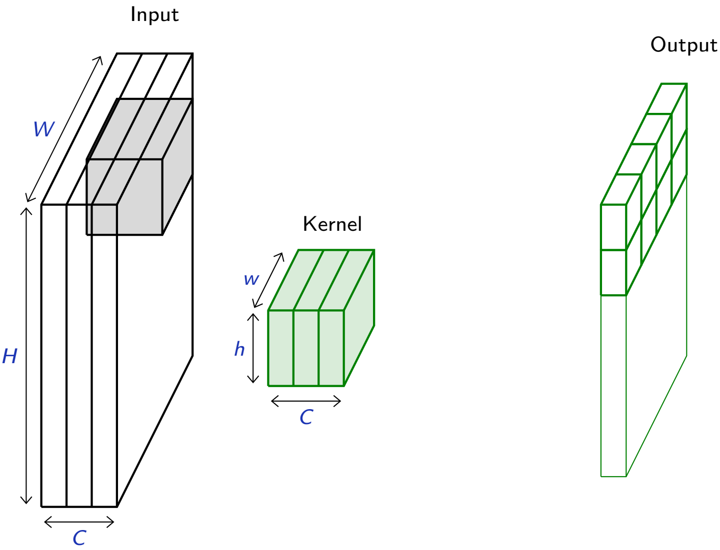

Input
W
H
C
Kernel
w
h
C
Output


Input
W
H
C
Kernel
w
h
C
Output

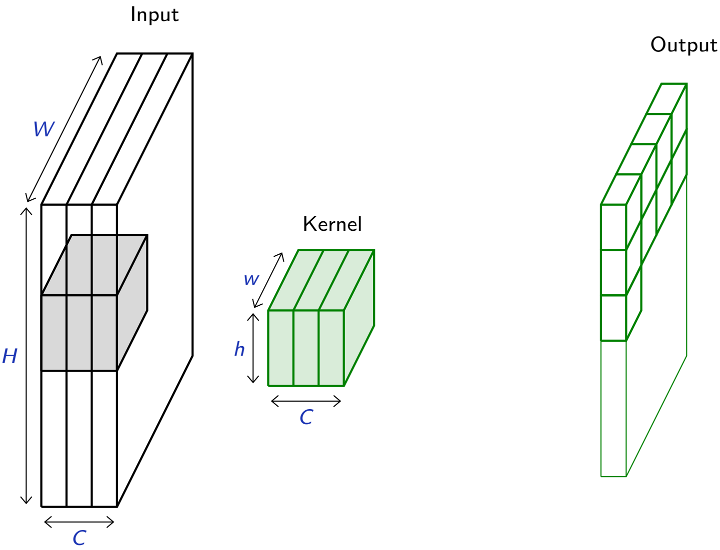

Input
W
H
C
Kernel
w
h
C
Output

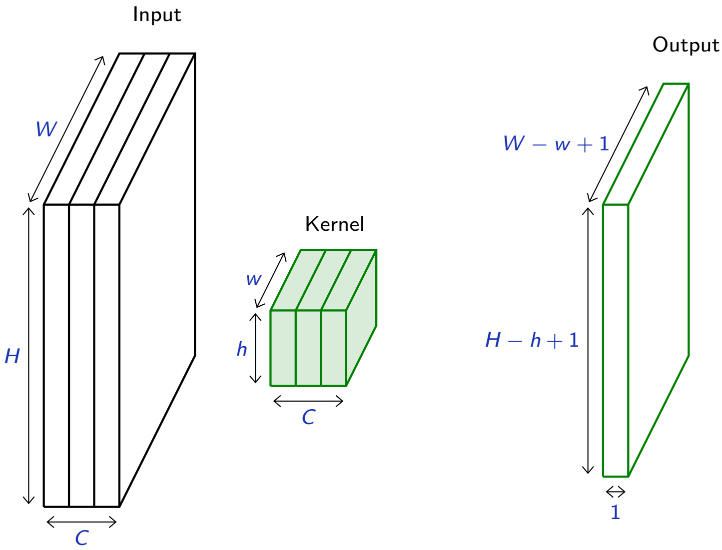

Input
W
H
C
Kernel
w
h
C
Output


Input
W
H
C
Kernel
w
h
C
Output

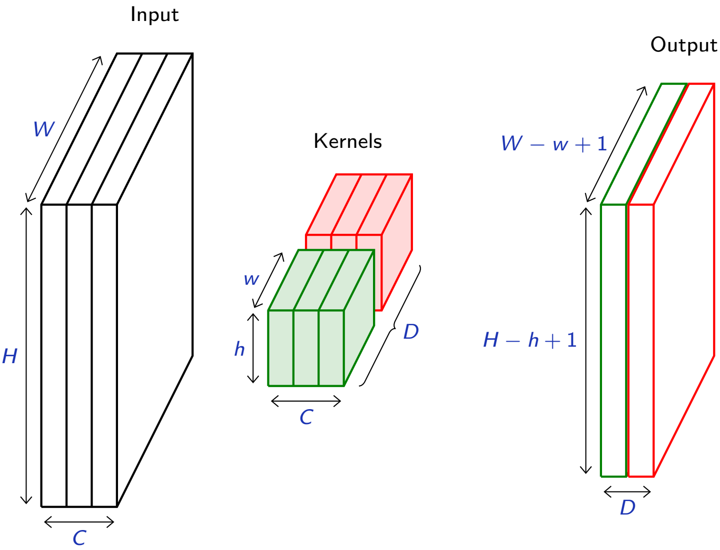


Input
W
H
C
Kernel
w
h
C
Output


Input
W
H
C
Kernel
w
h
C
Output



Input
W
H
C
Kernel
w
h
C
Output
W − w + 1
H − h + 1
1


Input
W
H
C
Kernels
w
h
C
D
Output
W − w + 1
H − h + 1
D

Note that a convolution **preserves the signal support structure**.

A 1d signal is converted into a 1d signal, a 2d signal into a 2d, and neighboring parts of the input signal influence neighboring parts of the output signal.

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A 1d signal is converted into a 1d signal, a 2d signal into a 2d, and neighboring parts of the input signal influence neighboring parts of the output signal.

A 3d convolution can be used if the channel index has some metric meaning, such as time for a series of grayscale video frames. Otherwise swiping across channels makes no sense.

We usually refer to one of the channels generated by a convolutional layer as an **activation map.**

The sub-area of an input map that influences a component of the output as the **receptive field** of the latter.

