

# Hypertuning

Search spaces & hypertune algorithms

deep learning 4

Raoul Grouls, 9 December 2025

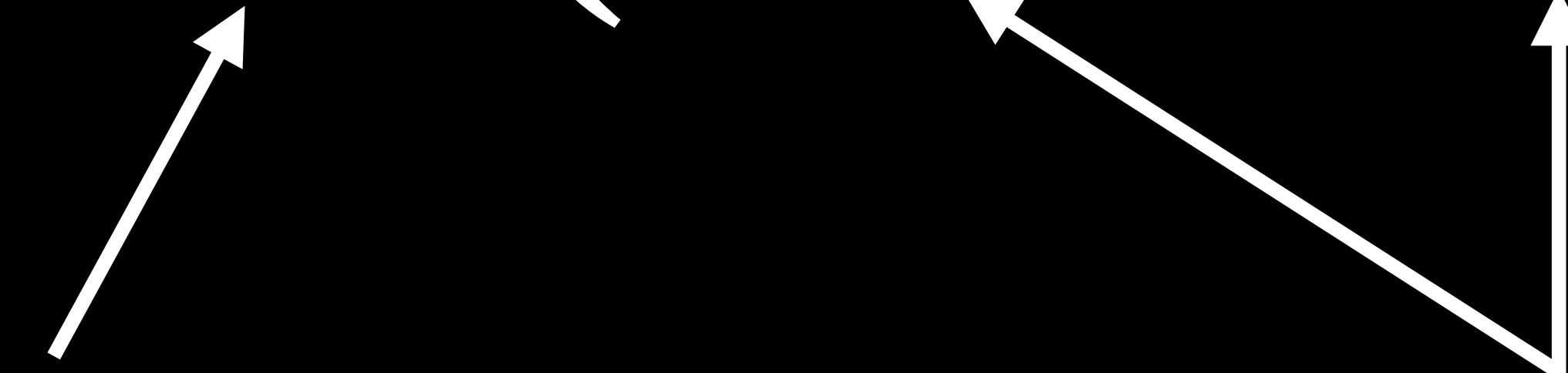
# Recap

# Neural networks

$$\sigma(wx + b)$$

# Neural networks

$$\sigma(wx + b)$$

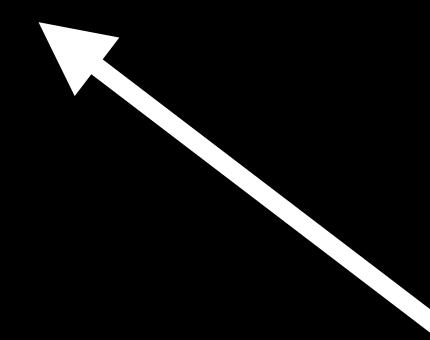


Non-linear transformation

Linear transformation

# Neural networks

$$\hat{y} = \sigma(wx + b)$$



Prediction

# Neural networks

$$\hat{y} = \sigma(wx + b)$$

$$z = (y - \hat{y})^2$$

Change  $w$  and  $b$  such that  $z$  is minimal

# Neural networks

$$w \leftarrow w + \eta \frac{\partial z}{\partial w}$$

$$b \leftarrow b + \eta \frac{\partial z}{\partial b}$$

Update the weights

# Neural networks

$$\left. \begin{aligned} w &\leftarrow w + \eta \frac{\partial z}{\partial w} \\ b &\leftarrow b + \eta \frac{\partial z}{\partial b} \end{aligned} \right\} \text{Optimizer}$$

# Convolutions

	1			
1	-1	1		
	-1			
1	-1			

0	0	0
0	1	0
0	0	0


# Convolutions

0	1	0	0	0
1	-1	1	0	0
0	0	0	0	0
0	-1	0	0	0
0	1	-1	0	0

0	0	0
0	1	0
0	0	0


# Convolutions

0	1	0	0	0
1	-1	1	0	0
0	0	0	0	0
0	-1	0	0	0
0	1	-1	0	0

0	0	0
0	1	0
0	0	0


# Convolutions

0	1	0	0	0
1	-1	1	0	0
0	0	0	0	0
0	-1	0	0	0
0	1	-1	0	0

0	0	0
0	1	0
0	0	0

-1		

# Convolutions

0	1	0	0	0
1	-1	1	0	0
0	0	0	0	0
0	-1	0	0	0
0	1	-1	0	0

0	0	0
0	1	0
0	0	0

-1	1	

# Convolutions

0	1	0	0	0
1	-1	1	0	0
0	0	0	0	0
0	-1	0	0	0
0	1	-1	0	0

0	0	0
0	1	0
0	0	0

-1	1	0

# Convolutions

0	1	0	0	0
1	-1	1	0	0
0	0	0	0	0
0	-1	0	0	0
0	1	-1	0	0

0	0	0
0	1	0
0	0	0

-1	1	0
0		

# Convolutions

0	1	0	0	0
1	-1	1	0	0
0	0	0	0	0
0	-1	0	0	0
0	1	-1	0	0

0	0	0
0	1	0
0	0	0

-1	1	0
0	0	

# Convolutions

0	1	0	0	0
1	-1	1	0	0
0	0	0	0	0
0	-1	0	0	0
0	1	-1	0	0

0	0	0
0	1	0
0	0	0

-1	1	0
0	0	0

# Convolutions

0	1	0	0	0
1	-1	1	0	0
0	0	0	0	0
0	-1	0	0	0
0	1	-1	0	0

0	0	0
0	1	0
0	0	0

-1	1	0
0	0	0
-1		

# Convolutions

0	1	0	0	0
1	-1	1	0	0
0	0	0	0	0
0	-1	0	0	0
0	1	-1	0	0

0	0	0
0	1	0
0	0	0

-1	1	0
0	0	0
-1	0	

# Convolutions

0	1	0	0	0
1	-1	1	0	0
0	0	0	0	0
0	-1	0	0	0
0	1	-1	0	0

0	0	0
0	1	0
0	0	0

-1	1	0
0	0	0
-1	0	0

# Convolutions

0	1	0	0	0
1	-1	1	0	0
0	0	0	0	0
0	-1	0	0	0
0	1	-1	0	0

0	0	0
0	1	0
0	0	0

-1	1	0
0	0	0
-1	0	0

Identity kernel

# Convolutions

x	x	x	x	x
x	x	x	x	x
x	x	x	x	x
x	x	x	x	x
x	x	x	x	x

w	w	w
w	w	w
w	w	w

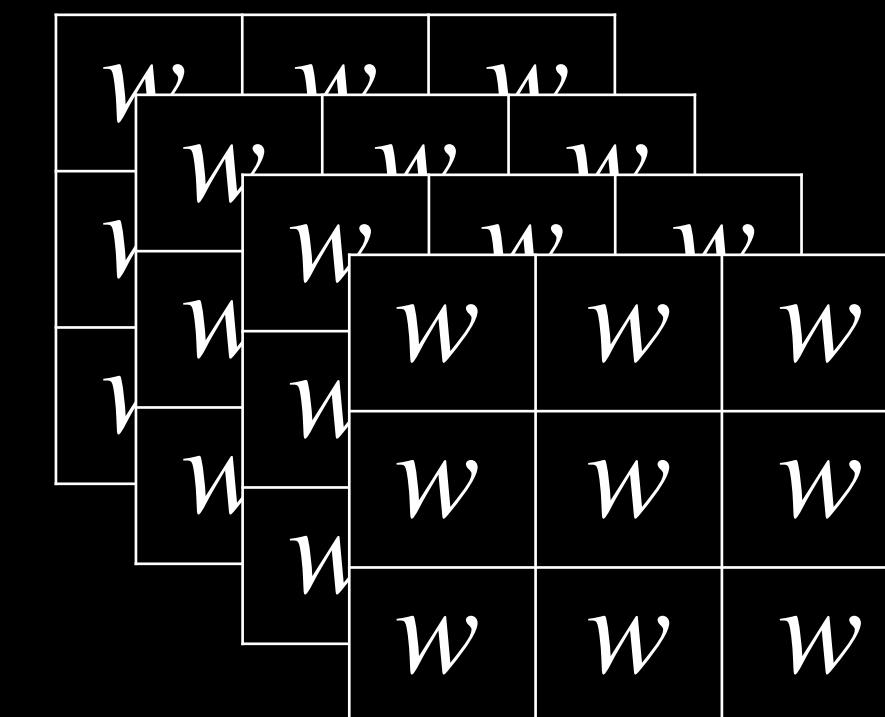
Learnable

$\hat{y}$	$\hat{y}$	$\hat{y}$
$\hat{y}$	$\hat{y}$	$\hat{y}$
$\hat{y}$	$\hat{y}$	$\hat{y}$

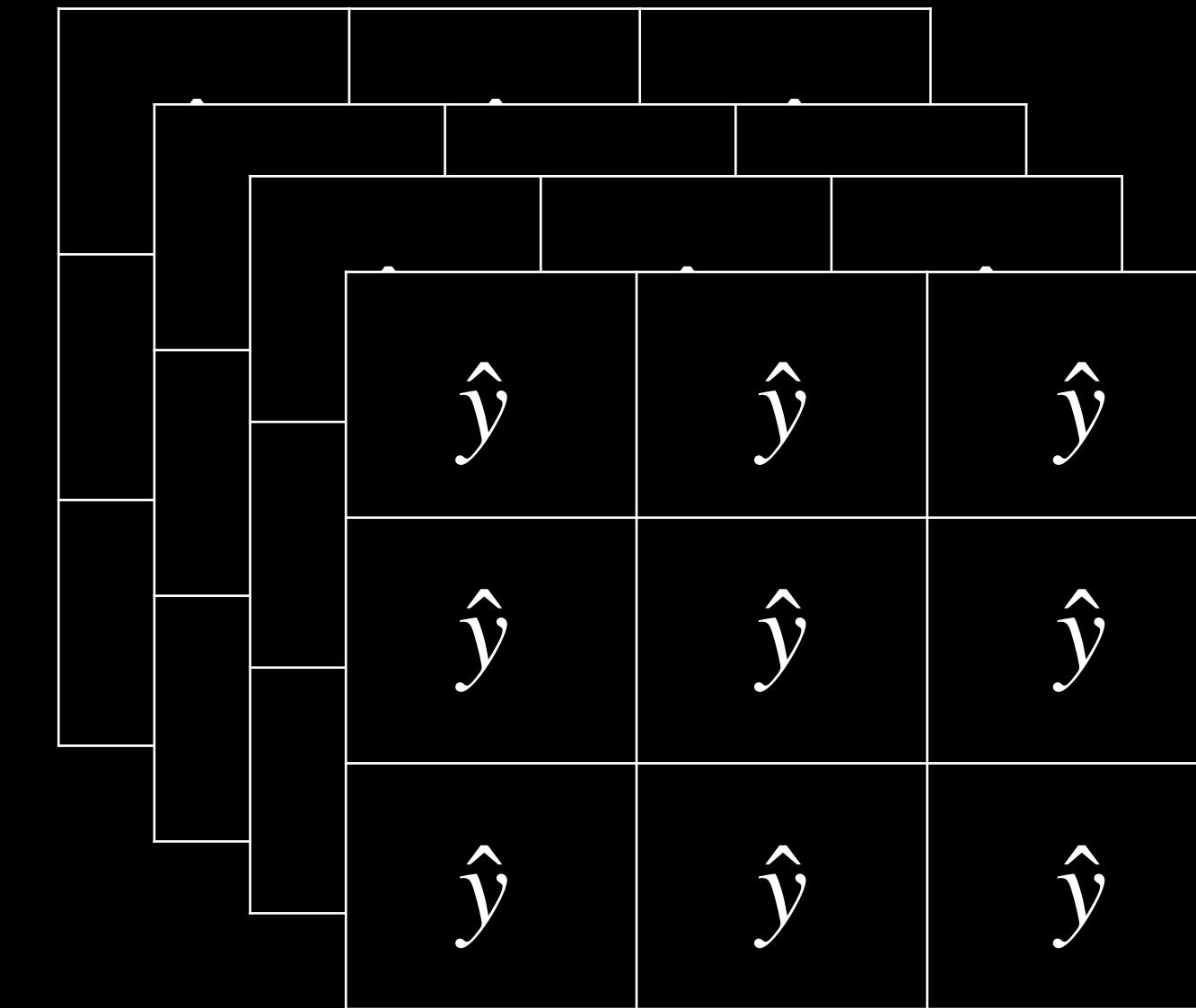
# Convolutions

x	x	x	x	x
x	x	x	x	x
x	x	x	x	x
x	x	x	x	x
x	x	x	x	x

Input



4 ( $1 \times 3 \times 3$ ) kernels

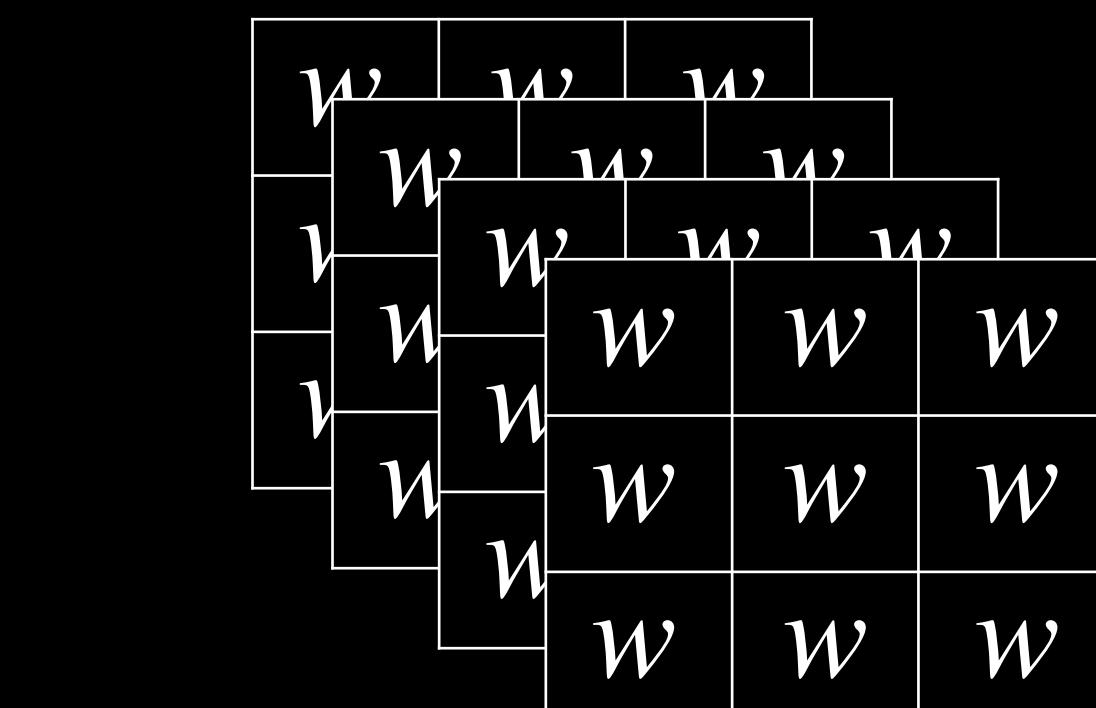


4 feature maps

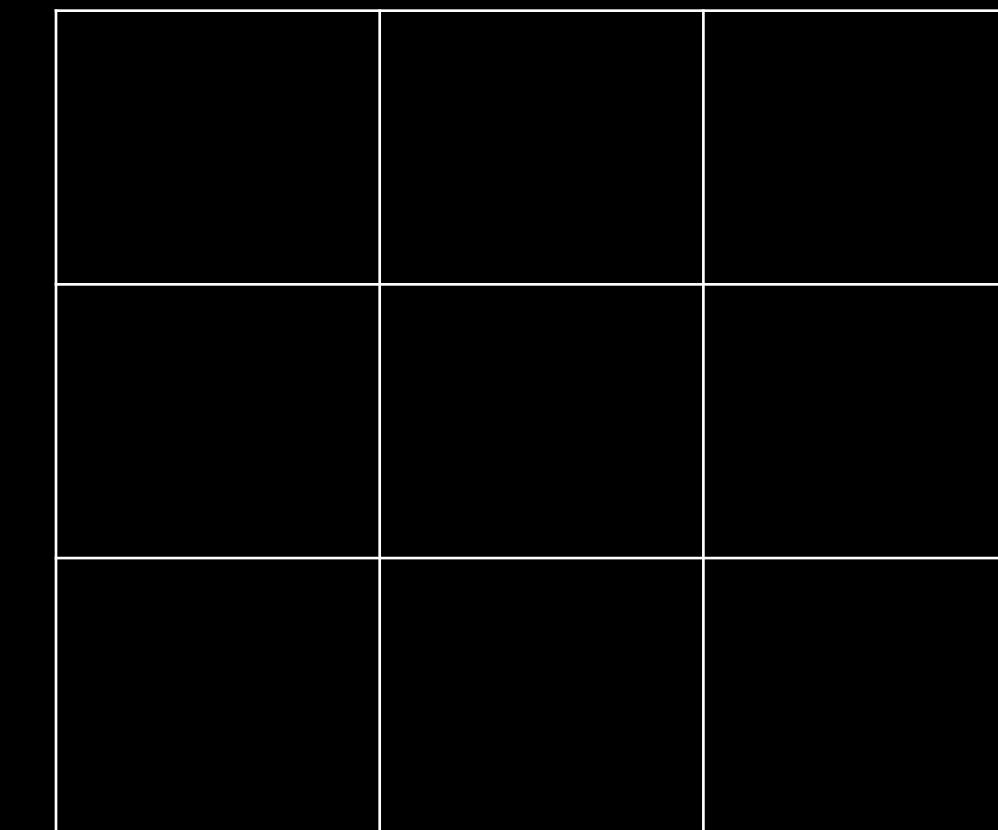
# Convolutions

1	1	0	0	0
0	1	1	0	0
1	0.5	1	0	0
1	-1	1	0	0
0	0	0	0	0
0	0	0	0	0
0	0	-1	0	0
0	1	-1	0	0

