

MXNet (<https://mxnet.incubator.apache.org>) > Autograd

# Autograd Package

## Overview

The `autograd` package enables automatic differentiation of `NDArray` operations. In machine learning applications, `autograd` is often used to calculate the gradients of loss functions with respect to parameters.

## Record vs Pause

`autograd` records computation history on the fly to calculate gradients later. This is only enabled inside a `with autograd.record():` block. A `with autograd.pause():` block can be used inside a `record()` block to temporarily disable recording.

To compute gradient with respect to an `NDArray` `x`, first call `x.attach_grad()` to allocate space for the gradient. Then, start a `with autograd.record()` block, and do some computation. Finally, call `backward()` on the result:

```
>>> x = mx.nd.array([1,2,3,4])
>>> x.attach_grad()
>>> with mx.autograd.record():
...     y = x * x + 1
>>> y.backward()
>>> print(x.grad)
[ 2.  4.  6.  8.]
```

## Train mode and Predict Mode

Some operators (Dropout, BatchNorm, etc) behave differently in training and making predictions. This can be controlled with `train_mode` and `predict_mode` scope.

By default, MXNet is in `predict_mode`. A `with autograd.record()` block by default turns on `train_mode` (equivalent to `with autograd.record(train_mode=True)`). To compute a gradient in prediction mode (as when generating adversarial examples), call `record` with `train_mode=False` and then call `backward(train_mode=False)`

Although training usually coincides with recording, this isn't always the case. To control *training vs predict\_mode* without changing *recording vs not recording*, use a `with autograd.train_mode():` or `with autograd.predict_mode():` block.

Detailed tutorials are available in Part 1 of the MXNet gluon book (<http://gluon.mxnet.io/>).

## Autograd

<code>record</code>	Returns an autograd recording scope context to be used in 'with' statement and captures code that needs gradients to be calculated.
<code>pause</code>	Returns a scope context to be used in 'with' statement for codes that do not need gradients to be calculated.
<code>train_mode</code>	Returns a scope context to be used in 'with' statement in which forward pass behavior is set to training mode, without changing the recording states.
<code>predict_mode</code>	Returns a scope context to be used in 'with' statement in which forward pass behavior is set to inference mode, without changing the recording states.
<code>backward</code>	Compute the gradients of heads w.r.t previously marked variables.
<code>set_training</code>	Set status to training/predicting.
<code>is_training</code>	Get status on training/predicting.
<code>set_recording</code>	Set status to recording/not recording.
<code>is_recording</code>	Get status on recording/not recording.
<code>mark_variables</code>	Mark NDArrays as variables to compute gradient for autograd.
<code>Function</code>	Customize differentiation in autograd.

## API Reference

Autograd for NDArray.

`mxnet.autograd.set_recording(is_recording)`

[source]

([../\\_modules/mxnet/autograd.html#set\\_recording](http://mxnet.incubator.apache.org/api/python/autograd/autograd.html#set_recording))

Set status to recording/not recording. When recording, graph will be constructed for gradient computation.

**Parameters:** `is_recording` (*bool*) –

**Returns:**

**Return type:** previous state before this set.

`mxnet.autograd. set_training (train_mode)`

[\[source\]](#)

[\(../../\\_modules/mxnet/autograd.html#set\\_training\)](#)

---

Set status to training/predicting. This affects `ctx.is_train` in operator running context. For example, Dropout will drop inputs randomly when `train_mode=True` while simply passing through if `train_mode=False`.

**Parameters:** `train_mode` (*bool*) –

**Returns:**

**Return type:** previous state before this set.

`mxnet.autograd. is_recording ()`

[\[source\]](#)

[\(../../\\_modules/mxnet/autograd.html#is\\_recording\)](#)

---

Get status on recording/not recording.

**Returns:**

**Return type:** Current state of recording.

`mxnet.autograd. is_training ()`

[\[source\]](#)

[\(../../\\_modules/mxnet/autograd.html#is\\_training\)](#)

---

Get status on training/predicting.