We usually refer to one of the channels generated by a convolutional layer as an **activation map.**

The sub-area of an input map that influences a component of the output as the **receptive field** of the latter.

In the context of convolutional networks, a standard linear layer is called a **fully connected layer** since every input influences every output.

Pooling

In many cases, a feed-forward network computes a low-dimension signal (*e.g.* a few scores) from a very high-dimension signal (*e.g.* an image).

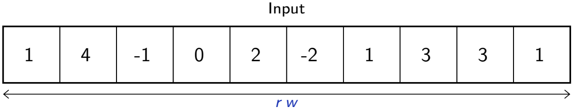
In many cases, a feed-forward network computes a low-dimension signal (*e.g.* a few scores) from a very high-dimension signal (*e.g.* an image).

As for convolution, it makes sense to reduce the signal's size in a way that preserves its structure, just "down-scaling it".

This operation is called **pooling**, and aims at grouping several activations into a single "more meaningful" one.

The most standard type of pooling is the **max-pooling**, which computes max values over non-overlapping blocks.

For instance in 1d with a kernel of size 2:



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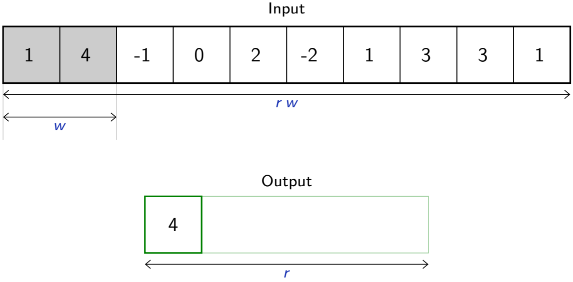

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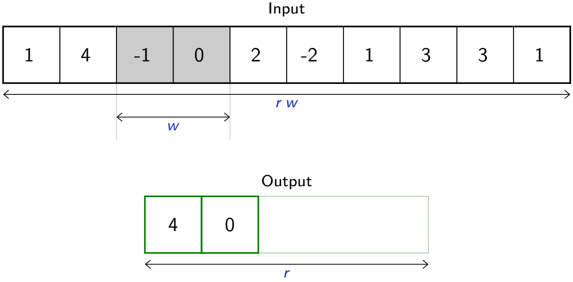