4 feature maps



1 ( $4 \times 3 \times 3$ ) kernel



1 feature map

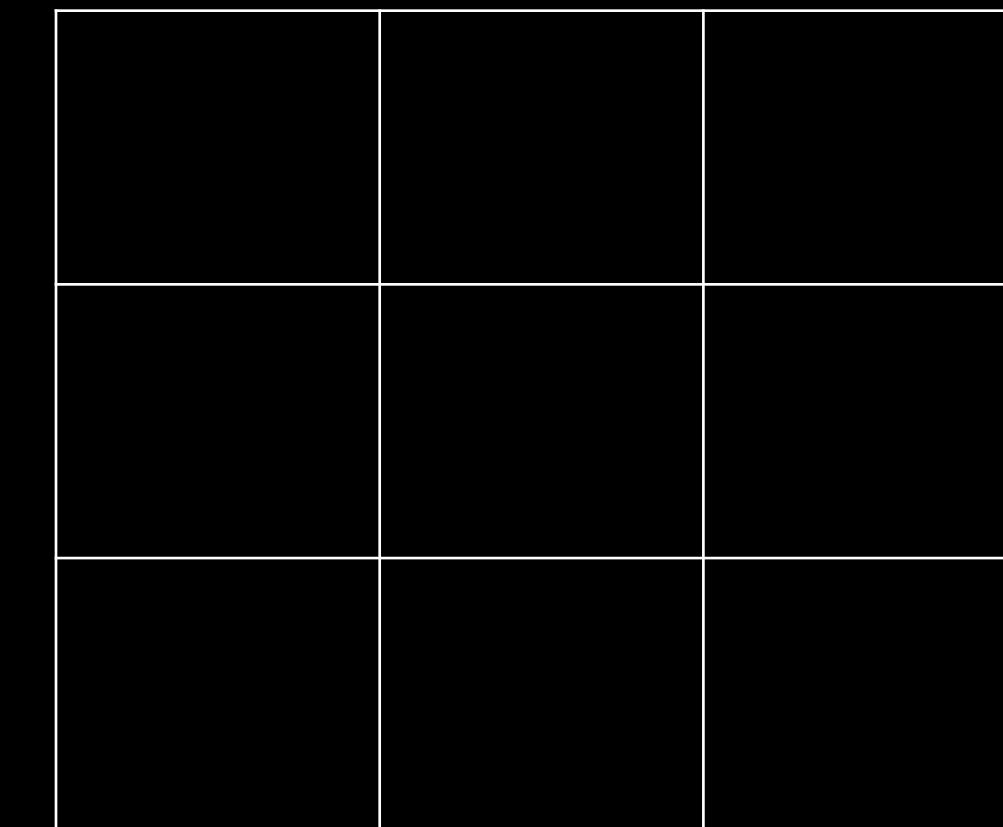
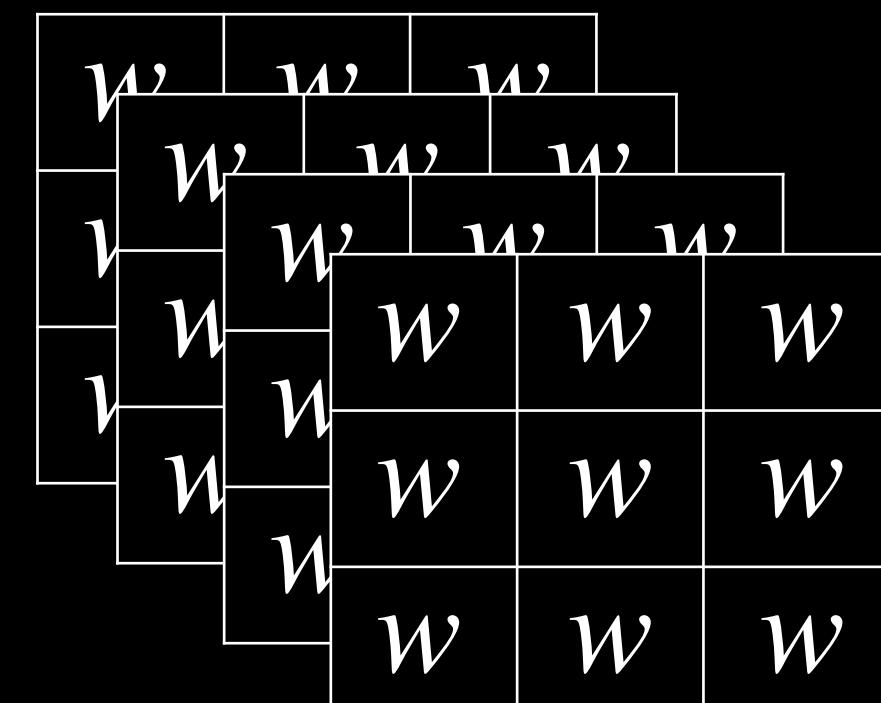
# Convolutions

1	1	0	0	0
0	1	1	0	0
1	0.5	1	0	0
1	1	-1	1	0
0	0	0	0	0
0	0	0	0	0
0	0	-1	0	0
0	1	-1	0	0

$n(c \times w \times h)$  feature maps

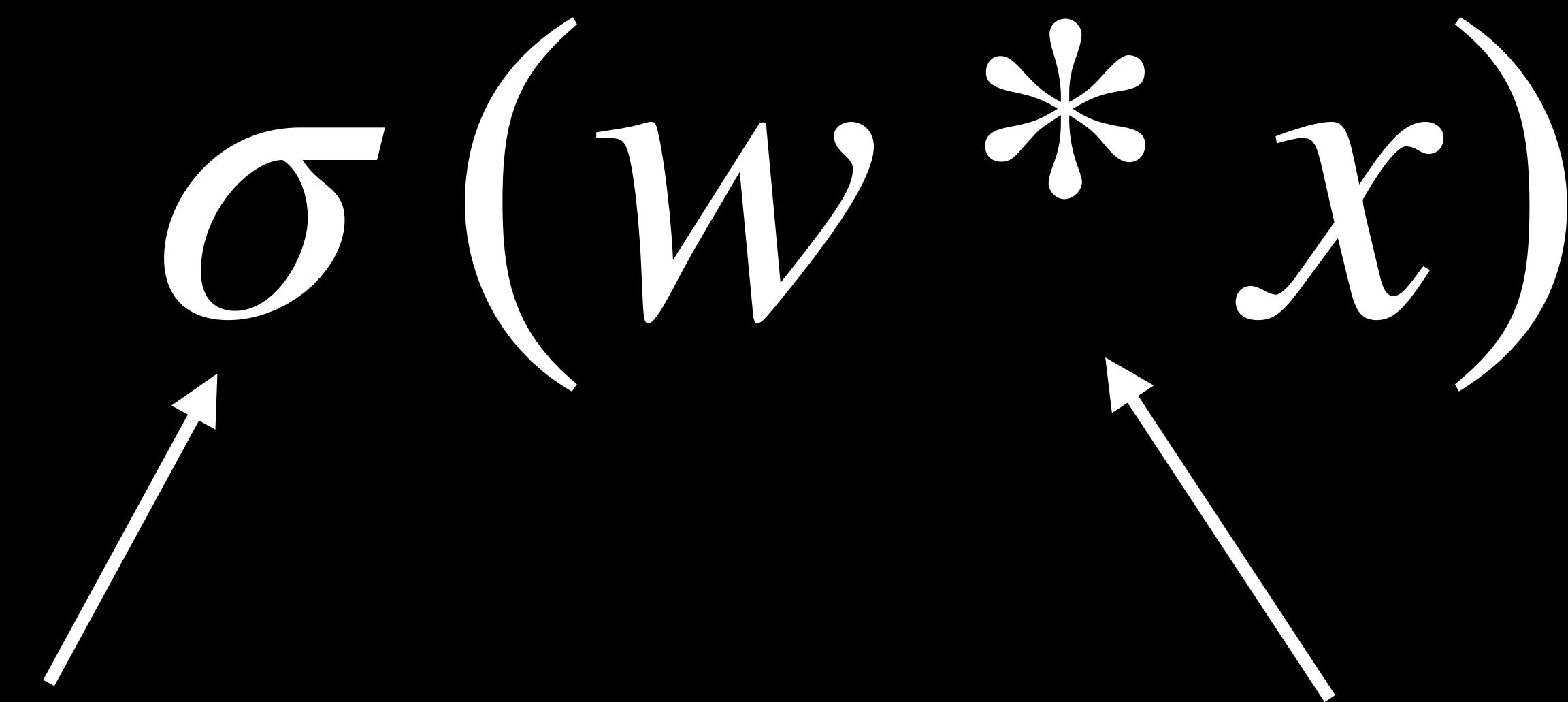
$m(c \times k \times k)$  kernel

$m(1 \times w \times h)$  feature map



$O(k)$

# Convolutions

$$\sigma(w * x)$$


The diagram illustrates the components of a convolution operation. At the top, the mathematical expression  $\sigma(w * x)$  is shown in white. Below it, two arrows point upwards towards the expression: one from the left pointing to the  $w$  term, labeled "Non-linear transformation", and another from the right pointing to the  $x$  term, labeled "Linear transformation".