**Returns:**

**Return type:** Current state of training/predicting.

`mxnet.autograd. record (train_mode=True)`

[\[source\]](#)

[\(../../\\_modules/mxnet/autograd.html#record\)](#)

---

Returns an autograd recording scope context to be used in 'with' statement and captures code that needs gradients to be calculated.

**Note**

When forwarding with `train_mode=False`, the corresponding backward should also use `train_mode=False`, otherwise gradient is undefined.

Example:

```
with autograd.record():
    y = model(x)
    backward([y])
metric.update(...)
optim.step(...)
```

**Parameters:** **train\_mode** (*bool, default True*) – Whether the forward pass is in training or predicting mode. This controls the behavior of some layers such as Dropout, BatchNorm.

mxnet.autograd. **pause** (train\_mode=False)

[source]

([../\\_modules/mxnet/autograd.html#pause](https://mxnet.incubator.apache.org/api/python/autograd/autograd.html#pause))

---

Returns a scope context to be used in ‘with’ statement for codes that do not need gradients to be calculated.

Example:

```
with autograd.record():
    y = model(x)
    backward([y])
    with autograd.pause():
        # testing, IO, gradient updates...
```

**Parameters:** **train\_mode** (*bool, default False*) – Whether to do forward for training or predicting.

mxnet.autograd. **train\_mode** ()

[source]

([../\\_modules/mxnet/autograd.html#train\\_mode](https://mxnet.incubator.apache.org/api/python/autograd/autograd.html#train_mode))

---

Returns a scope context to be used in ‘with’ statement in which forward pass behavior is set to training mode, without changing the recording states.

Example:

```
y = model(x)
with autograd.train_mode():
    y = dropout(y)
```

mxnet.autograd. **predict\_mode** ()

[source]

([../\\_modules/mxnet/autograd.html#predict\\_mode](https://mxnet.incubator.apache.org/api/python/autograd/autograd.html#predict_mode))

---

Returns a scope context to be used in ‘with’ statement in which forward pass behavior is set to inference mode, without changing the recording states.

Example:

```
with autograd.record():
    y = model(x)
    with autograd.predict_mode():
        y = sampling(y)
    backward([y])
```

**mxnet.autograd. mark\_variables** (variables, gradients, grad\_reqs='write') [\[source\]](#)  
[\(../..../\\_modules/mxnet/autograd.html#mark\\_variables\)](#)

Mark NDArrays as variables to compute gradient for autograd.

- Parameters:**
- **variables** (*NDArray* ([../ndarray/ndarray.html#mxnet.ndarray.NDArray](#)) or list of *NDArray*) –
  - **gradients** (*NDArray* ([../ndarray/ndarray.html#mxnet.ndarray.NDArray](#)) or list of *NDArray*) –
  - **grad\_reqs** (*str* or list of *str*) –

**mxnet.autograd. backward** (heads, head\_grads=None, retain\_graph=False, train\_mode=True) [\[source\]](#)  
[\(../..../\\_modules/mxnet/autograd.html#backward\)](#)

Compute the gradients of heads w.r.t previously marked variables.

- Parameters:**
- **heads** (*NDArray* ([../ndarray/ndarray.html#mxnet.ndarray.NDArray](#)) or list of *NDArray*) – Output *NDArray(s)*
  - **head\_grads** (*NDArray* ([../ndarray/ndarray.html#mxnet.ndarray.NDArray](#)) or list of *NDArray* or *None*) – Gradients with respect to heads.
  - **train\_mode** (*bool*, optional) – Whether to do backward for training or predicting.

**mxnet.autograd. grad** (heads, variables, head\_grads=None, retain\_graph=None, create\_graph=False, train\_mode=True) [\[source\]](#)  
[\(../..../\\_modules/mxnet/autograd.html#grad\)](#)

Compute the gradients of heads w.r.t variables. Gradients will be returned as new NDArrays instead of stored into *variable.grad*. Supports recording gradient graph for computing higher order gradients.

#### Note

Currently only a very limited set of operators support higher order gradients.