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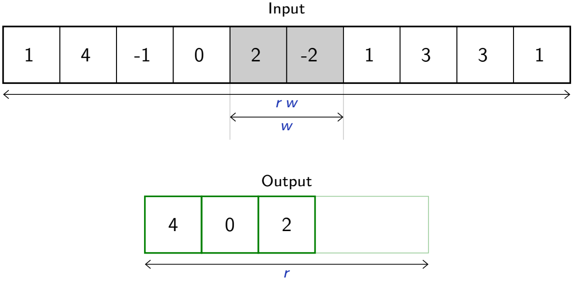

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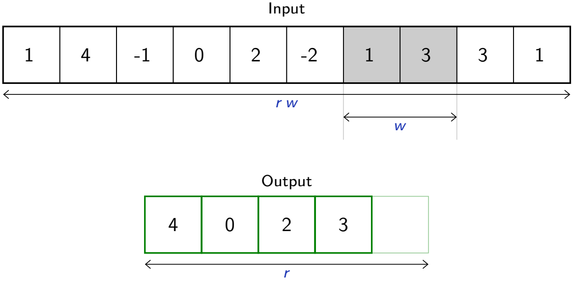

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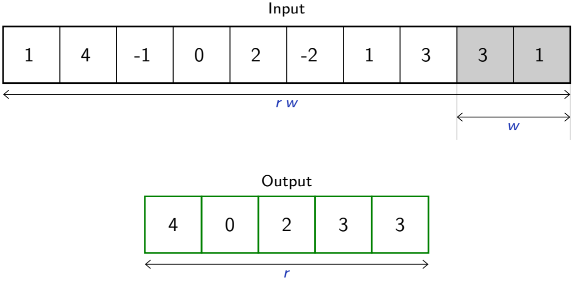

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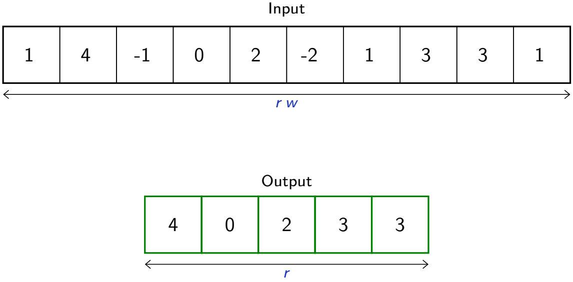

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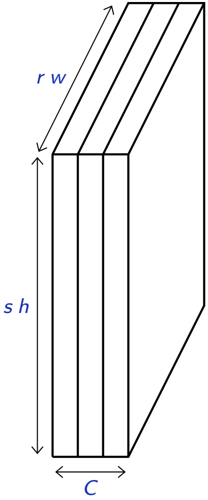
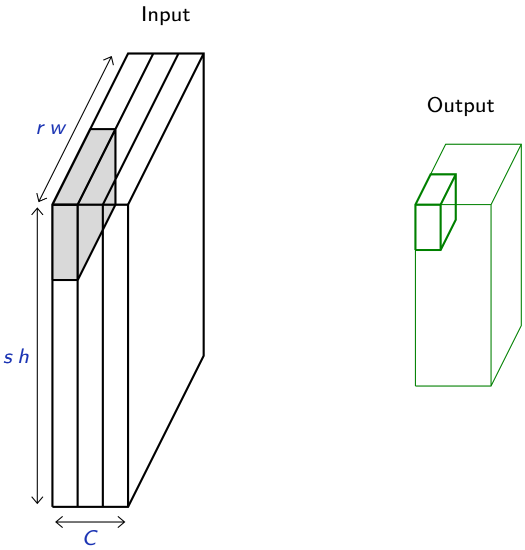
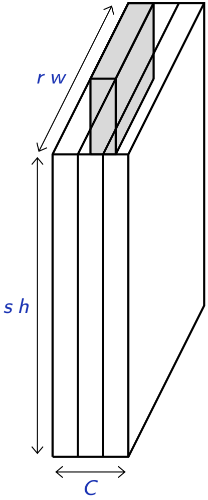
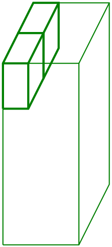