# RNN: Concatenation

0	1	0	0	0
1	-1	1	0	0
0	0	0	0	0
0	-1	0	0	0
0	1	-1	0	0

$h_{t-1}$

1	1	-1	0	1
---	---	----	---	---

$x_t$

0	1	0	0	0
1	-1	1	0	0
0	0	0	0	0
0	-1	0	0	0
0	1	-1	0	0
1	1	-1	0	1

$[x_t, h_{t-1}]$

# RNN

$$\sigma(w[x_t, h_{t-1}] + b)$$

# Gates

0	1	0	0
1	-1	1	0
1	1	0	-1
0	-1	0	0

1	1	1	1
1	1	1	1
1	1	1	1
1	1	1	1

0	1	0	0
1	-1	1	0
1	1	0	-1
0	-1	0	0

 $X$  $\otimes$  $\Gamma$  $=$  $Y$

# Gates

0	1	0	0
1	-1	1	0
1	1	0	-1
0	-1	0	0

 $\otimes$ 

0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0

 $\Gamma$  $=$  $Y$ 

0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0

# Gates

0	1	0	0
1	-1	1	0
1	1	0	-1
0	-1	0	0

1	1	1	1
1	1	1	1
0.5	0.5	0.5	0.5
0	0	0	0

0	1	0	0
1	-1	1	0
0.5	0.5	0	-0.5
0	0	0	0

 $X$  $\otimes$  $\Gamma$  $=$  $Y$

# GRU

$$\Gamma = \sigma(W_{\Gamma}[X_t, h_{t-1}] + b_{\Gamma})$$

$$\tilde{h}_t = \sigma(W_H[X_t, h_{t-1}] + b_H)$$

$$h_t = \Gamma \otimes h_{t-1} + (1 - \Gamma) \otimes \tilde{h}_t$$

# GRU

$$\Gamma = \sigma(W_\Gamma[X_t, h_{t-1}] + b_\Gamma)$$

$$\tilde{h}_t = \sigma(W_H[X_t, h_{t-1}] + b_H)$$