- Parameters:**
- **heads** (*NDArray* ([../ndarray/ndarray.html#mxnet.ndarray.NDArray](http://ndarray.ndarray.html#mxnet.ndarray.NDArray)) or list of *NDArray*) – Output *NDArray*(s)
  - **variables** (*NDArray* ([../ndarray/ndarray.html#mxnet.ndarray.NDArray](http://ndarray.ndarray.html#mxnet.ndarray.NDArray)) or list of *NDArray*) – Input variables to compute gradients for.
  - **head\_grads** (*NDArray* ([../ndarray/ndarray.html#mxnet.ndarray.NDArray](http://ndarray.ndarray.html#mxnet.ndarray.NDArray)) or list of *NDArray* or *None*) – Gradients with respect to heads.
  - **retain\_graph** (*bool*) – Whether to keep computation graph to differentiate again, instead of clearing history and release memory. Defaults to the same value as `create_graph`.
  - **create\_graph** (*bool*) – Whether to record gradient graph for computing higher order
  - **train\_mode** (*bool, optional*) – Whether to do backward for training or prediction.

**Returns:** Gradients with respect to variables.

**Return type:** *NDArray* ([../ndarray/ndarray.html#mxnet.ndarray.NDArray](http://ndarray.ndarray.html#mxnet.ndarray.NDArray)) or list of *NDArray*

## Examples

```
>>> x = mx.nd.ones((1,))
>>> x.attach_grad()
>>> with mx.autograd.record():
...     z = mx.nd.elemwise_add(mx.nd.exp(x), x)
>>> dx = mx.autograd.grad(z, [x], create_graph=True)
>>> print(dx)
[
[ 3.71828175]
]
```

`mxnet.autograd.get_symbol(x)`

[\[source\]](#)

[../ndarray/ndarray.html#mxnet.ndarray.NDArray](http://ndarray.ndarray.html#mxnet.ndarray.NDArray) or list of *NDArray*

Retrieve recorded computation history as *Symbol*.

**Parameters:** *x* (*NDArray* ([../ndarray/ndarray.html#mxnet.ndarray.NDArray](http://ndarray.ndarray.html#mxnet.ndarray.NDArray))) – Array representing the head of computation graph.

**Returns:** The retrieved *Symbol*.

**Return type:** *Symbol* ([../symbol/symbol.html#mxnet.symbol.Symbol](http://symbol.symbol.html#mxnet.symbol.Symbol))

class `mxnet.autograd.Function`

[\[source\]](#)

[\(../..../\\_modules/mxnet/autograd.html#Function\)](#)

---

Customize differentiation in autograd.

If you don't want to use the gradients computed by the default chain-rule, you can use `Function` to customize differentiation for computation. You define your computation in the forward method and provide the customized differentiation in the backward method. During gradient computation, autograd will use the user-defined backward function instead of the default chain-rule. You can also cast to numpy array and back for some operations in forward and backward.

For example, a stable sigmoid function can be defined as:

```
class sigmoid(mx.autograd.Function):
    def forward(self, x):
        y = 1 / (1 + mx.nd.exp(-x))
        self.save_for_backward(y)
        return y

    def backward(self, dy):
        # backward takes as many inputs as forward's return value,
        # and returns as many NDArrays as forward's arguments.
        y, = self.saved_tensors
        return dy * y * (1-y)
```

Then, the function can be used in the following way:

```
func = sigmoid()
x = mx.nd.random.uniform(shape=(10,))
x.attach_grad()

with mx.autograd.record():
    m = func(x)
    m.backward()
dx = x.grad.asnumpy()
```

**forward** (\*inputs)

[\[source\]](#)

[\(../..../\\_modules/mxnet/autograd.html#Function.forward\)](#)

---

Forward computation.

**backward** (\*output\_grads)

[\[source\]](#)

[\(../..../\\_modules/mxnet/autograd.html#Function.backward\)](#)

---

Backward computation.

Takes as many inputs as forward's outputs, and returns as many NDArrays as forward's inputs.

