LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

Deeplearning

Chapter 2: Regularization

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Winter term 2018

REVISION OF OVERFITTING

- A model finds a pattern in the data that is actually not true in the real world. That means the model **overfits** the data.
  - Humans also overfit when they overgeneralize from an incomplete picture of the world.
  - Every powerful model can “hallucinate” patterns.
- Happens when you have too many hypotheses and not enough data to tell them apart.
  - The more data, the more “bad” hypotheses are eliminated.
  - If the hypothesis space is not constrained, there may never be enough data.
  - There is often a parameter that allows you to constrain (**regularize**) the model.

AVOIDING OVERFITTING

- You should never believe your model until you've *verified it on data that it didn't see*.
- Scientific method applied to machine learning: model must make new predictions that can be experimentally verified.
- Randomly divide the data into:
  - *Training set* $\mathcal{D}_{\text{train}}$, which we will feed the model with.
  - *Test set* $\mathcal{D}_{\text{test}}$, which we will hide to verify its predictive performance.

OVERFITTING AND NOISE

- Overfitting is seriously exacerbated by *noise* (errors in the training data).
- An unconstrained learner will model that noise.
- A popular misconception is that overfitting is always caused by noise.
- It can also arise when relevant features are missing in the data.
- In general, it's better to make some mistakes on training data ("ignore some observations") than trying to get all correct.

TRIPLE TRADE-OFF

In all learning algorithms that are trained from example data, there is a trade-off between three factors:

- the complexity of the hypothesis we fit to data
- the amount of training data
- the generalization error on new examples

The generalization error decreases with the amount of training data. As the complexity of the hypothesis space H increases, the generalization error decreases first and then starts to increase (overfitting).

- Training error and test error evolve in the opposite direction with increasing complexity:

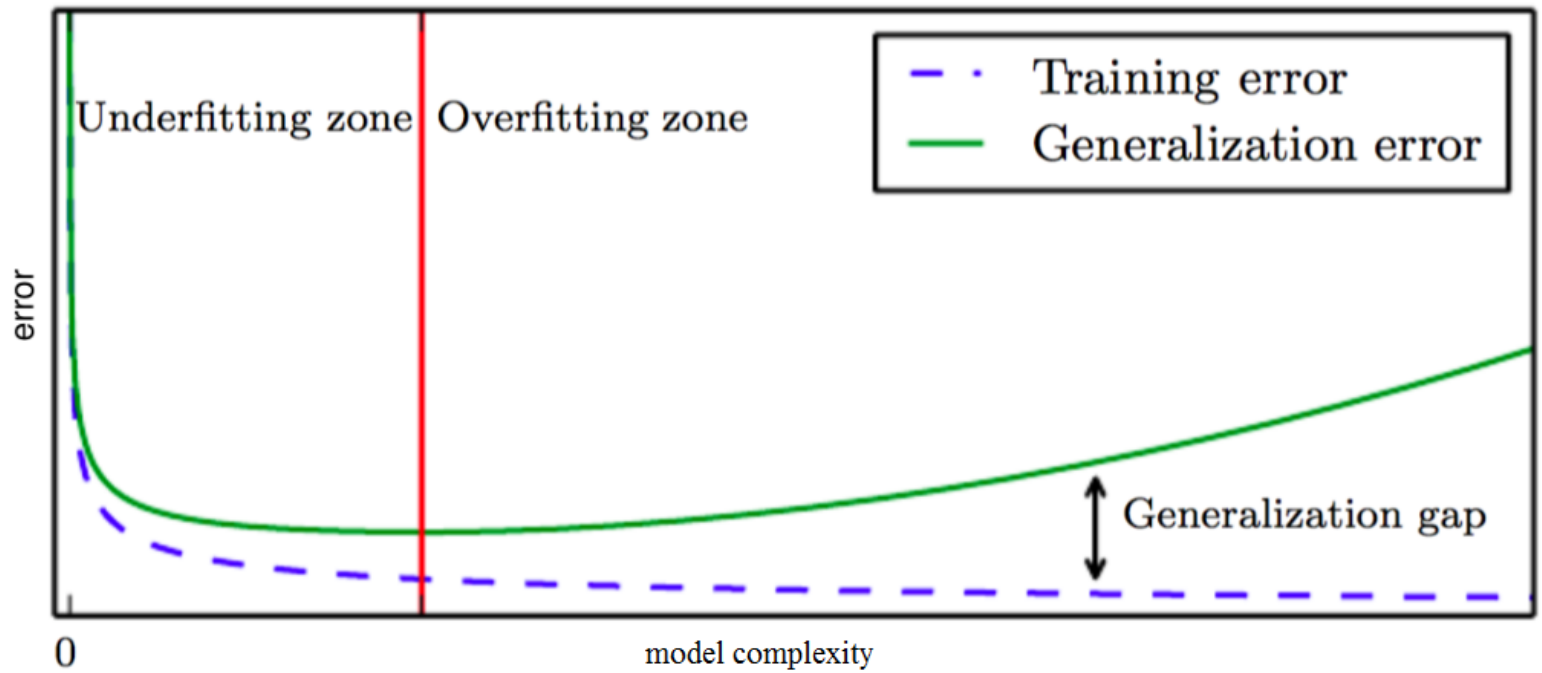


Figure: Underfitting vs. overfitting (Goodfellow et al. (2016))

$\Rightarrow$ Optimization regarding the model complexity is desirable!

GENERALIZATION ERROR

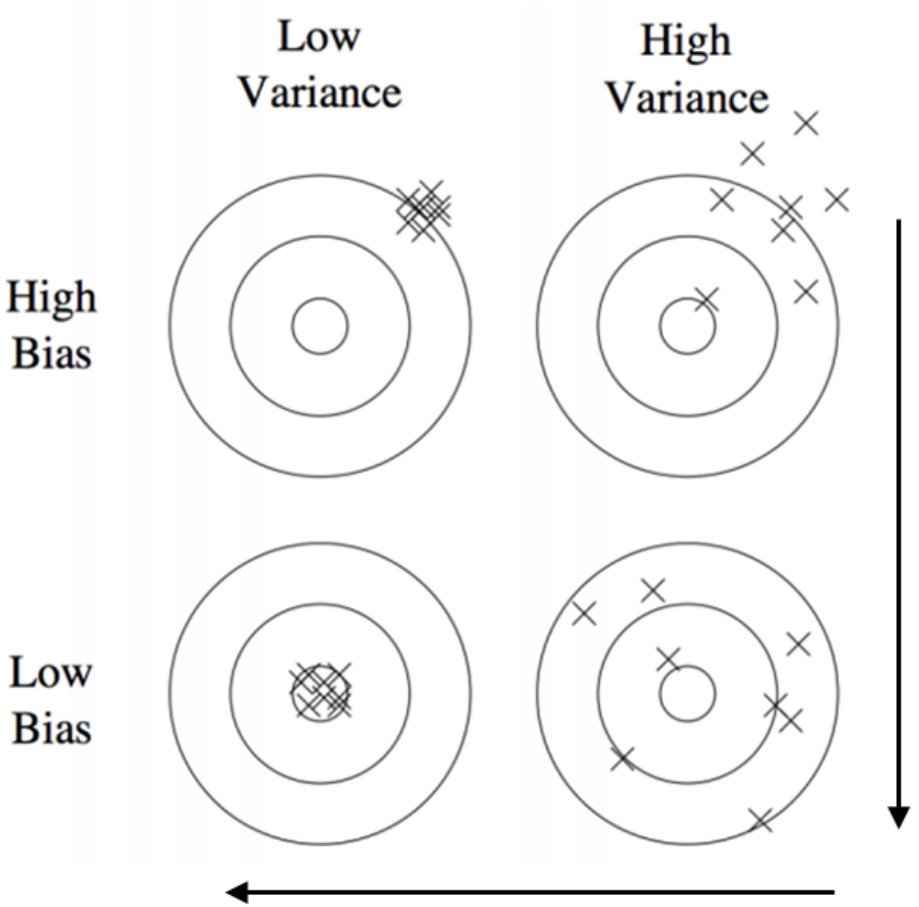
The *generalization error* is defined as the error that occurs when a model $\hat{f}_{\mathcal{D}}$ that was trained on observed data $\mathcal{D}$ is applied to (unseen) data:

$$GE(\hat{f}_{\mathcal{D}}) = \mathbb{E}(L(y, \hat{f}_{\mathcal{D}}(x))|\mathcal{D}),$$

where

- $\hat{f}_{\mathcal{D}}$ is the prediction model that was estimated using the data $\mathcal{D}$,
- the expectation is conditional on $\mathcal{D}$ that was used to build the prediction model and
- L is an *outer* loss function that tries to measure the model performance (which can be different from the *inner* loss function that was used for the empirical risk minimization).