$$h_t = \Gamma \otimes h_{t-1} + (1 - \Gamma) \otimes \tilde{h}_t$$

$$\sigma(wx+b)$$

$$\sigma(w^{\ast}x)$$

$$\sigma(w[x_t,h_{t-1}] + b)$$

# Hyperparameters

# Neural networks

$$\sigma(f(x))$$

# Neural networks

$$f_2(\sigma(f_1(x)))$$

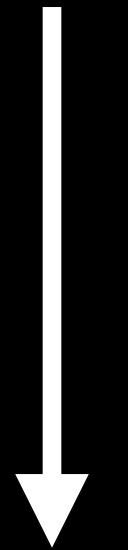
# Neural networks

$f_2 \circ \sigma \circ f_1$

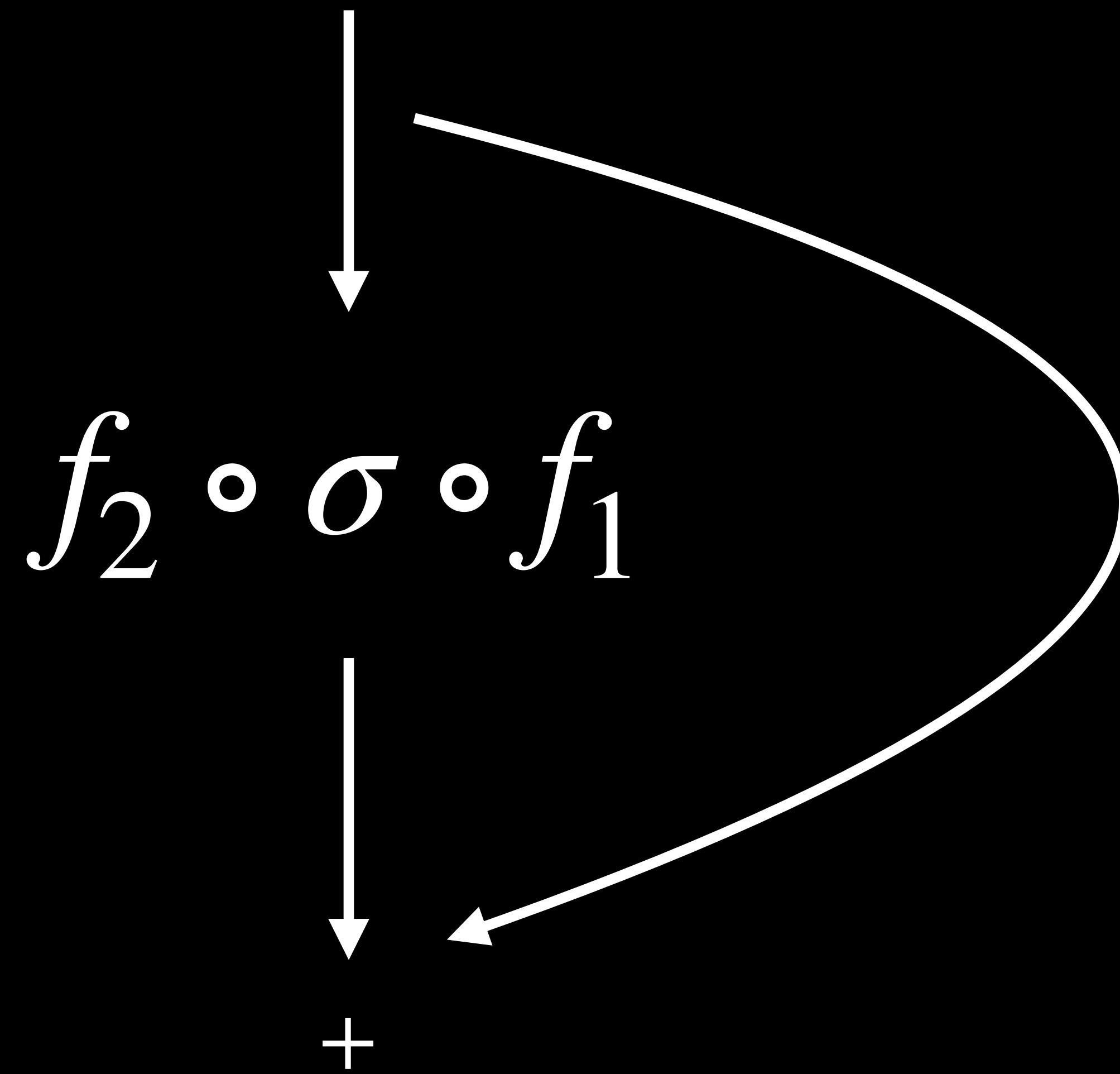
# Deep neural networks



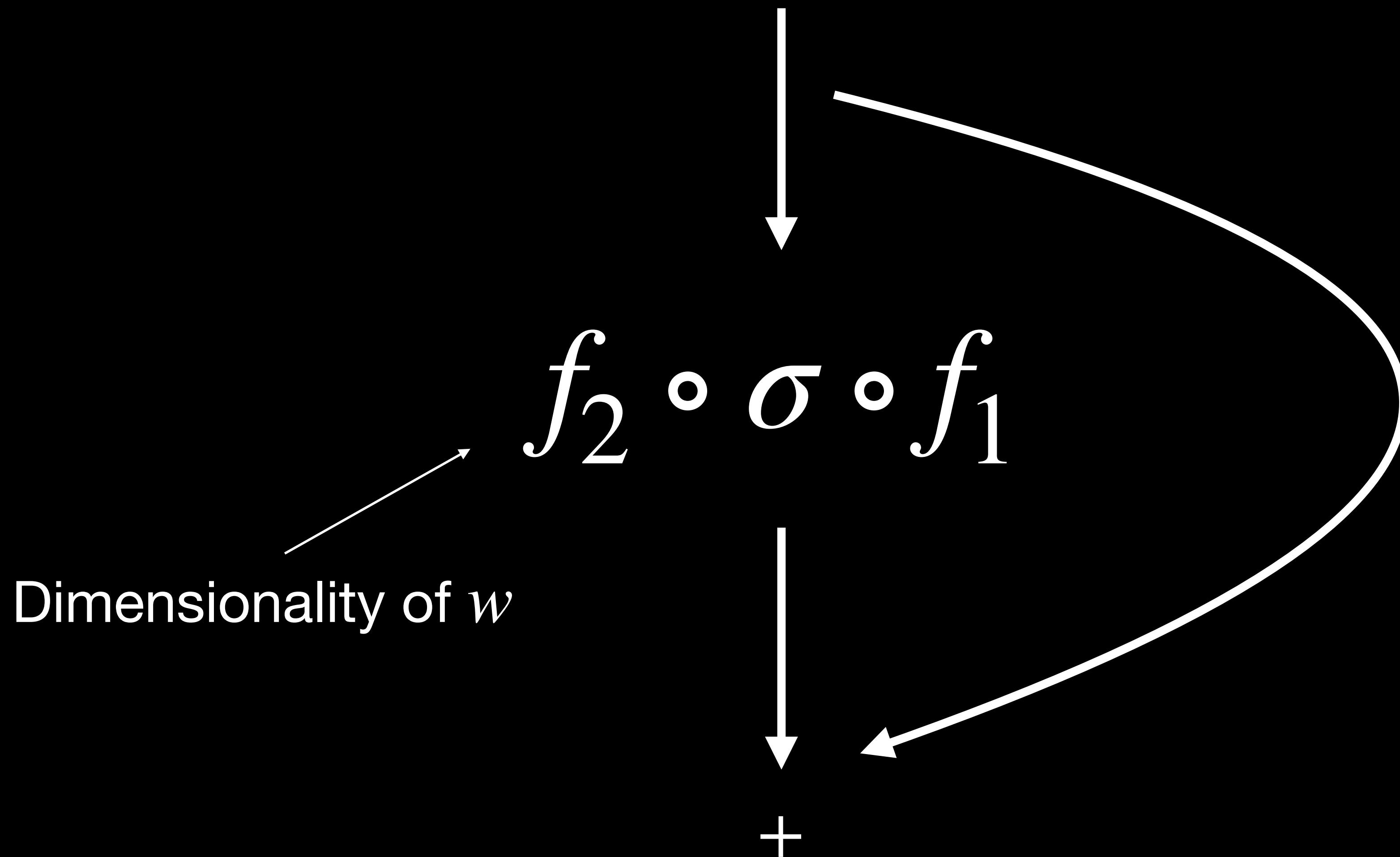
$$f_2 \circ \sigma \circ f_1$$



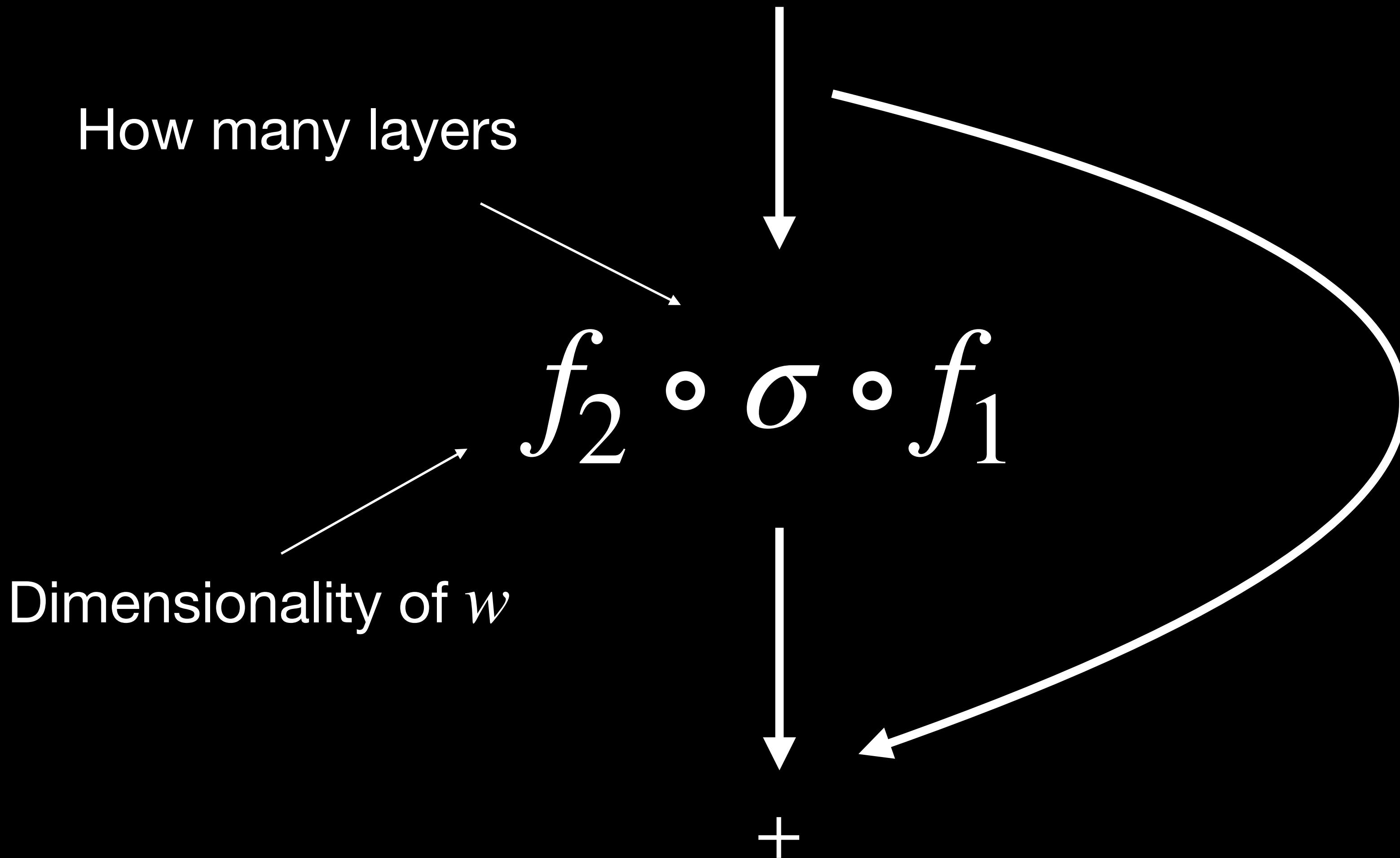
# Deep neural networks



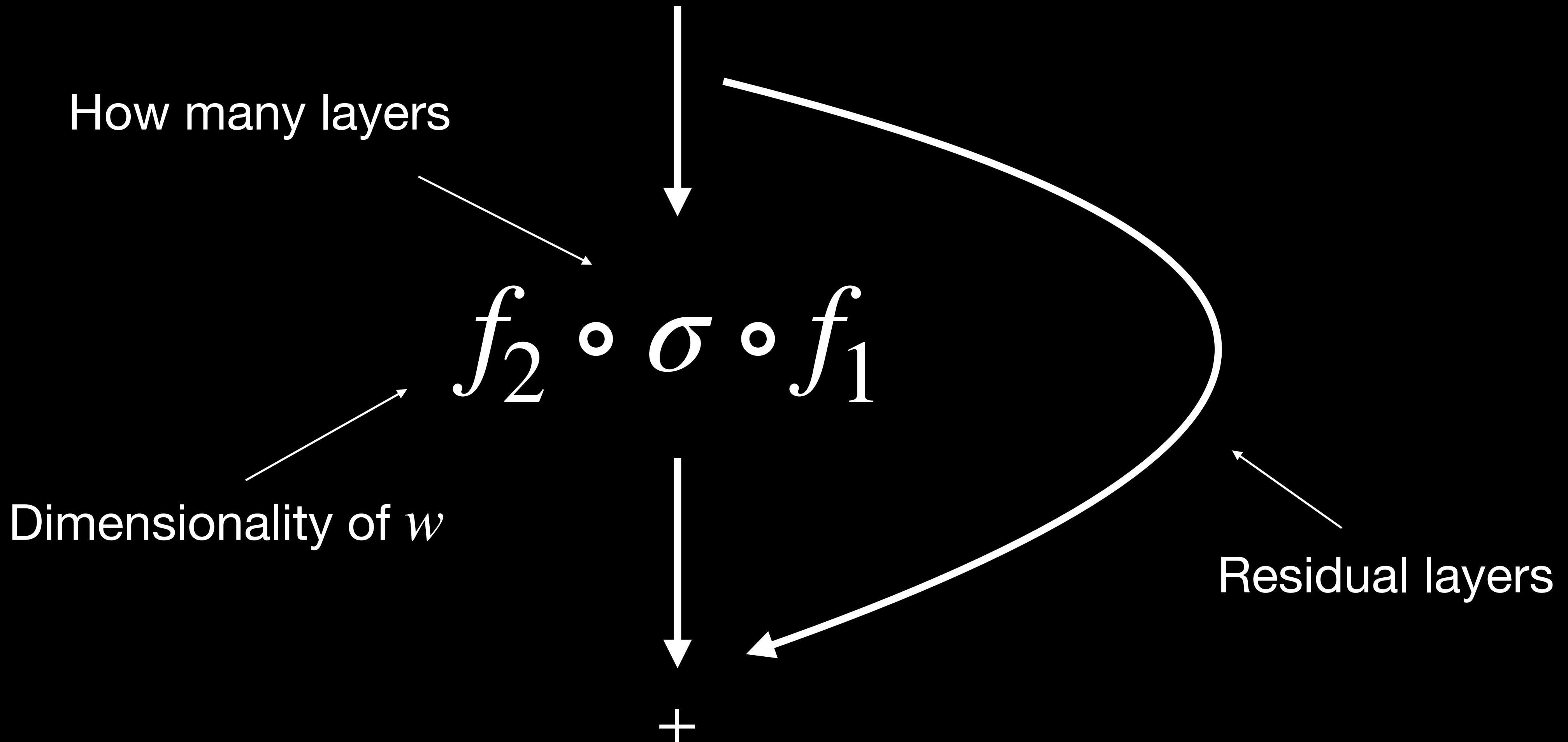
# Hyperparameters



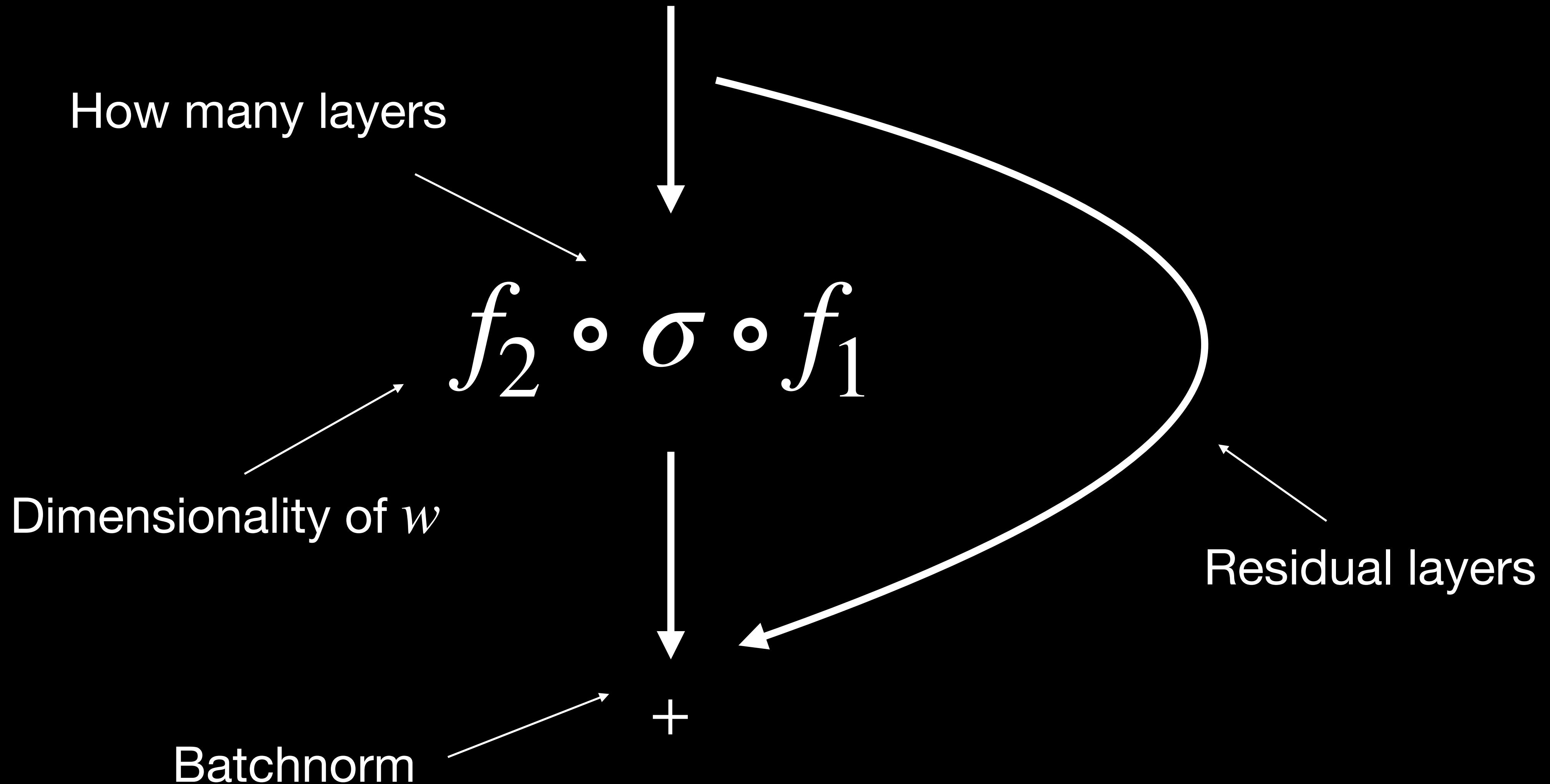
# Hyperparameters



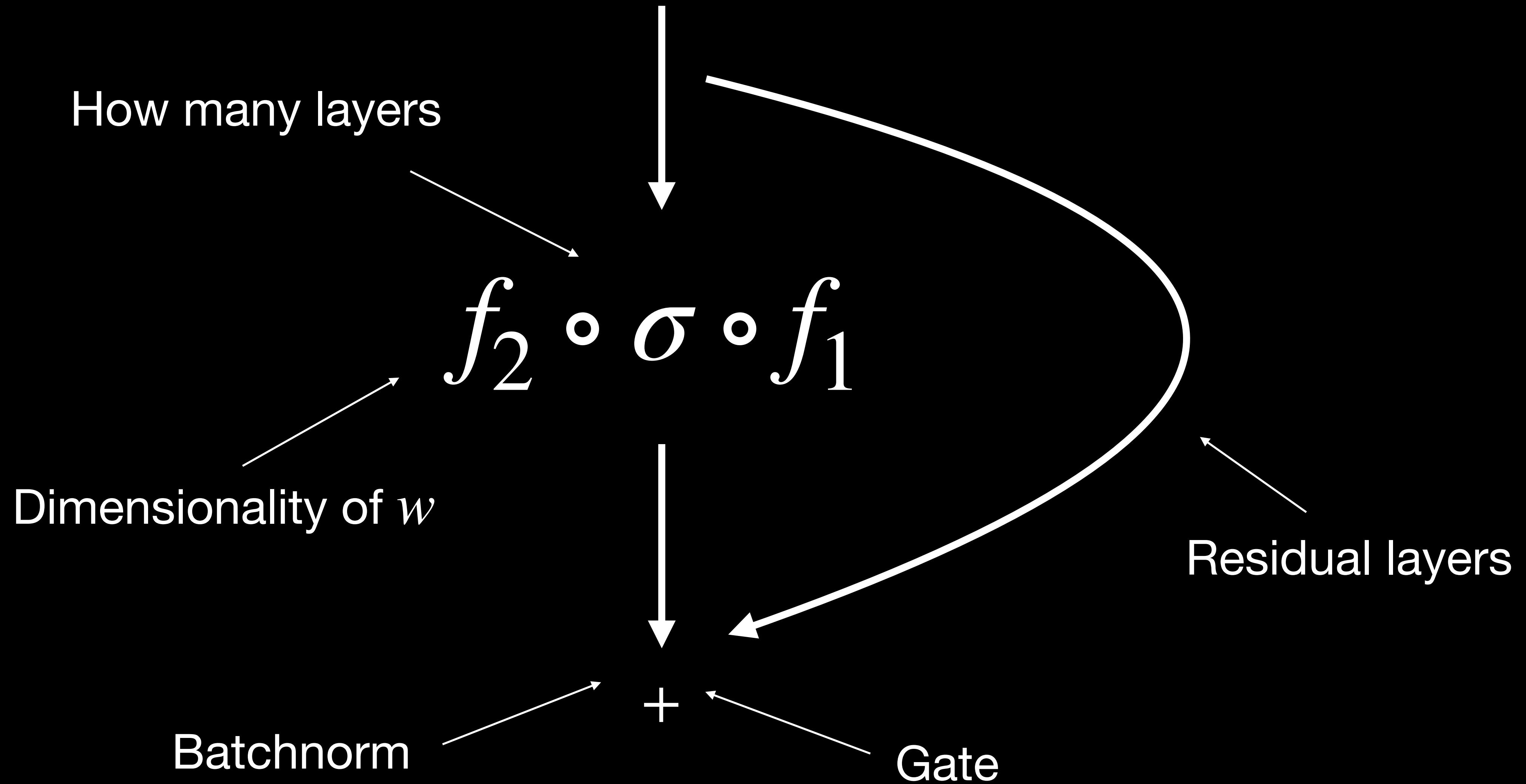
# Hyperparameters



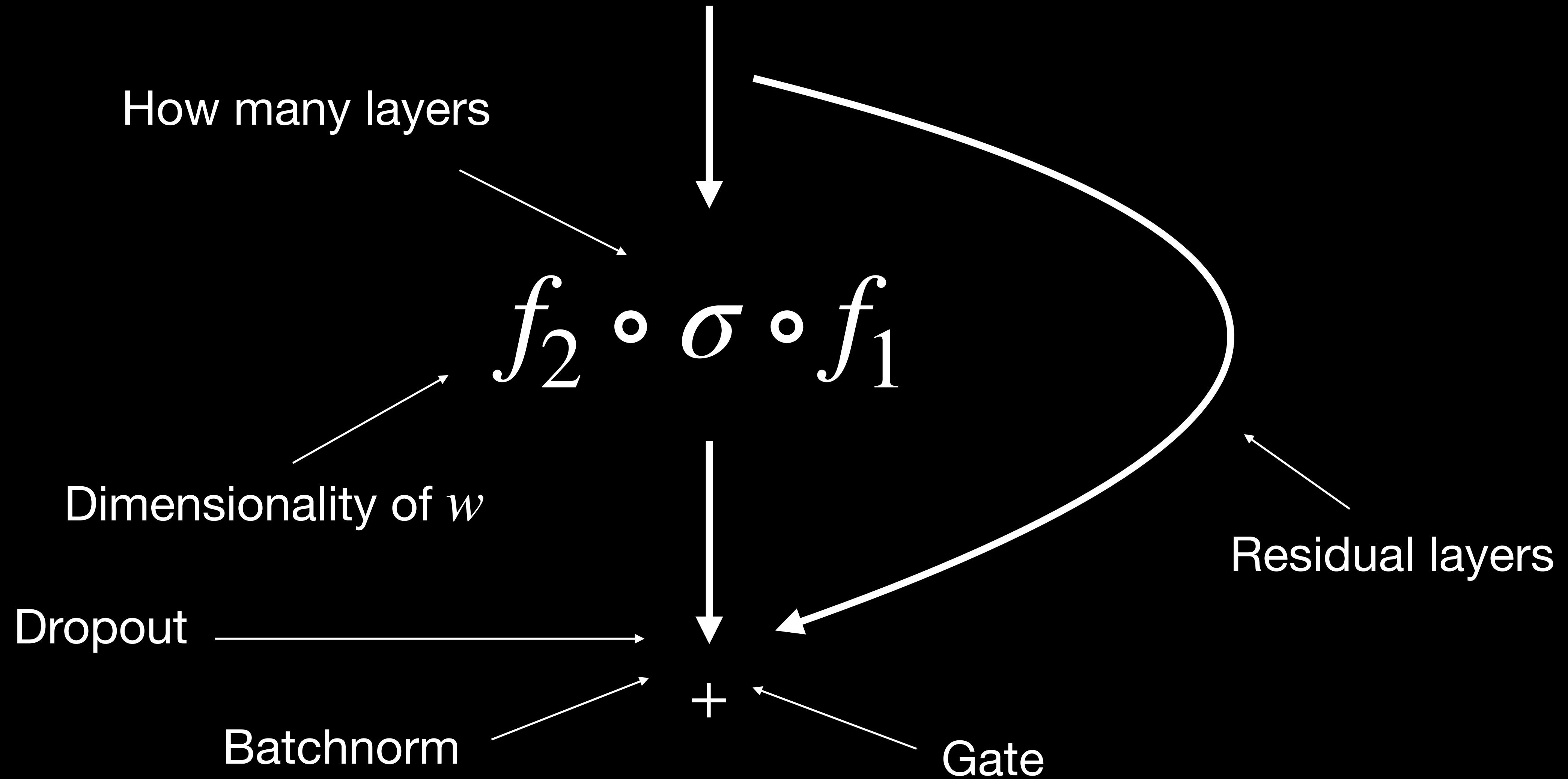
# Hyperparameters



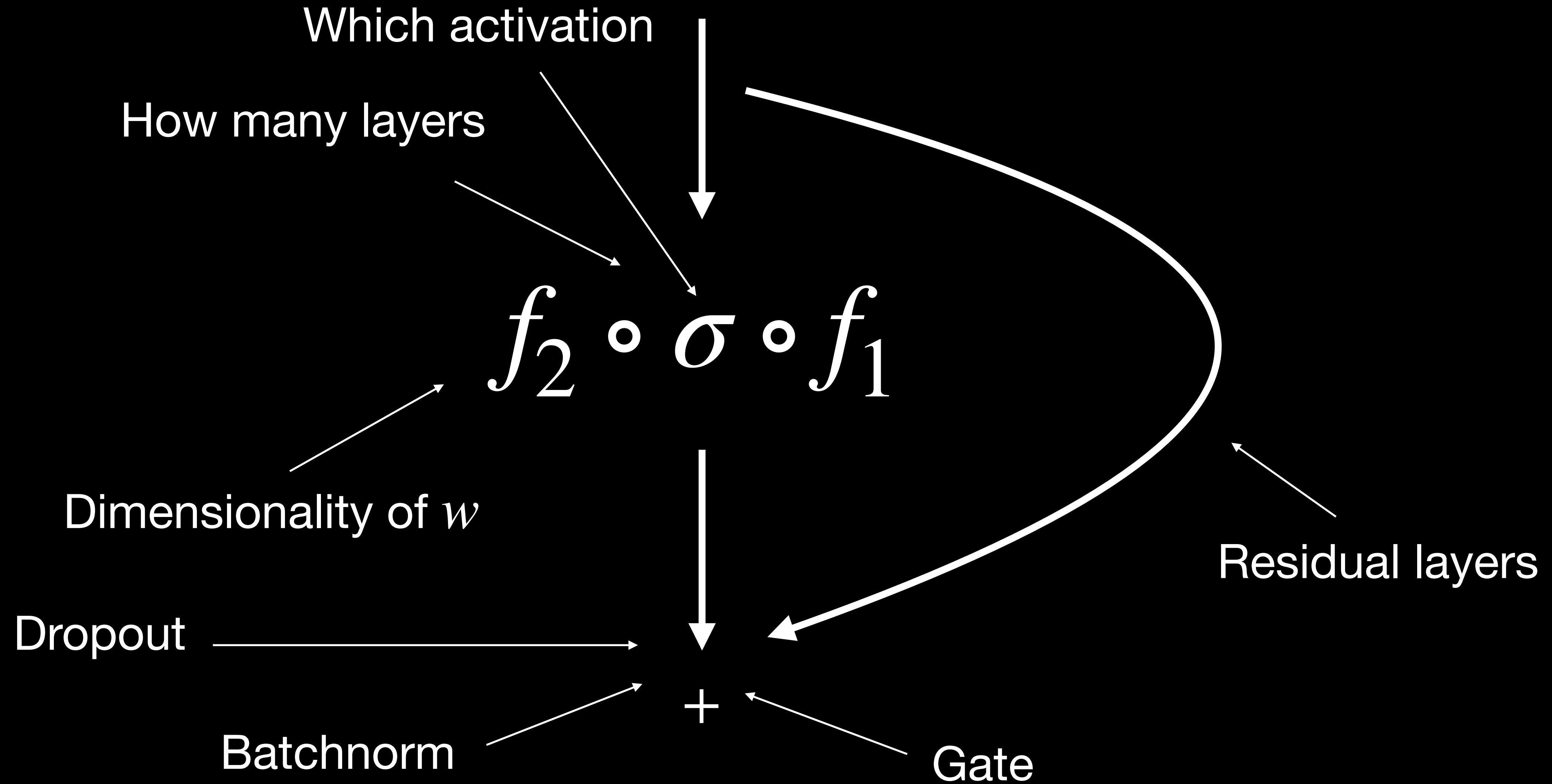
# Hyperparameters

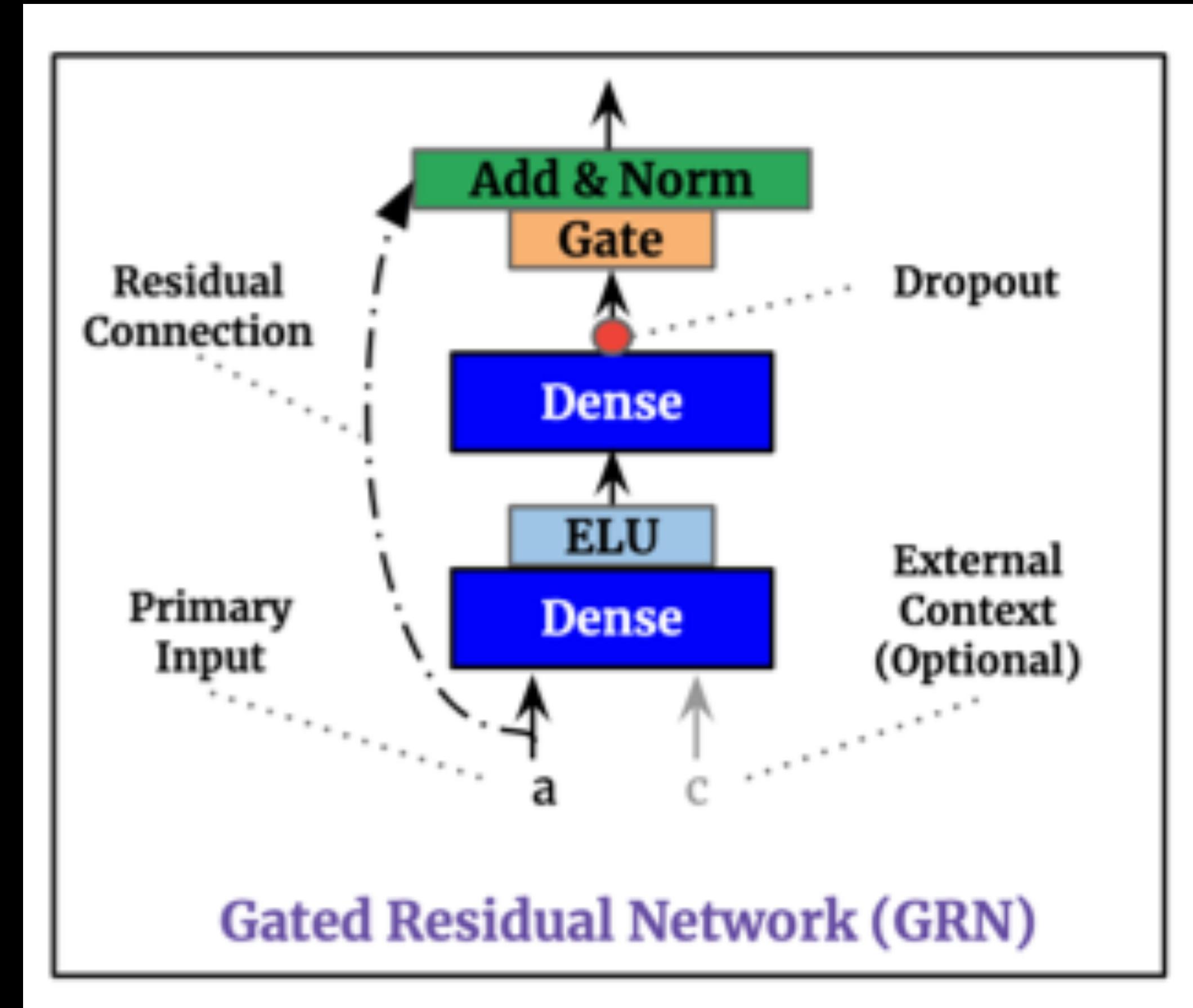


# Hyperparameters



# Hyperparameters





# Transfer learning

Input



Layer



Layer

Some task



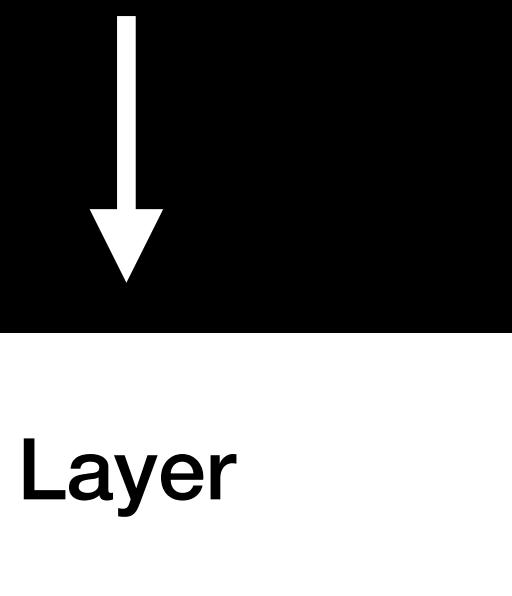
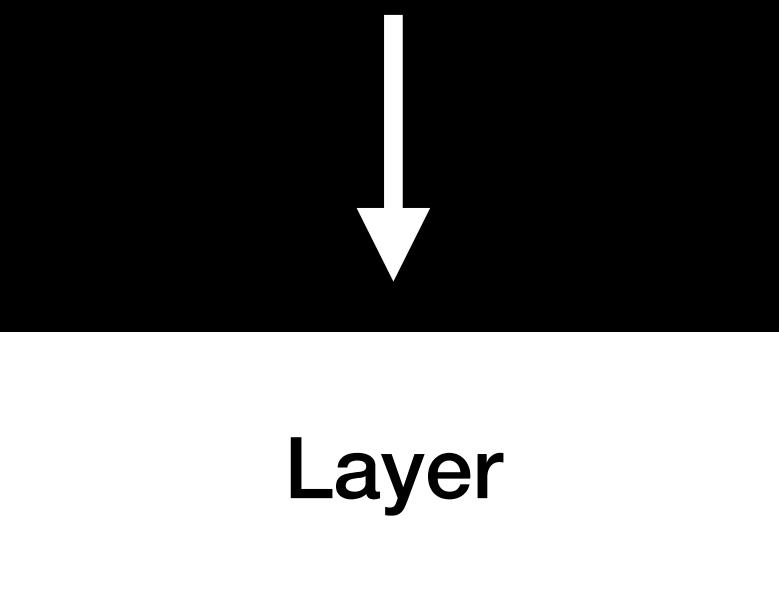
Layer