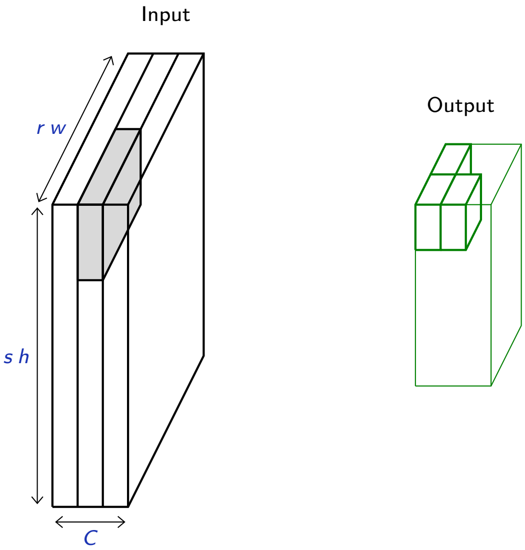

Input
r w
s h
C
Output

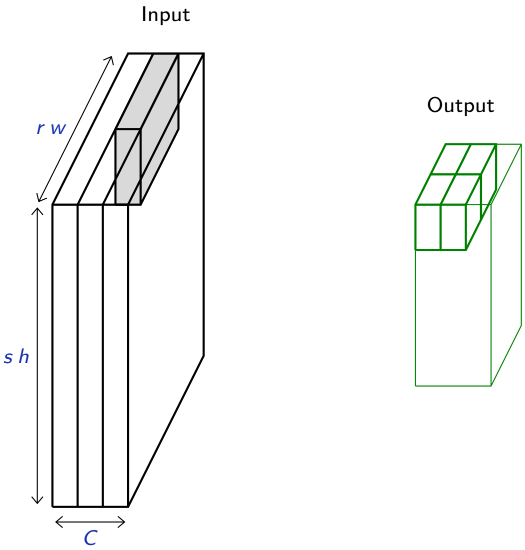
Input



Output




Input
Output
$r\ w$
$s\ h$
C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r w
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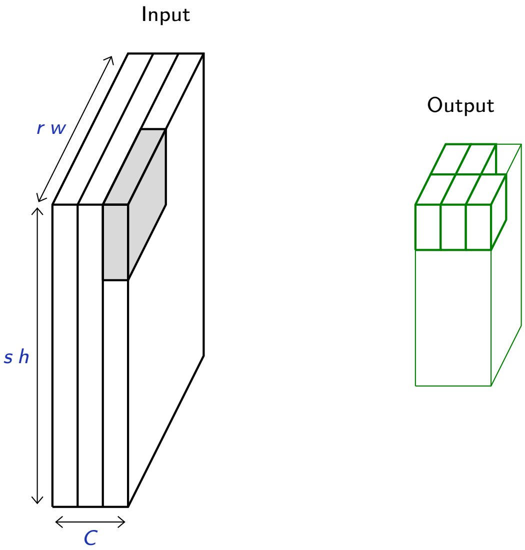
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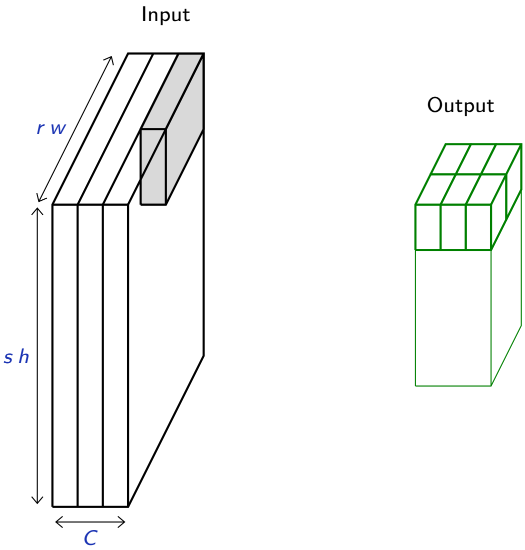
Input
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r w
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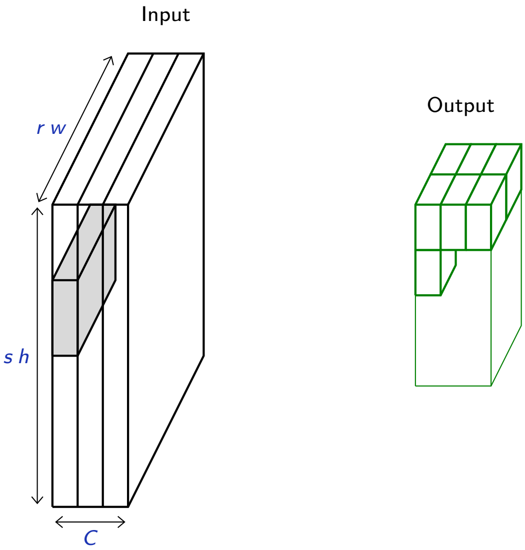