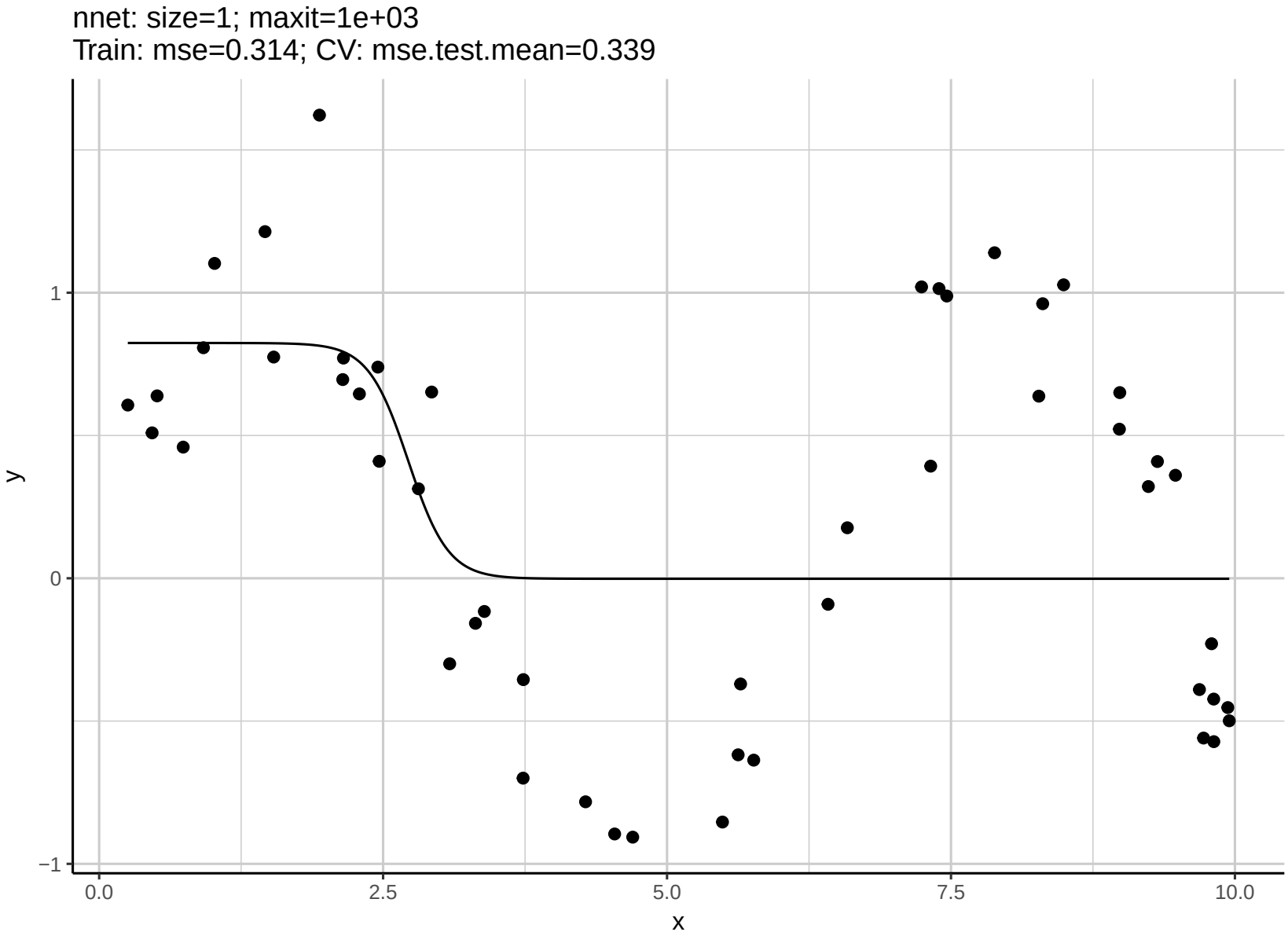
BIAS-VARIANCE DECOMPOSITION



Reduce bias
$\Rightarrow$ reduce underfitting
$\Rightarrow$ make model more flexible.