Output

Input

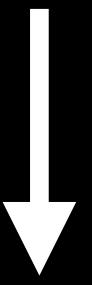
Other input



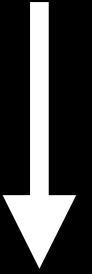
Some task

Some other task

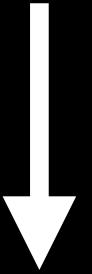
Input



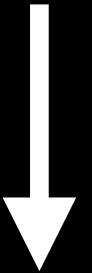
Layer



Layer

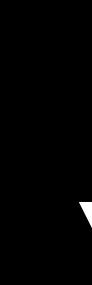


Layer

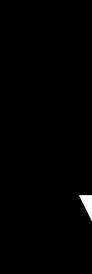


Output

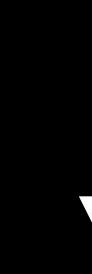
Other input



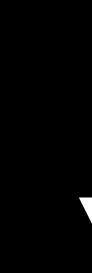
Layer



Layer



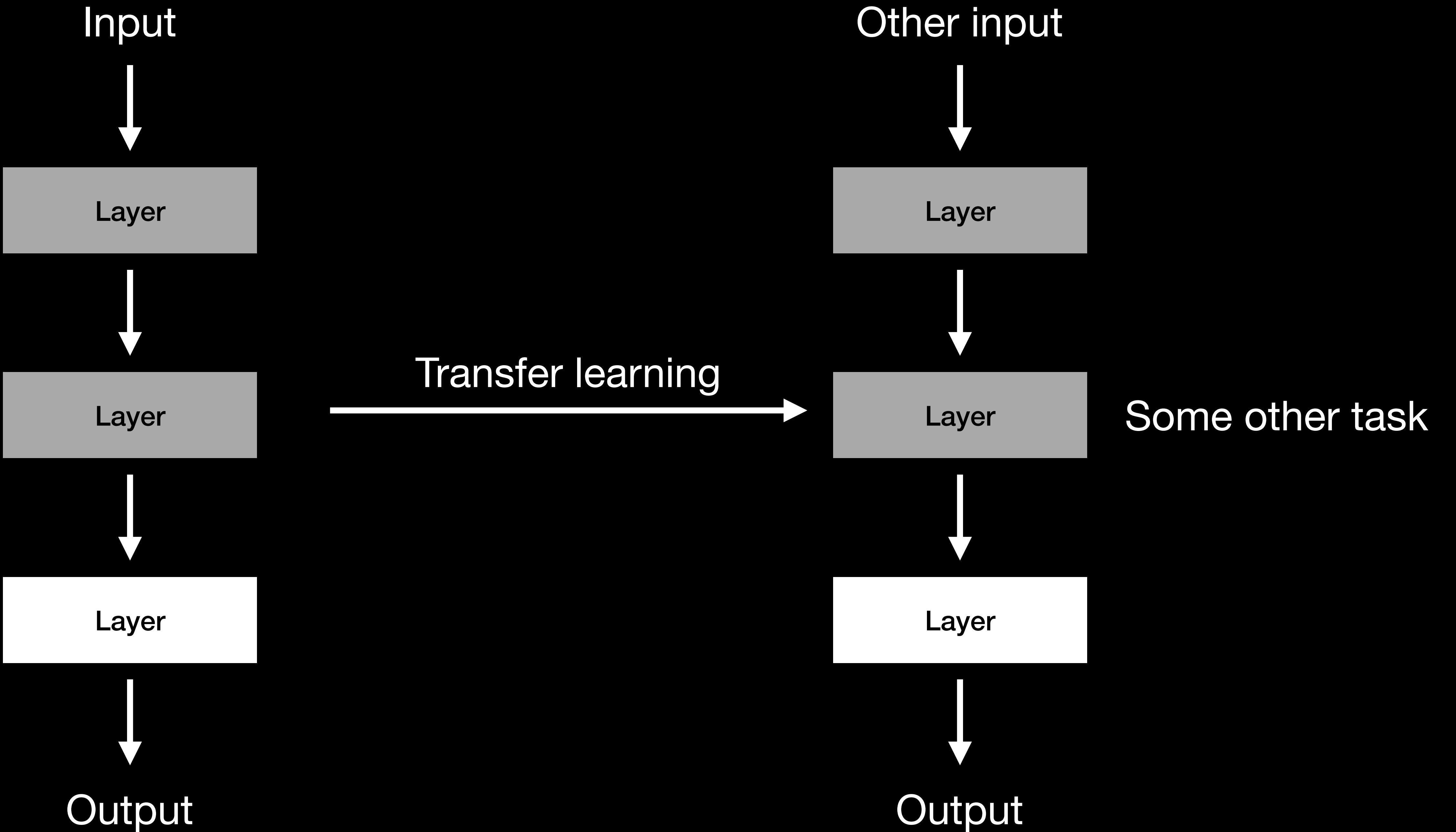
Layer



Output

Freeze weights





Other input



Layer



Layer



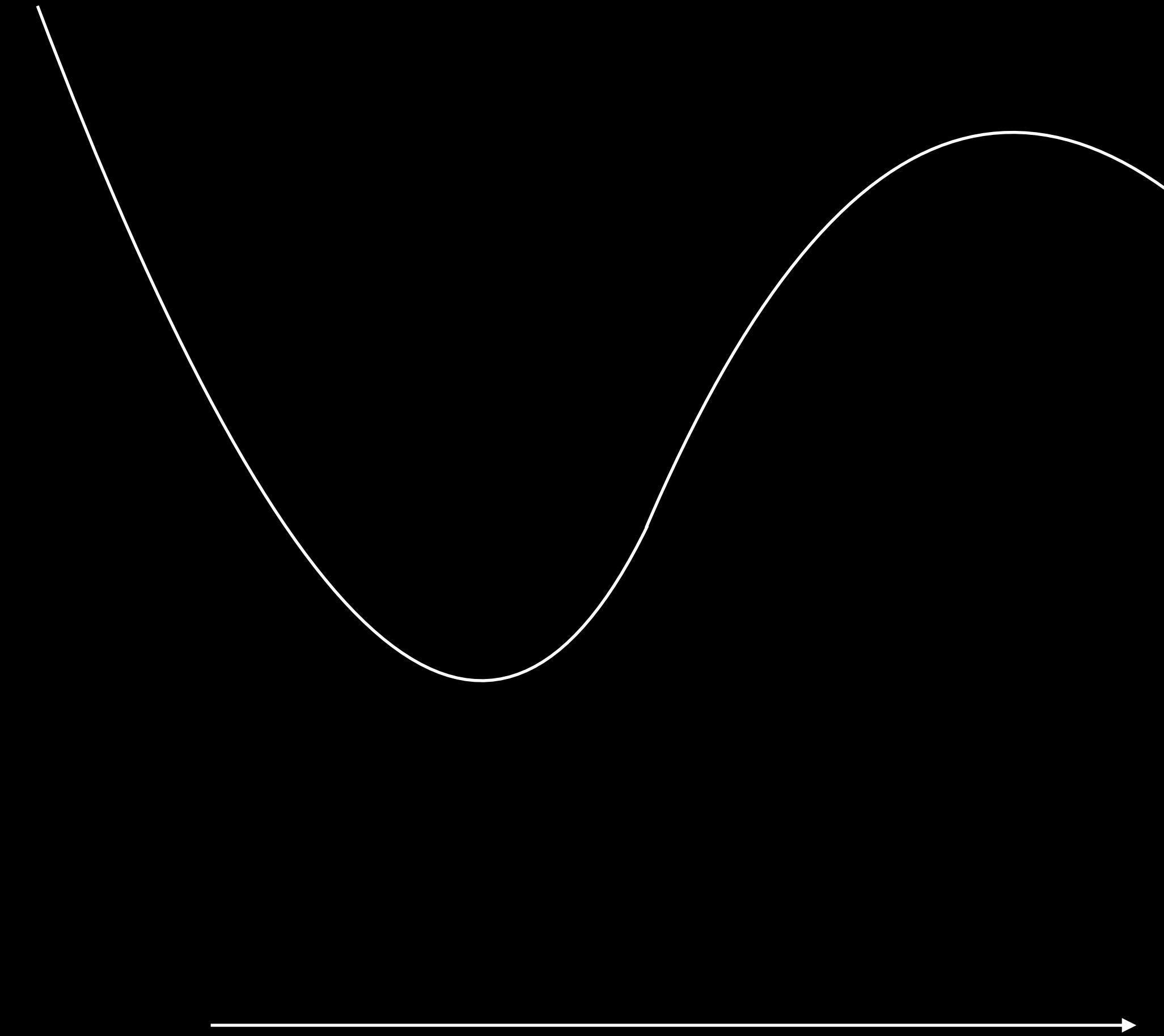
Finetuning

Layer



Output

# Search spaces

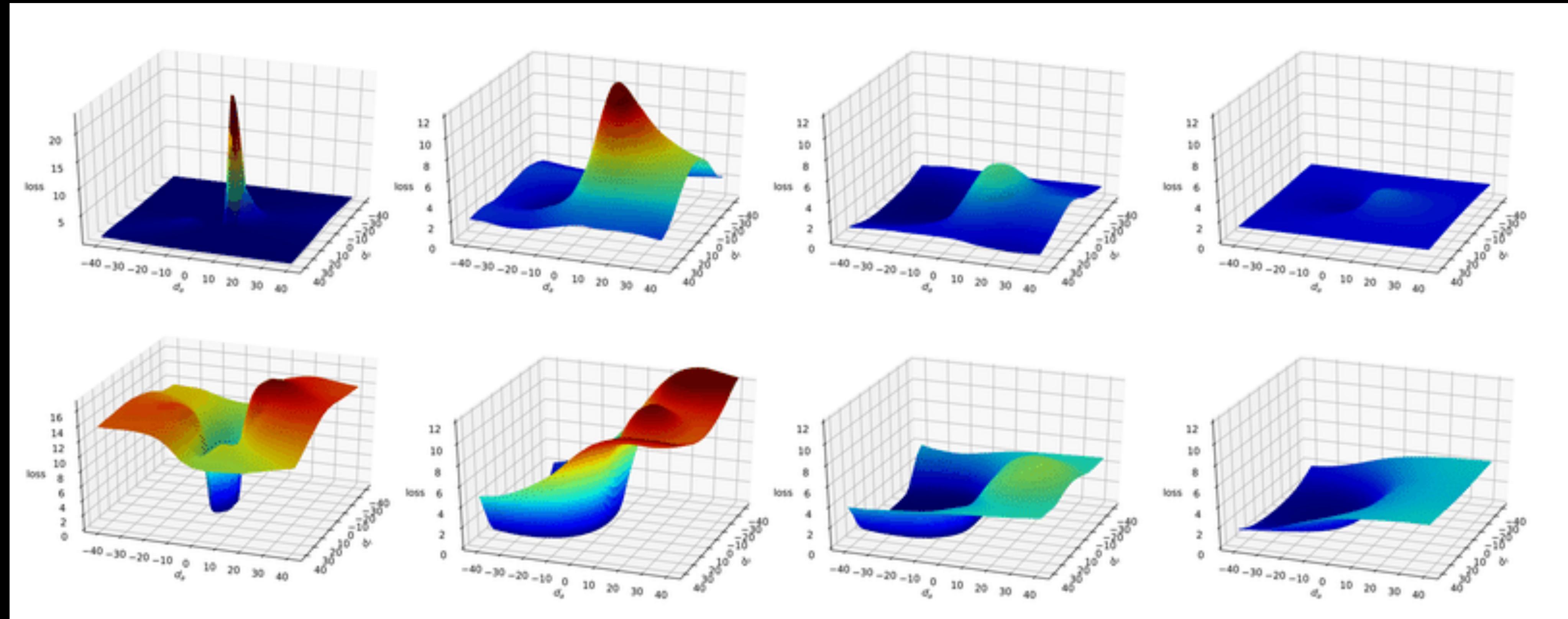


One hyperparameter



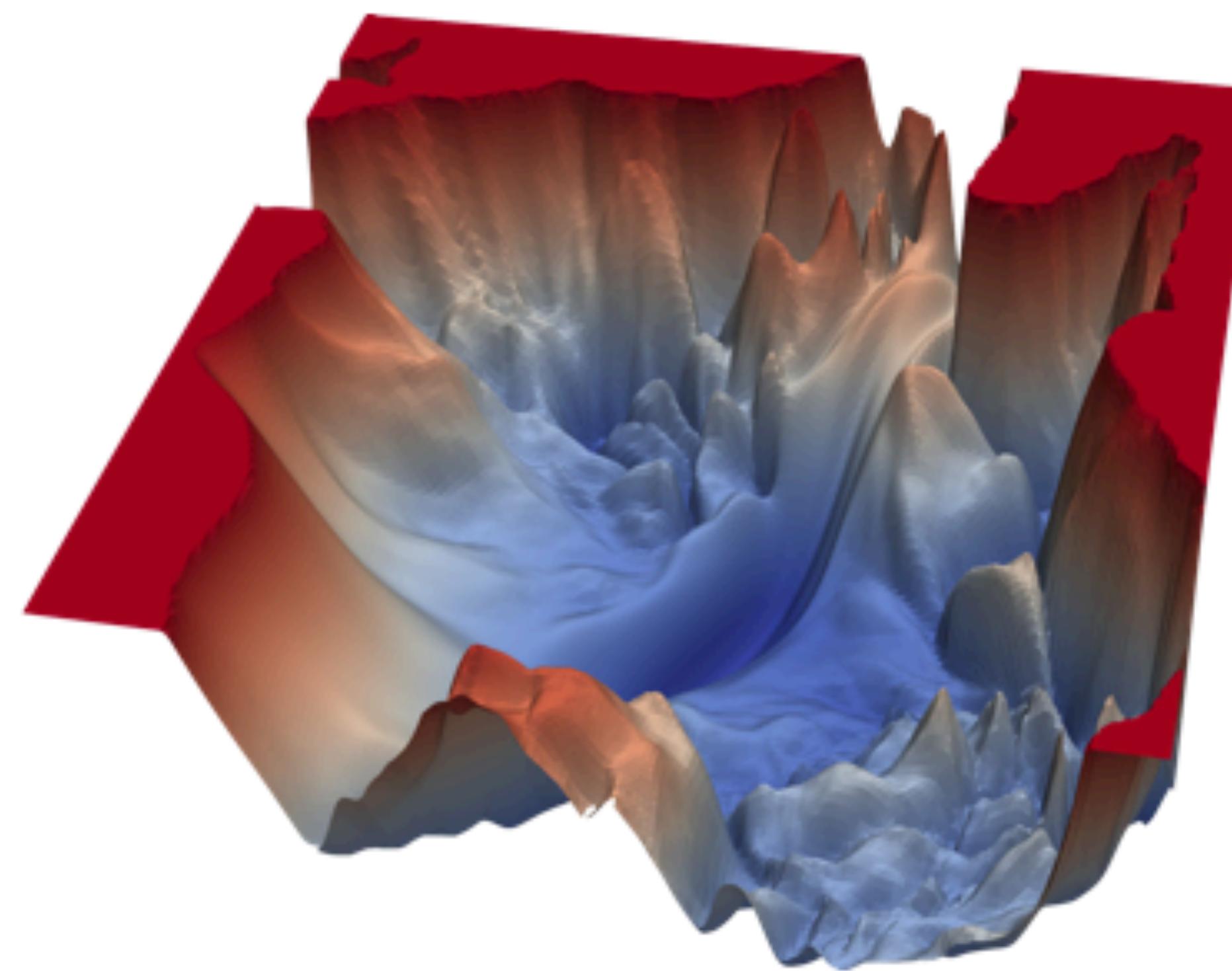
Minimum

One hyperparameter

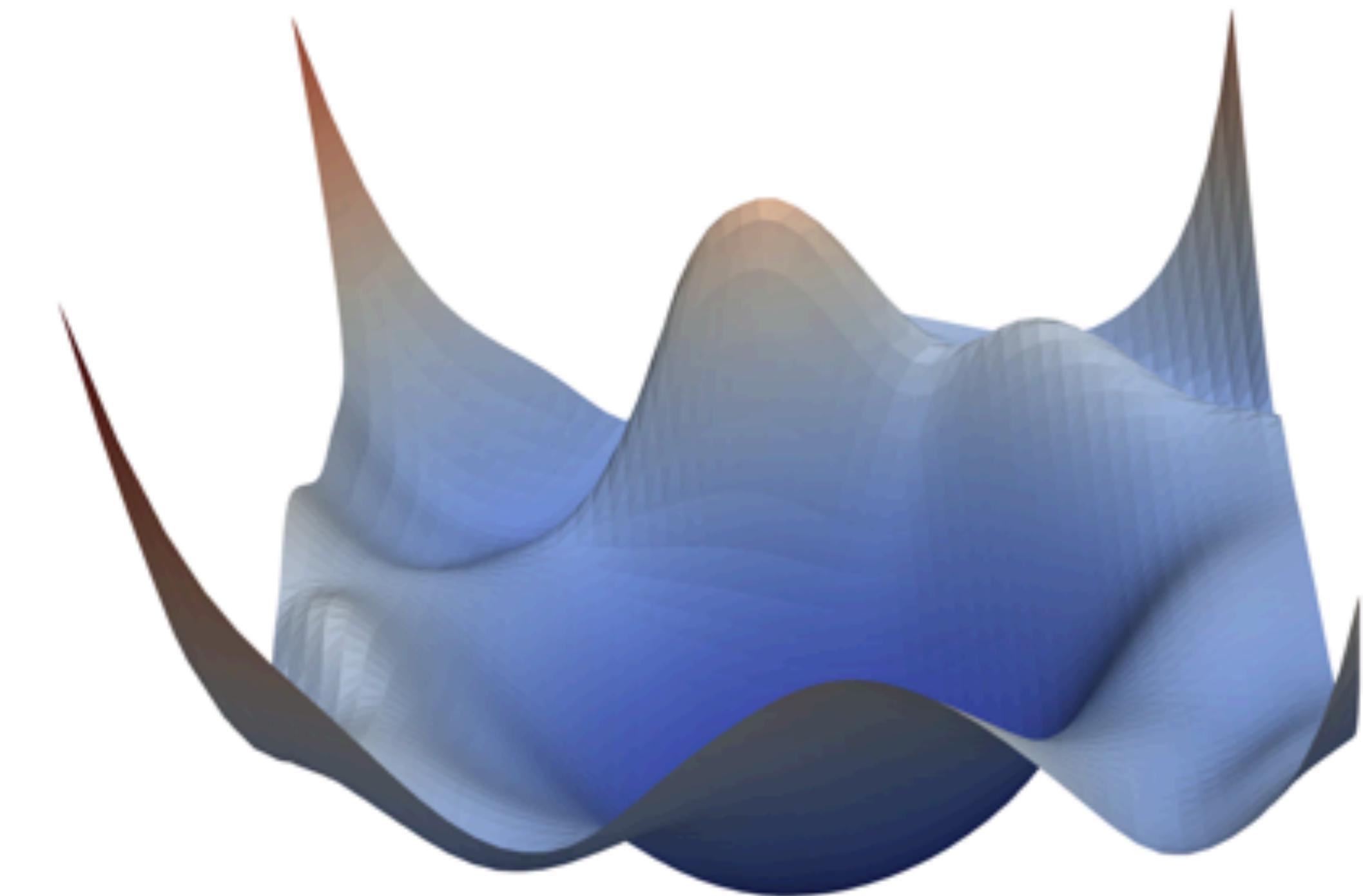


Two hyperparameters

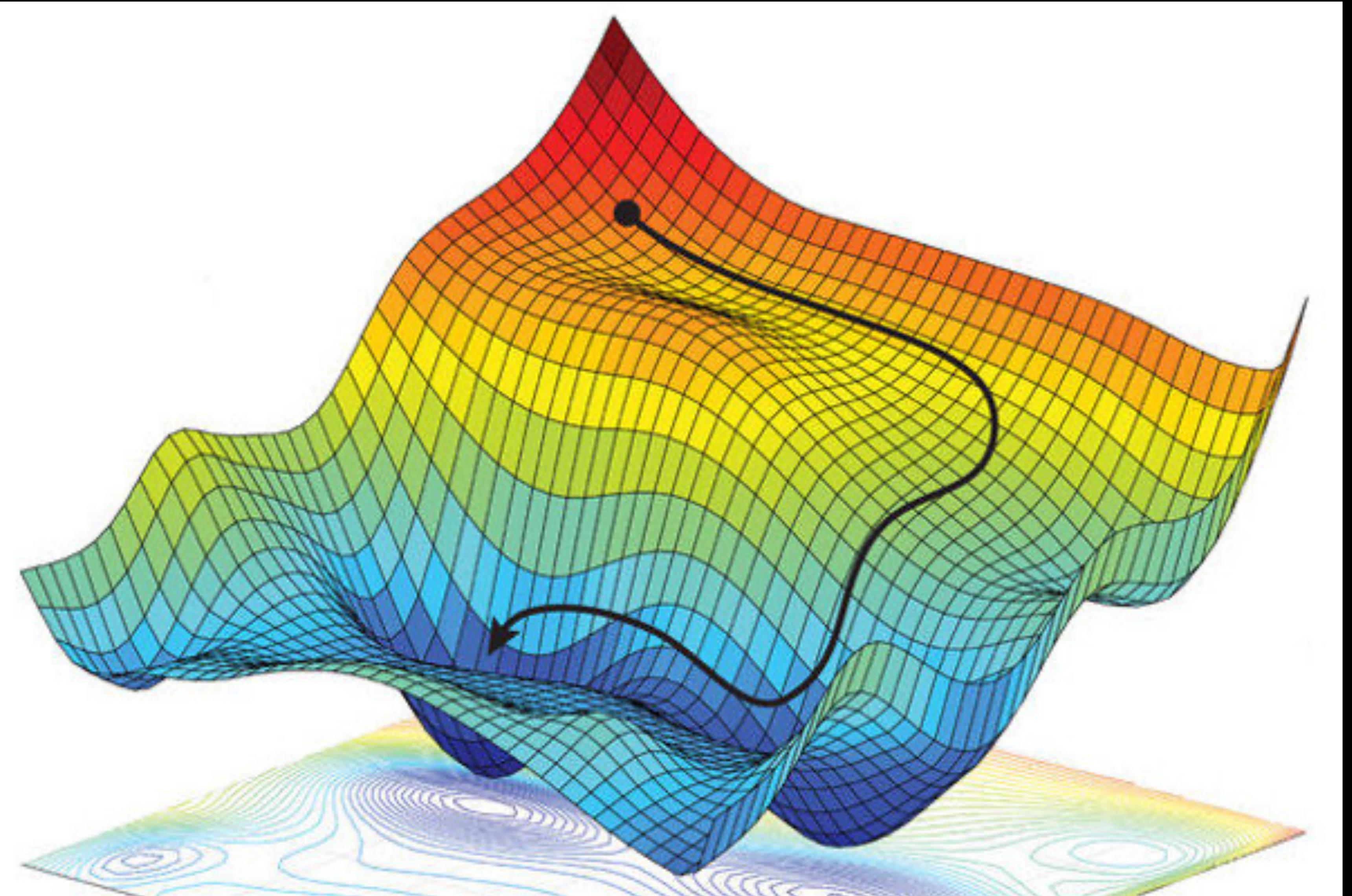
No residual connections



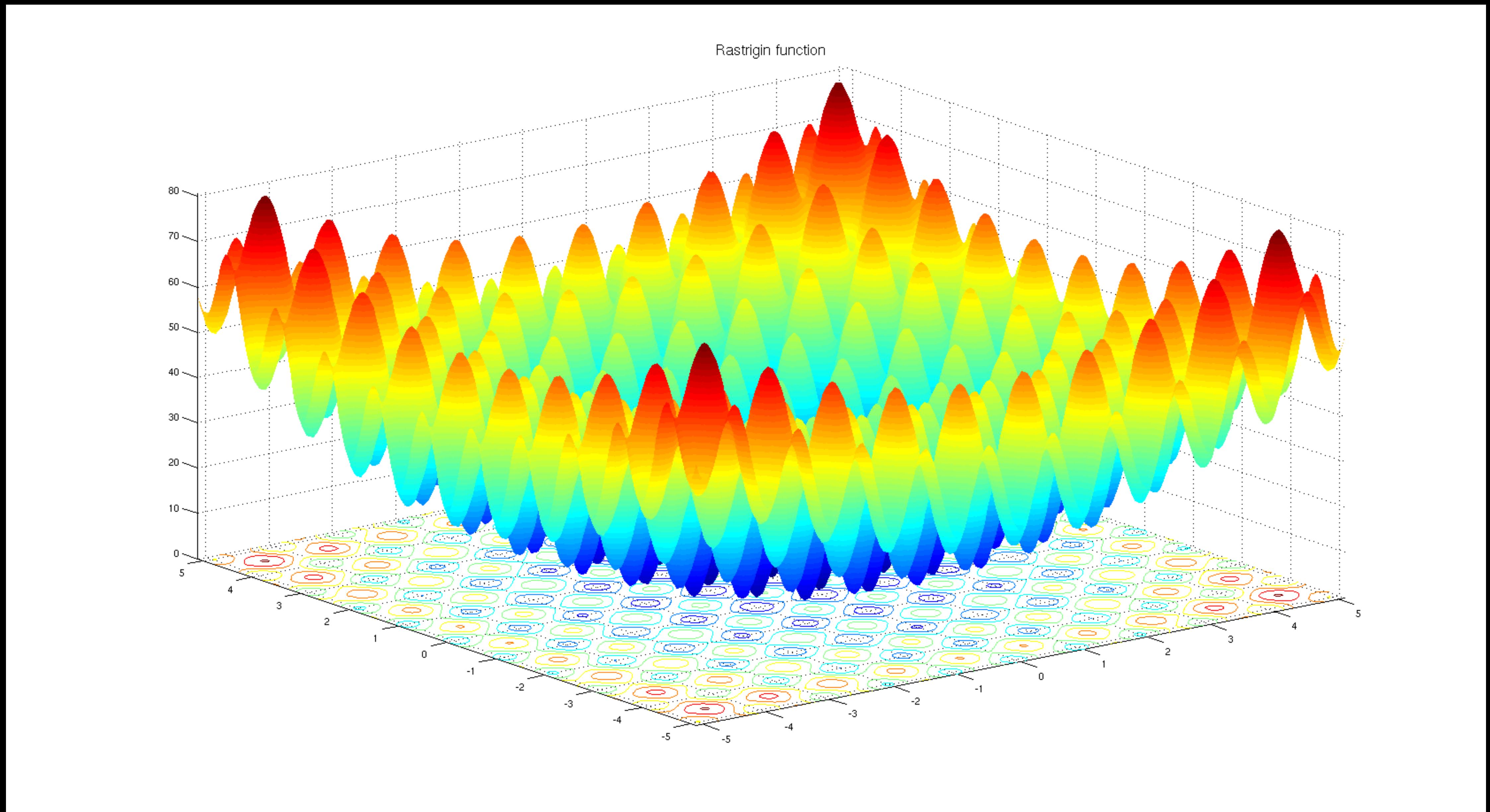
With residual connections



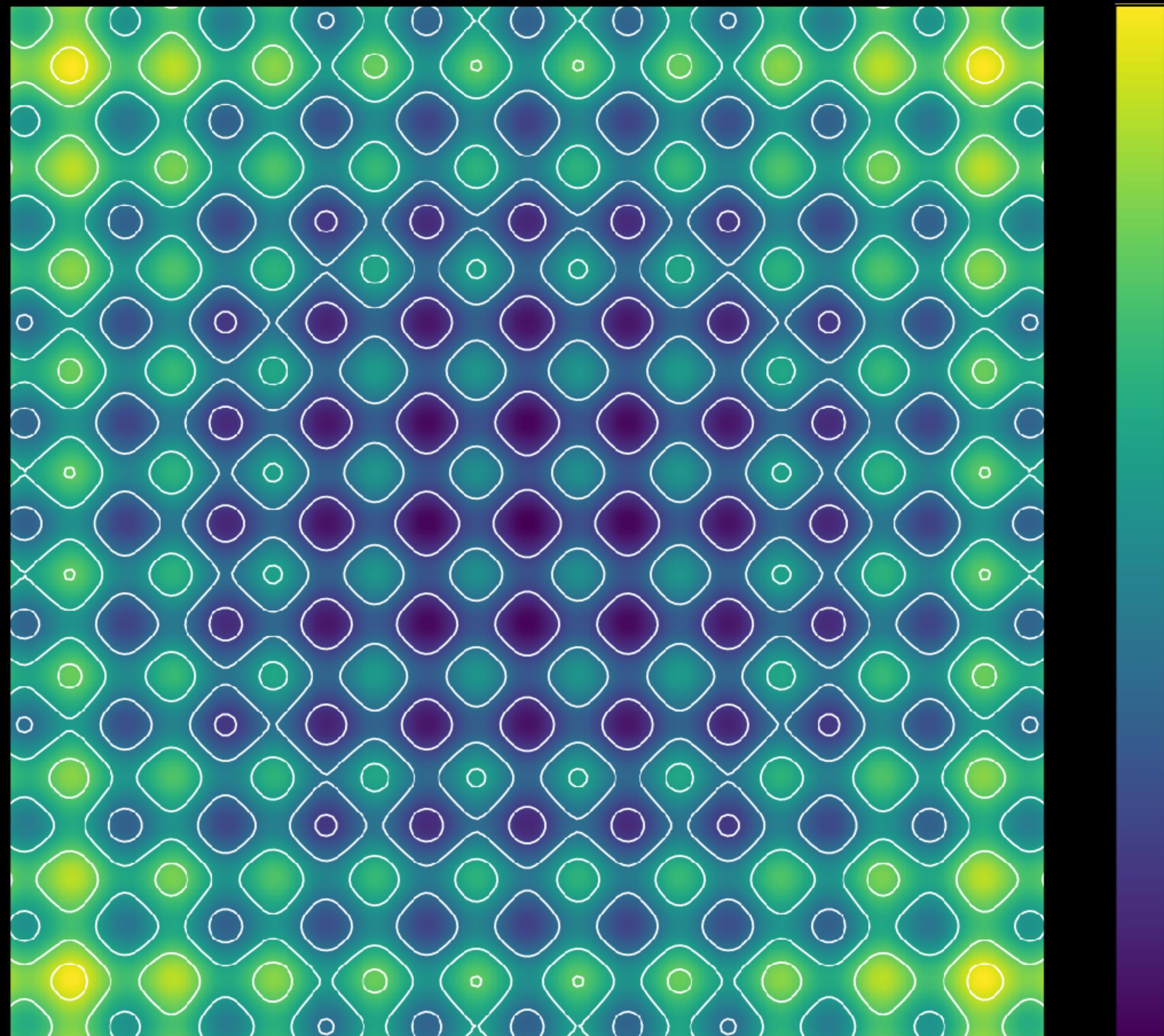
Same general network architecture



Find the minimum without getting stuck



Rastrigin function



Rastrigin function

# Search space size

Let's say you want to hypertune:

- Linear units (between 16 and 256)
- Depth of linear layers (between 1 and 10)
- Convolution filters (between 16 and 64)
- kernel size (between 3 and 5)
- dropout (4 options)
- depth of convolutions (between 1 and 5)
- learning rate (4 options)
- optimizers (3 options)
- activation functions (3 options)
- batchsize (between 16 and 128)

Can you calculate how big the search space is?

# Search space size

- $256 \times 10 \times 64 \times 3 \times 4 \times 5 \times 4 \times 3 \times 3 \times 128$

# Search space size

- $256 \times 10 \times 64 \times 3 \times 4 \times 5 \times 4 \times 3 \times 3 \times 128$
- 45.298.483.200

# Search space size

- $256 \times 10 \times 64 \times 3 \times 4 \times 5 \times 4 \times 3 \times 3 \times 128$
- 45.298.483.200
- $4.5 \times 10^{10}$

# Search space size

- $256 \times 10 \times 64 \times 3 \times 4 \times 5 \times 4 \times 3 \times 3 \times 128$
- 45.298.483.200
- $4.5 \times 10^{10}$  with 3 minutes per test

# Search space size

- $256 \times 10 \times 64 \times 3 \times 4 \times 5 \times 4 \times 3 \times 3 \times 128$