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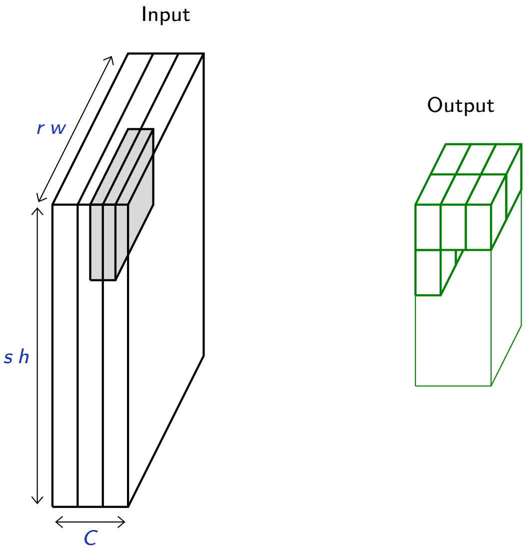
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r w
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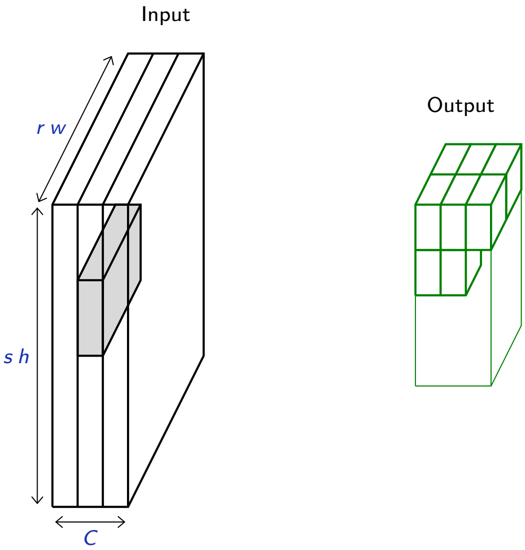
Input
r w
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C
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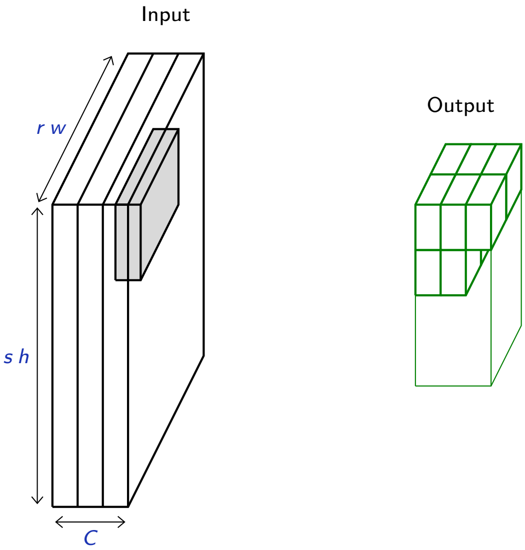
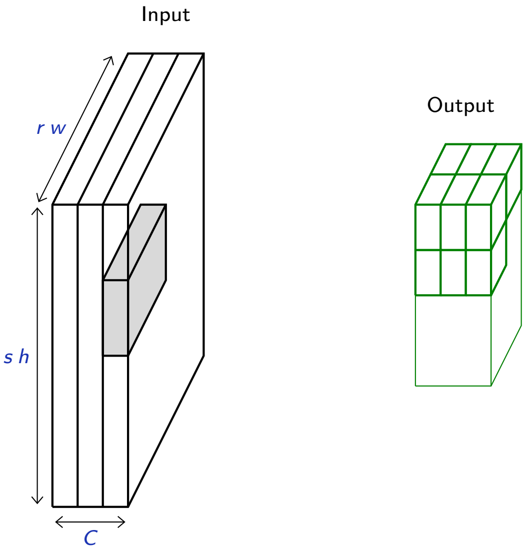


Input
r w
s h
C
Output


Input
Output
r w
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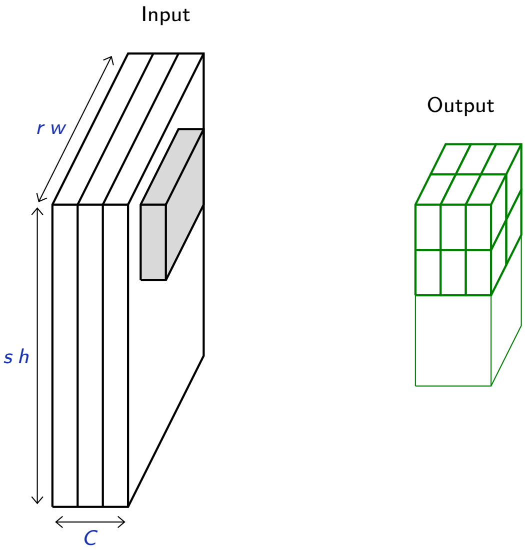
C