- 45.298.483.200
- $4.5 \times 10^{10}$  with 3 minutes per test
- about  $1.3 \times 10^{11}$  minutes

# Search space size

- $256 \times 10 \times 64 \times 3 \times 4 \times 5 \times 4 \times 3 \times 3 \times 128$
- 45.298.483.200
- $4.5 \times 10^{10}$  with 3 minutes per test
- about  $1.3 \times 10^{11}$  minutes
- about 258.000 years

# The curse of dimensionality

The search space has about  $4.5 \times 10^{10}$  options. This is roughly the amount of sand when you fill your  $40m^2$  living room with 50 cm of sand.

If you test at random 50 options, you are just scanning a very small fraction of all options.

You shouldn't be surprised if the result of **random** hypertuning would be worse than the result of your manual hypertuning!

searchspace too big



# Manual search

Manual tuning is necessary to develop some intuition about complexity of models.

When encountering a problem, you will be able to make a reasonable guess:

- Have you already solved problems that are sort-of-similar?
- What are ranges of parameters you have seen working in similar complexity?
- How much time does it take / do you have to hypertune a problem?
- How do you spot learning (or a lack of it) in tensorboard?

# Manual search

When encountering a problem, it helps to have reference points:

- This problem seems more complex than MNIST, but not as complex as the flower photos;

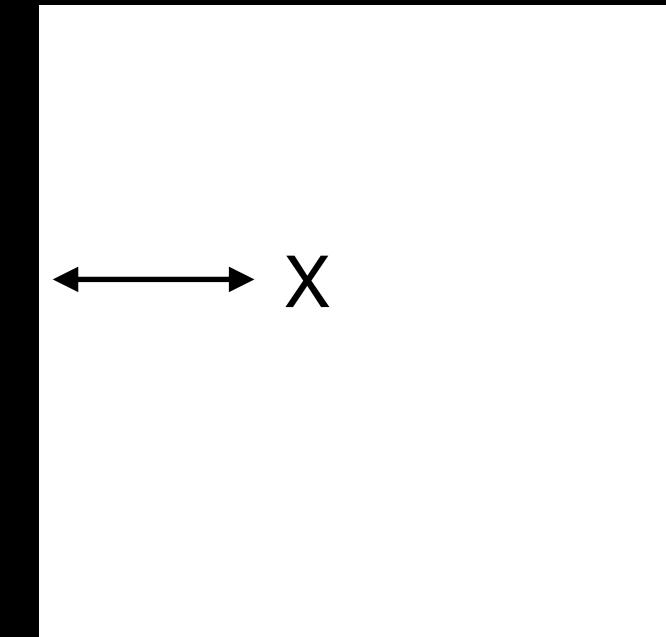
So let's start with settings somewhere between what worked for those two.

However, *after* you have an intuition, we can get the help of algorithms.

# Things behave different in high-dimensional space

Pick a random point in a  $d$ -dimensional unit square/hypercube. Let the distance from the border be  $\delta$ .

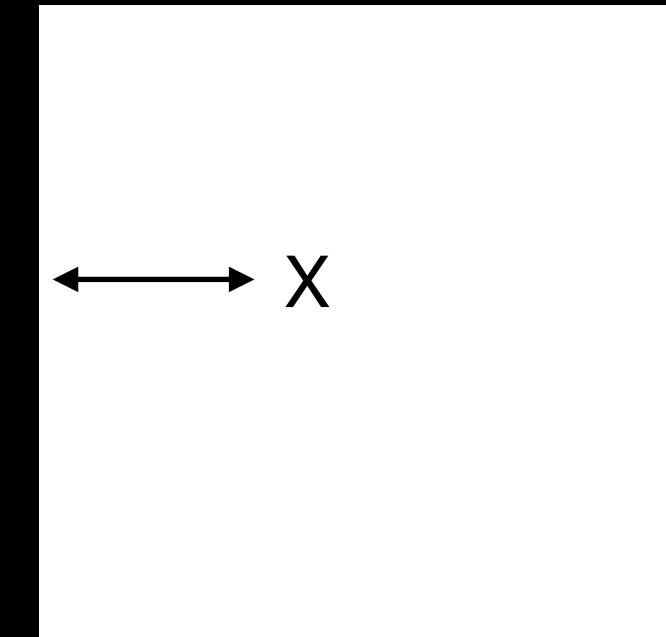
1. For  $d = 2$  (square),  $P(\delta < 0.001) =$



# Things behave different in high-dimensional space

Pick a random point in a  $d$ -dimensional unit square/hypercube. Let the distance from the border be  $\delta$ .

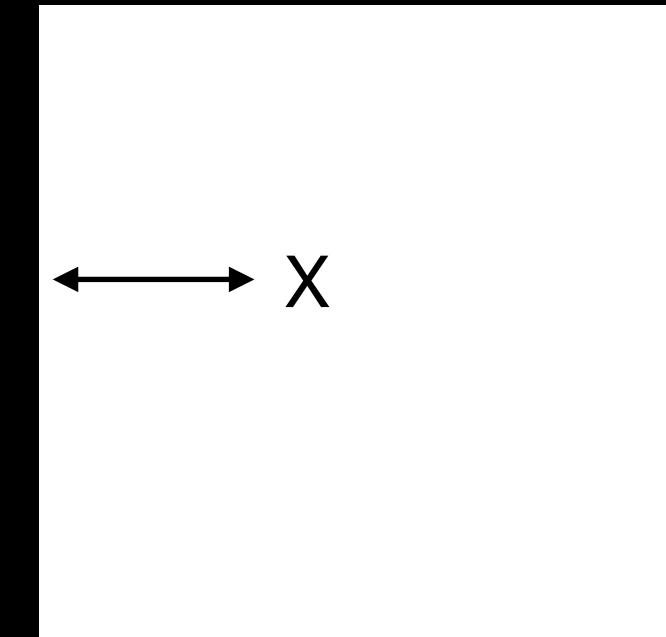
1. For  $d = 2$  (square),  $P(\delta < 0.001) = 0.004$



# Things behave different in high-dimensional space

Pick a random point in a  $d$ -dimensional unit square/hypercube. Let the distance from the border be  $\delta$ .

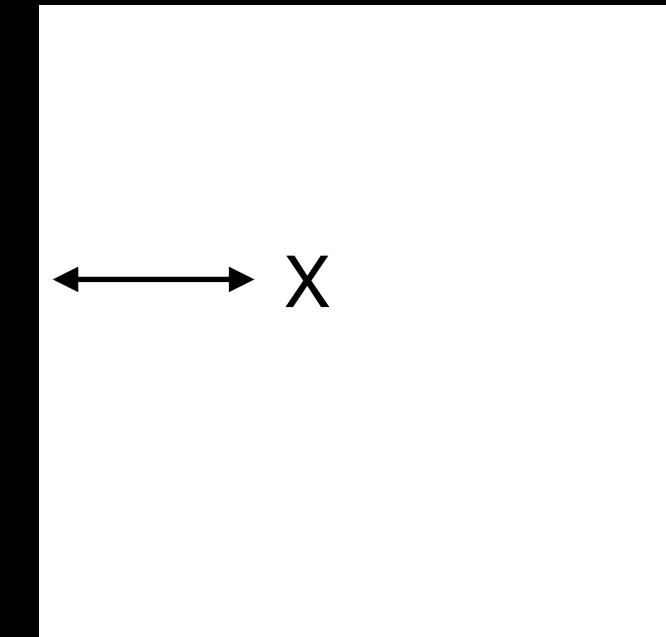
1. For  $d = 2$  (square),  $P(\delta < 0.001) = 0.004$
2. For  $d = 10,000$ ,  $P(\delta < 0.001) = ?$



# Things behave different in high-dimensional space

Pick a random point in a  $d$ -dimensional unit square/hypercube. Let the distance from the border be  $\delta$ .

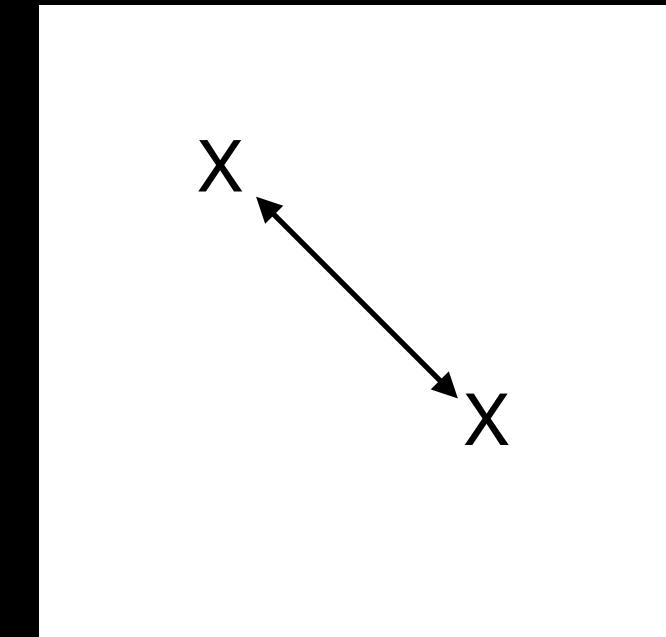
1. For  $d = 2$  (square),  $P(\delta < 0.001) = 0.004$
2. For  $d = 10,000$ ,  $P(\delta < 0.001) = 0.99999999$



# Things behave different in high-dimensional space

Pick two points randomly in a  $d$ -dimensional unit-square/cube/hypercube.

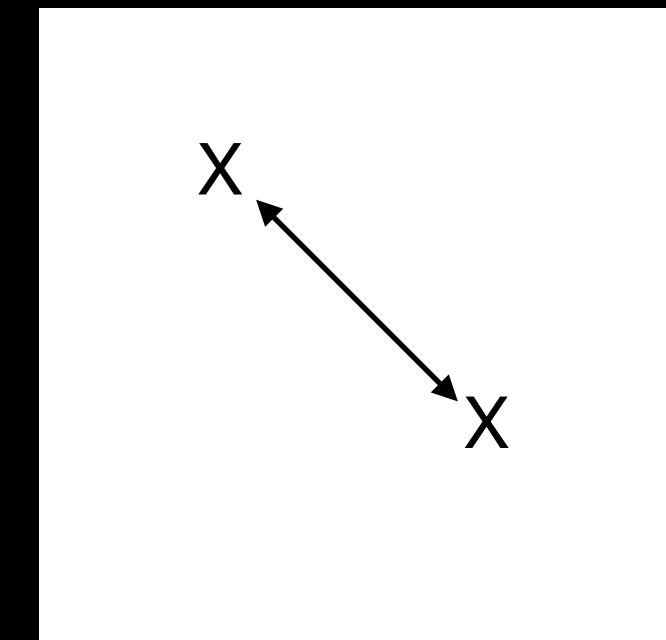
1. For  $d = 2$  (square), expected distance is 0.52



# Things behave different in high-dimensional space

Pick two points randomly in a  $d$ -dimensional unit-square/cube/hypercube.

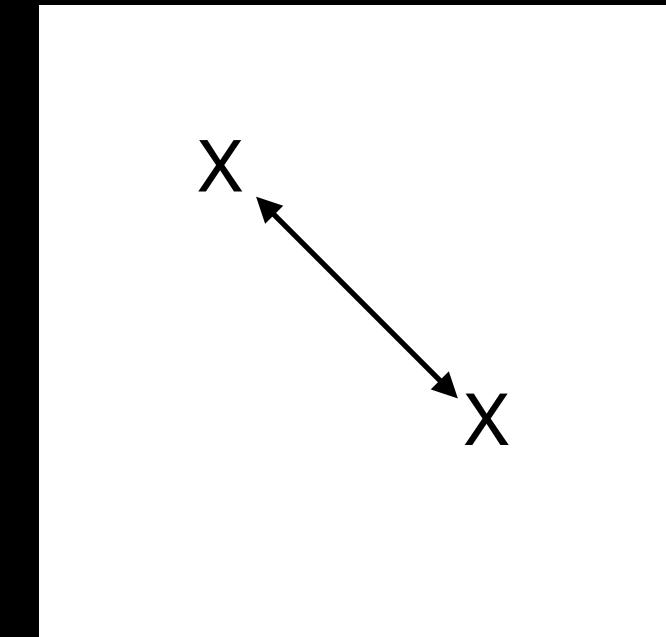
1. For  $d = 2$  (square), expected distance is 0.52
2. For  $d = 3$  (cube), expected distance is 0.66



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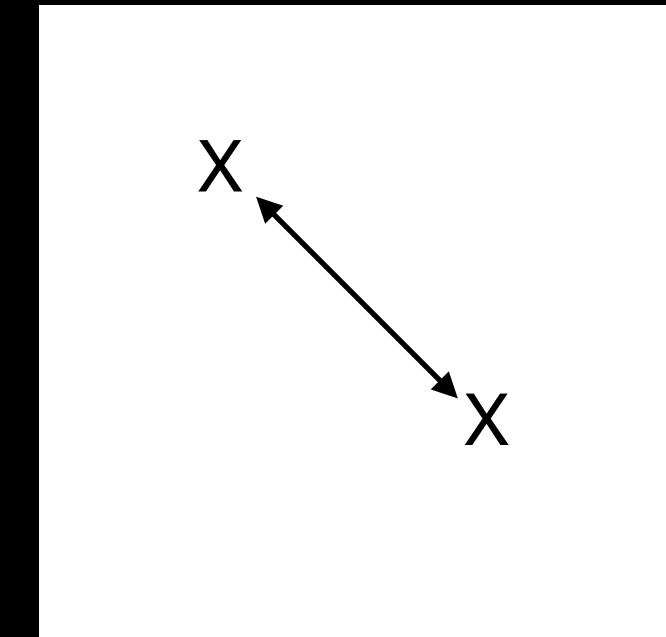
1. For  $d = 2$  (square), expected distance is 0.52
2. For  $d = 3$  (cube), expected distance is 0.66
3. For  $d = 1,000,000$ , expected distance is ?



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3. For  $d = 1,000,000$ , expected distance is 408.25



# Hypertuning

- Manual tuning helps you to restrict your hyperparameter search
- Combined with your theoretical knowledge,
- you will be able to use hypertuning at scale with an algorithm

# Tuning frameworks

## Algorithms for tuning algorithms

- we will use [Ray tune](#)
- [HyperOpt](#) is another alternative
- You want a framework that is agnostic to ML frameworks; this way you dont have to switch if your framework changes.
- Ray offers parallel computing, also for training, data preprocessing, etc.



	HyperOpt	Optuna	Keras-Tuner	HpBandSter	Tune
Distributed Execution	✓	✓	□	✓	✓
Fault Tolerance	□	□	□	□	✓
Search algorithms	2	4	3	3	6
Framework Support (TF/Keras, Sklearn, PyTorch)	✓	✓	□	□	✓

# Keeping track

There are a lot of ways to keep track of your experiments.

- **tomlserializer**: uses small toml files to log your hyperparameters
- **TensorBoard**: integrated in vscode, nice to have fast feedback on your manual hypertuning
- **MLflow**: database and dashboard, ready for production
- **Ray**: An open source framework to build and scale (distributed) ML: batch inference, model training, hyperparameter tuning, model serving.

# Hypertune algorithms

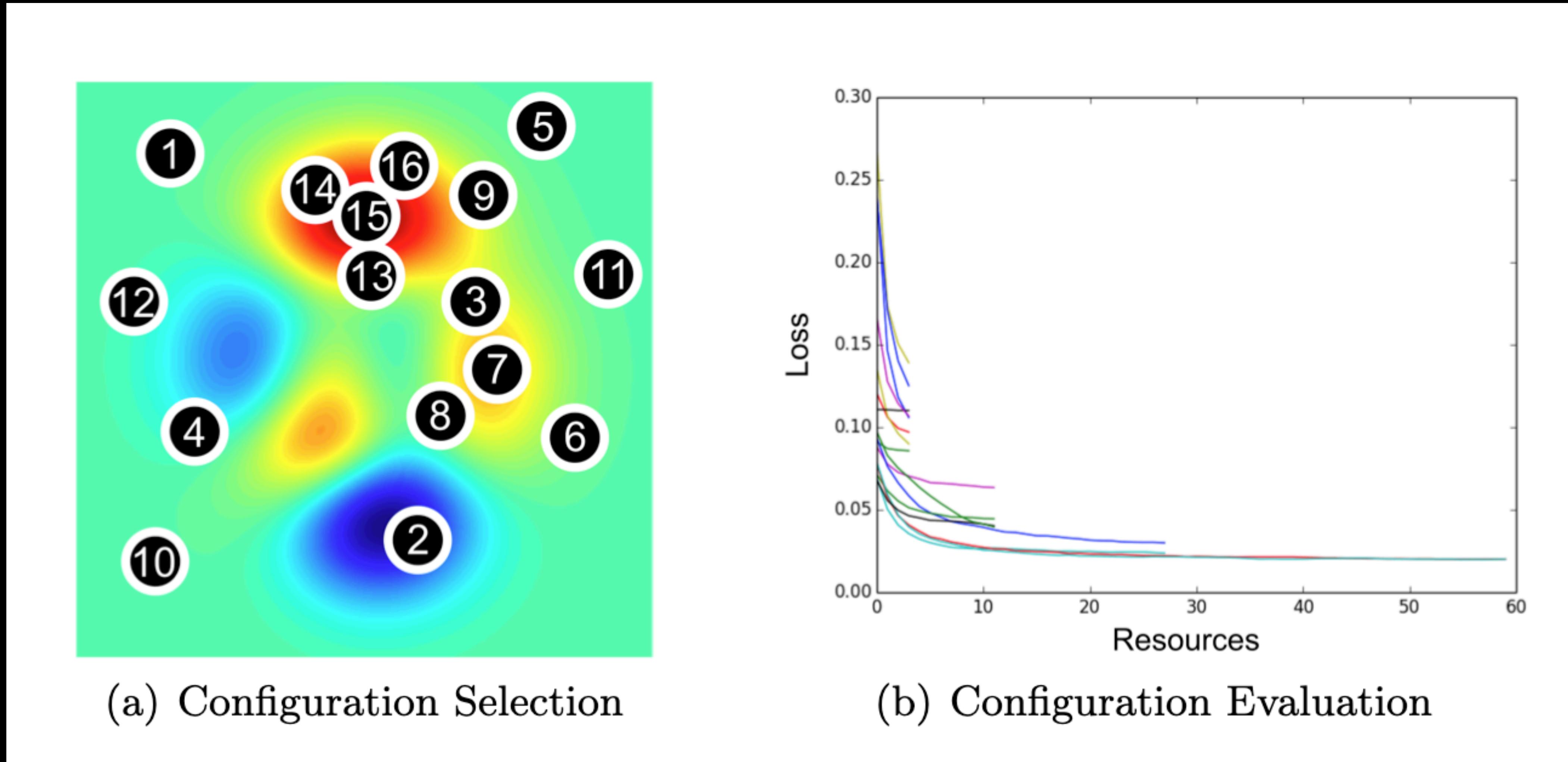
- bayesian search
- hyperband



Baysian: how high is the probability that you find value in this area?



Hyperband: only the best performing configurations stay in the game



Baysian

Hyperband

# Hypertune algorithms

- bayesian search
- hyperband
- Bayesian Optimization and Hyperband (BOHB) combines bayesian & hyperband techniques.

# Hypertune algorithms

- bayesian search
- hyperband
- Bayesian Optimization and Hyperband (BOHB)
- Tree Parzen Estimators (bayesian optimization over awkward search spaces with real, discrete and conditional parameters)
- PSO: Particle Swarm Optimization, swarm intelligence for difficult loss surfaces (eg rastrigin). Can be used via ray with NevergradSearch

Table III  
RESULT OF BENCHMARK-I

Dataset	Method	Score	Time
dna	HyperOpt Random	0.9538178	366
	HyperOpt TPE	0.9579369	322
	Optuna Random	0.9580583	94
	Optuna TPE	0.9602619	521
	Optunity PSO	0.925369	200
	SMAC	0.9595218	807
electricity	HyperOpt Random	0.6969229	546
	HyperOpt TPE	0.7011213	341
	Optuna Random	0.6942903	494
	Optuna TPE	0.7011213	167
	Optunity PSO	0.9074971	190
	SMAC	0.7011213	393
gas drift	HyperOpt Random	0.850121	23869
	HyperOpt TPE	0.88168	14105
	Optuna Random	0.868639	14549
	Optuna TPE	0.882114	4403
	Optunity PSO	0.982105	11923
	SMAC	0.825001	12966
nomao	HyperOpt Random	0.926516	1711
	HyperOpt TPE	0.931569	1441
	Optuna Random	0.93677	1064
	Optuna TPE	0.937144	1124
	Optunity PSO	0.938943	1554
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	Optuna Random	0.982508	336
	Optuna TPE	0.983886	897
	Optunity PSO	0.958028	2980
	SMAC	0.984226	860
semeion	HyperOpt Random	0.901575	762
	HyperOpt TPE	0.915246	458
	Optuna Random	0.92832	895
	Optuna TPE	0.934616	1989
	Optunity PSO	0.700295	538
	SMAC	0.929794	1647

Table IV  
CONFIGURATION SPACE FOR MLP TUNING. THE TYPE, NATURE OF SEARCH SPACE AND THE RANGE OF VALUES FOR SEARCHING ARE GIVEN AS COLUMNS.

Hyper-parameter	Type	Space	Range
hidden layer size	integer	linear	(50, 200)
alpha	real	log	( $10^{-5}$ , 10)
batch size	integer	linear	(10, 250)
learning rate	real	log	( $10^{-5}$ , $10^{-1}$ )
tolerance	real	log	( $10^{-5}$ , $10^{-1}$ )
validation fraction	real	real	(0.1, 0.9)
beta 1	real	logit	(0.5, 0.99)
beta 2	real	logit	(0.9, 1.0- $10^{-6}$ )
epsilon	real	log	( $10^{-9}$ , $10^{-6}$ )

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lowest

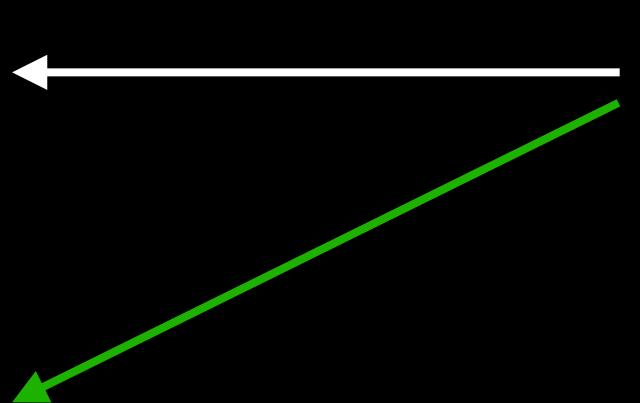
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← Slowest

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Highest

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← Fastest

No free lunch theorem:  
if an algorithm performs well on a certain class of problems  
then it necessarily has degraded performance on all the  
remaining problems