Input
r w
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C
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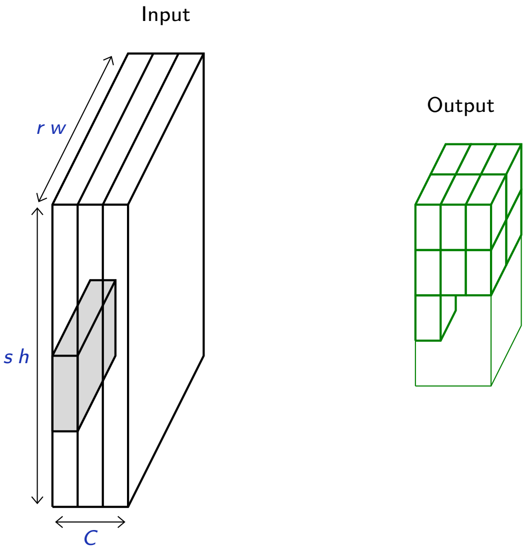
Input
r w
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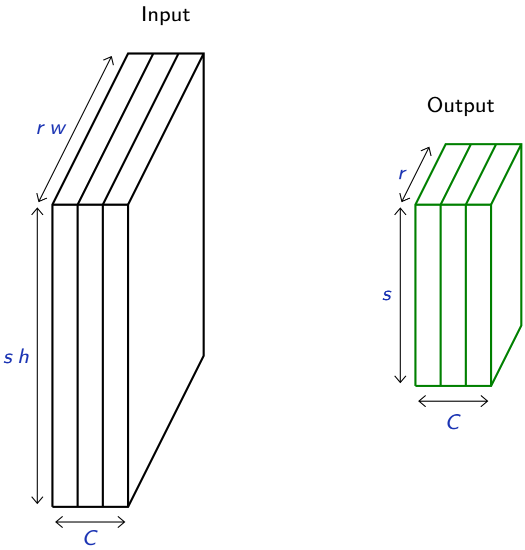
Output


Input
r w
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r
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Pooling provides invariance to any permutation inside one of the cell.

More practically, it provides a pseudo-invariance to deformations that result into local translations.

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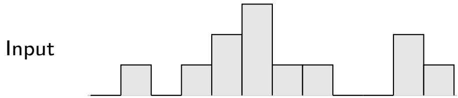

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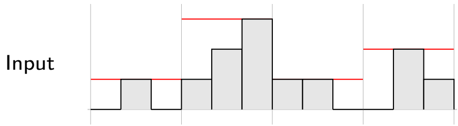

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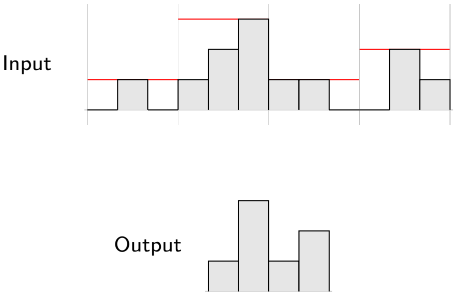

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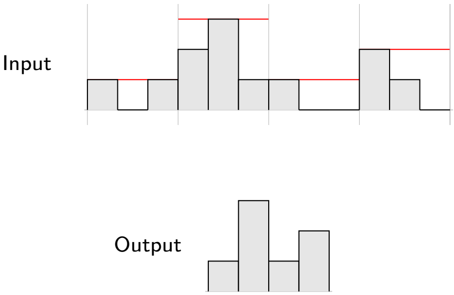

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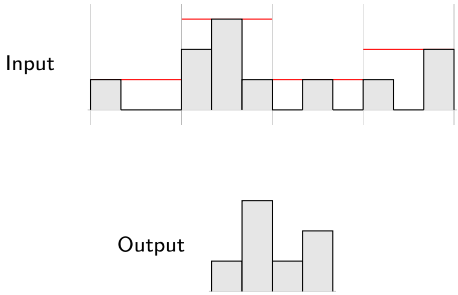

The end