# Learning rate schedulers

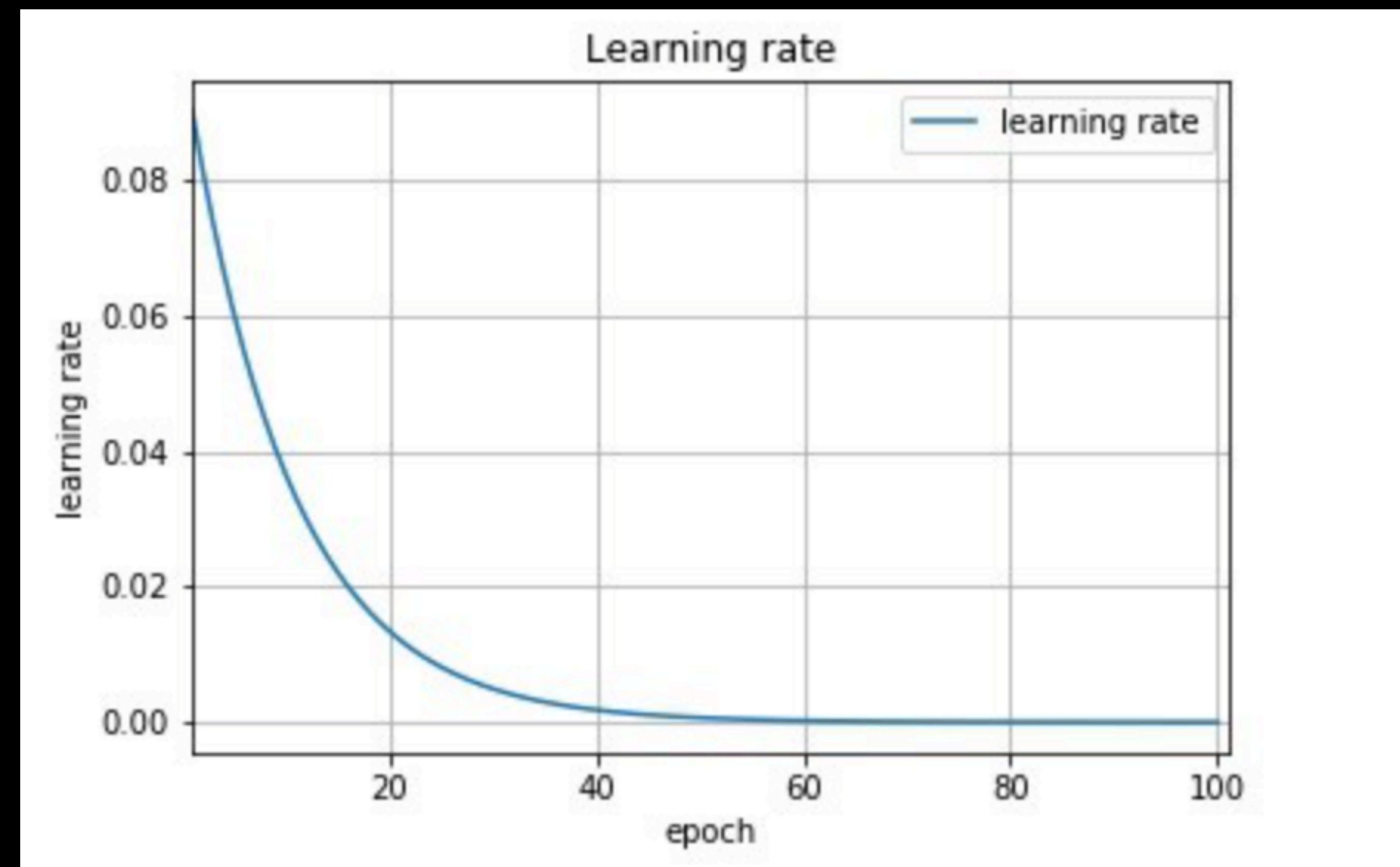
# Learning rate schedulers

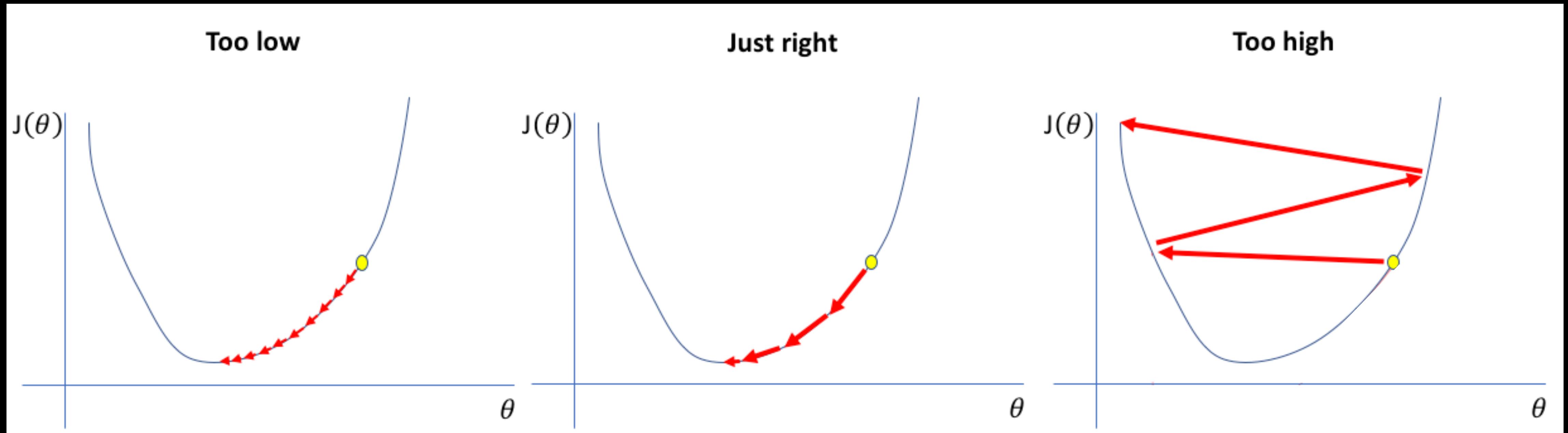
The learning rate  $\eta$  tells how fast weights are adjusted

$$W_{t+1} \leftarrow W_t - \eta \times \text{gradient}$$

The learning rate can be compared to different sizes of tools to carve wood. Big tools go fast, but miss the details.

So, often a decay of the learning rate is a good idea.

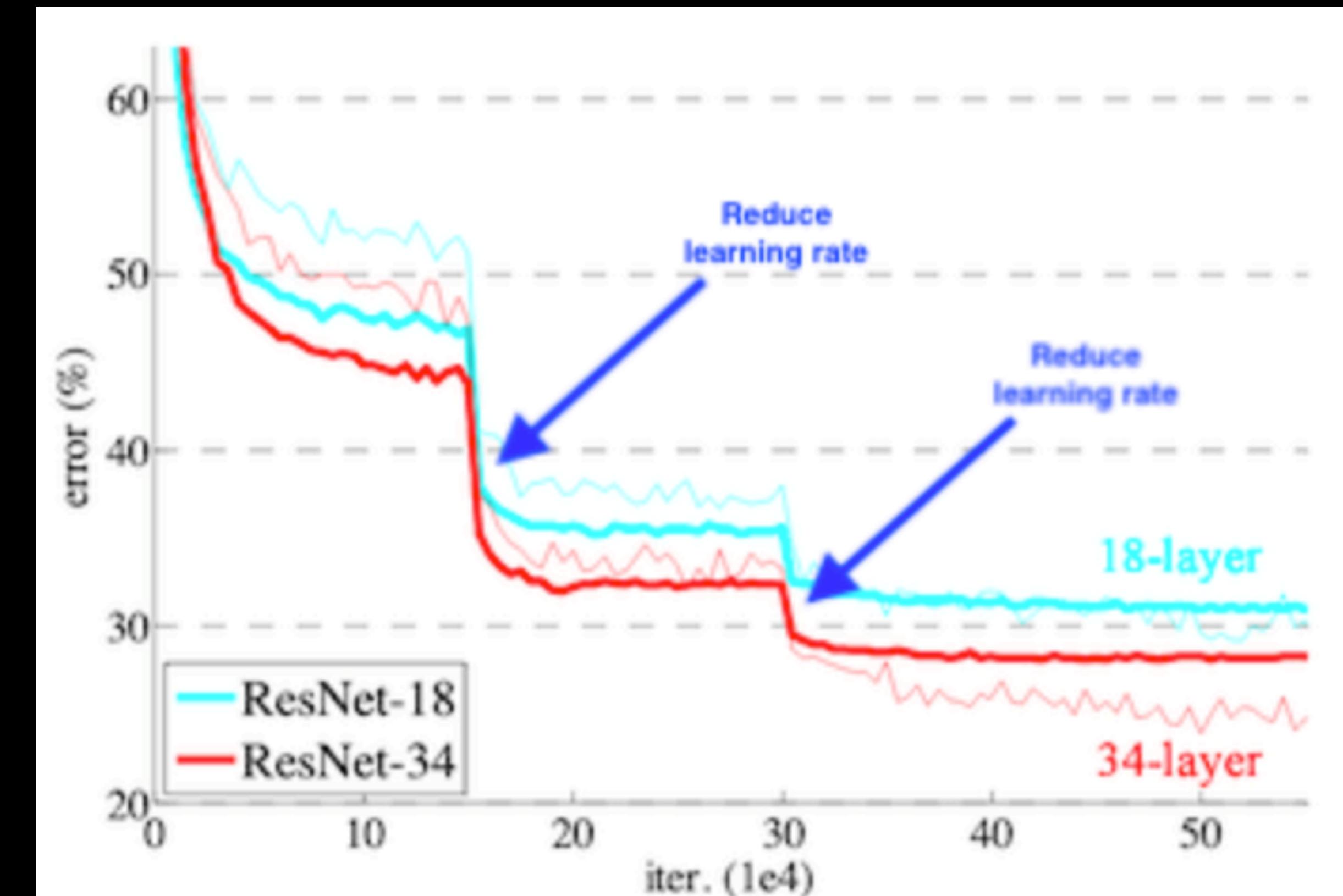




# Learning rate schedulers

ResNet can be trained for very long. From the paper:

*“The learning rate starts from 0.1 and is divided by 10 when the error plateaus, and the models are trained for up to  $60 \times 10^4$  iterations”*

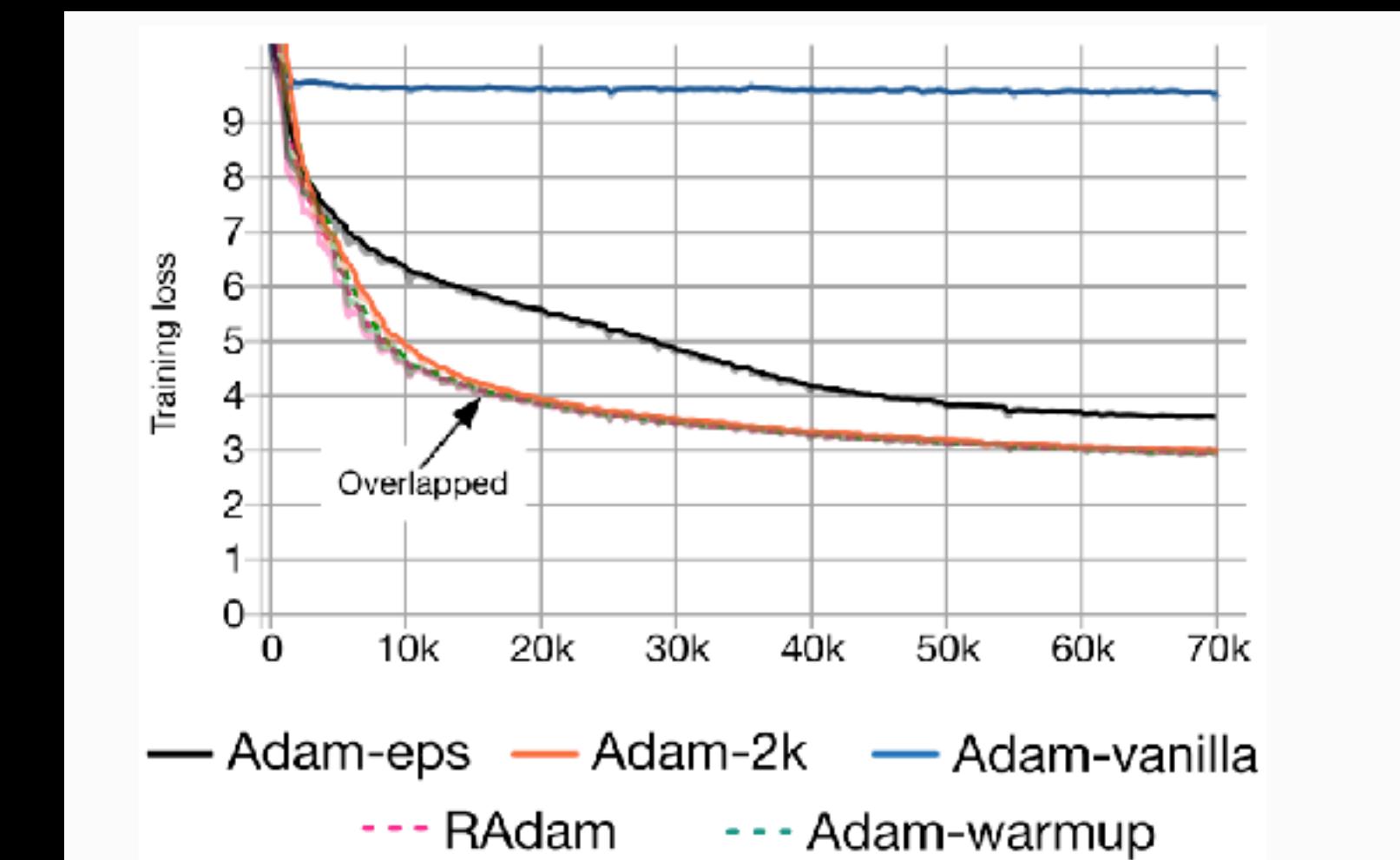
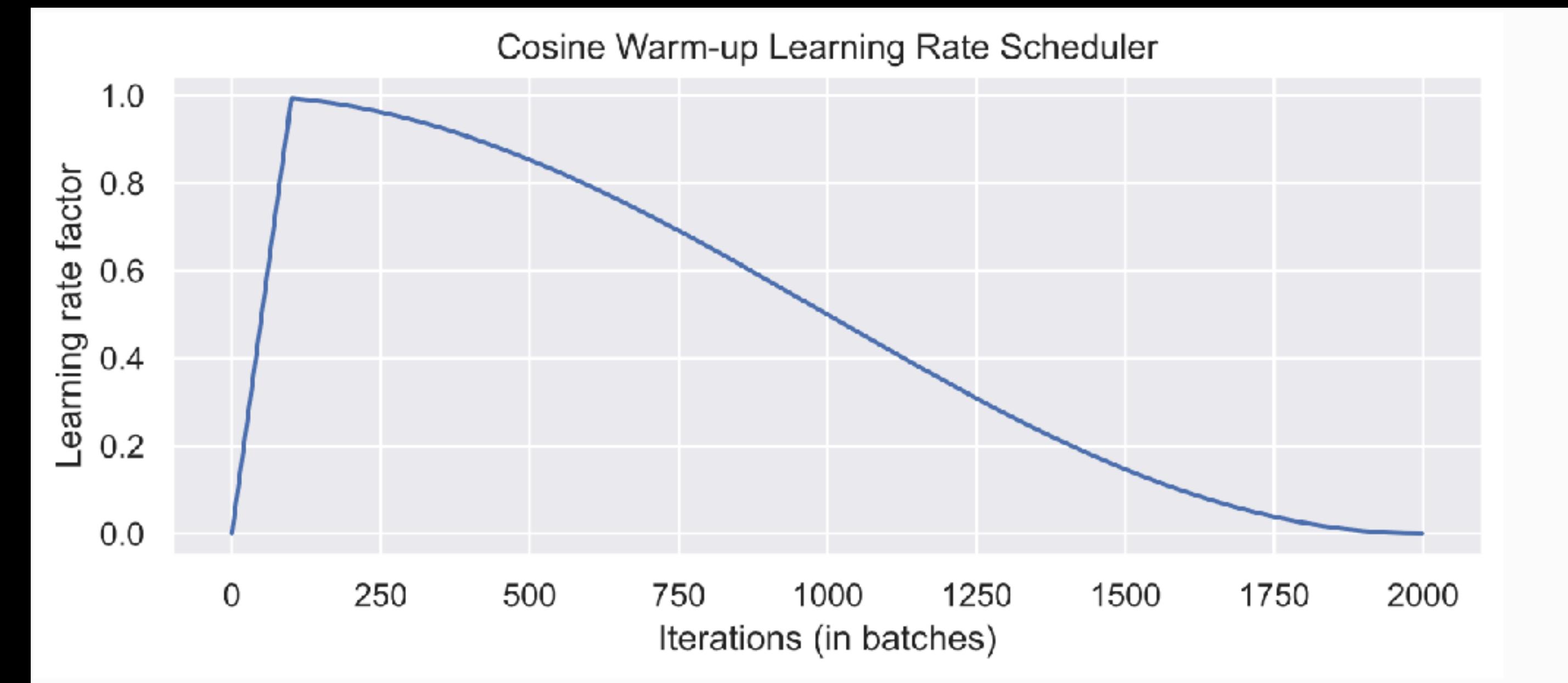


# Learning rate schedulers

The first iterations can have very high gradients, and could “lock” the model in the wrong direction.

A solution is to gradually increase the learning rate from 0 on to the originally specified learning rate in the first few iterations.

This is typically used with transformer architectures.



```
10d, 7 months ago | 3 authors (R.Grouis and others)
class Trainer:
    def __init__(
        self,
        model: torch.nn.Module,
        settings: TrainerSettings,
        loss_fn: Callable,
        optimizer: Type[Optimizer],
        traindataloader: Iterator,
        validdataloader: Iterator,
        scheduler: Optional[Callable],
        device: Optional[str] = None,
    ) -> None:
        self.model = model
        self.settings = settings
        self.loss_fn = loss_fn
        self.optimizer = optimizer
        self.traindataloader = traindataloader
        self.validdataloader = validdataloader
        self.scheduler = scheduler
        self.device = device
```

```
        if scheduler:
            if settings.scheduler_kwargs is None:
                raise ValueError("Missing 'scheduler_kwargs' in TrainerSettings.")
            self.scheduler = scheduler(self.optimizer, **settings.scheduler_kwargs)
        else:
            self.scheduler = None
```