Reduce variance $\Rightarrow$ Reduce overfitting
$\Rightarrow$ make model less flexible
$\Rightarrow$ **regularization**, or add more data.

OVERFITTING IN REGRESSION



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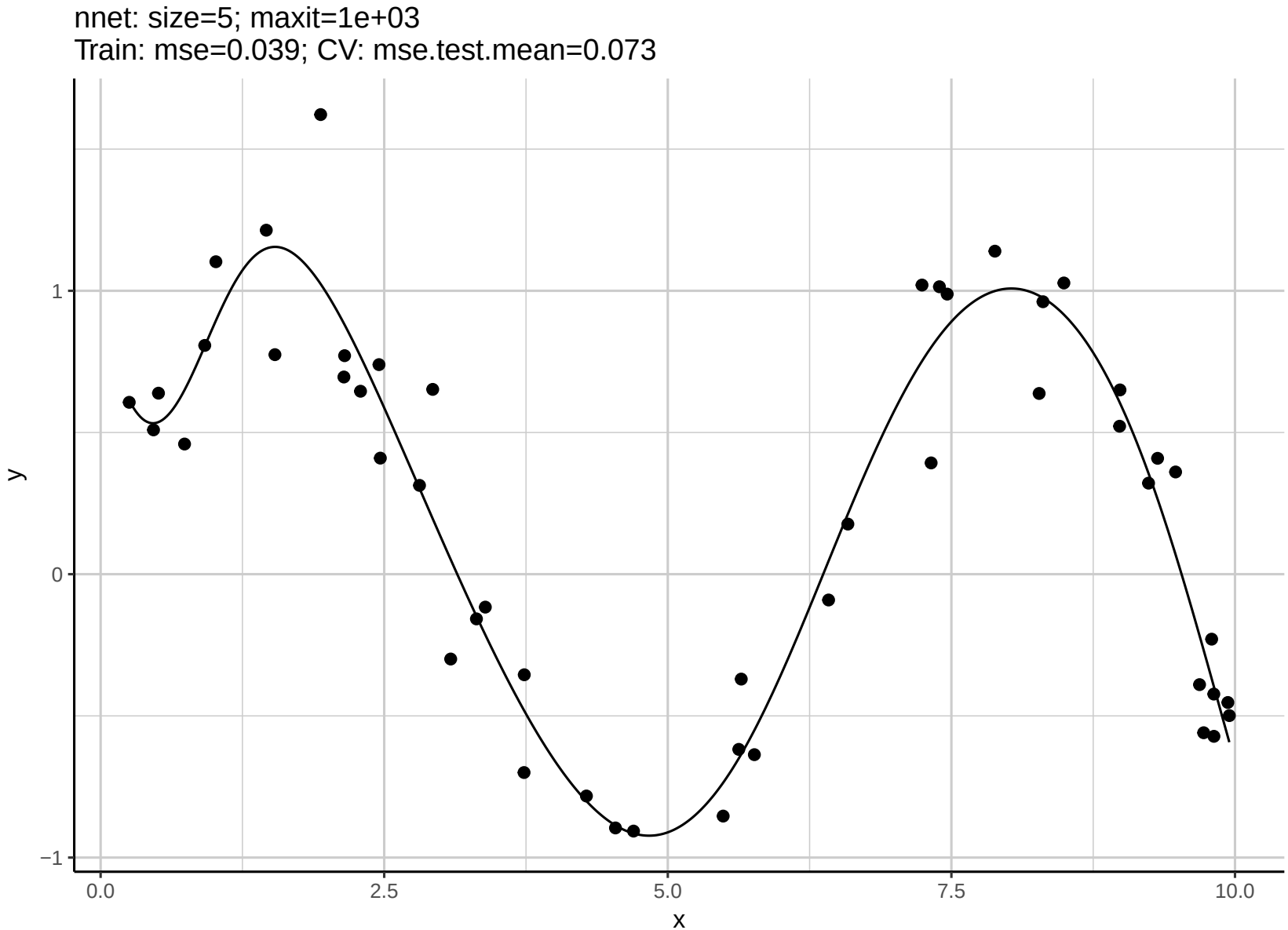
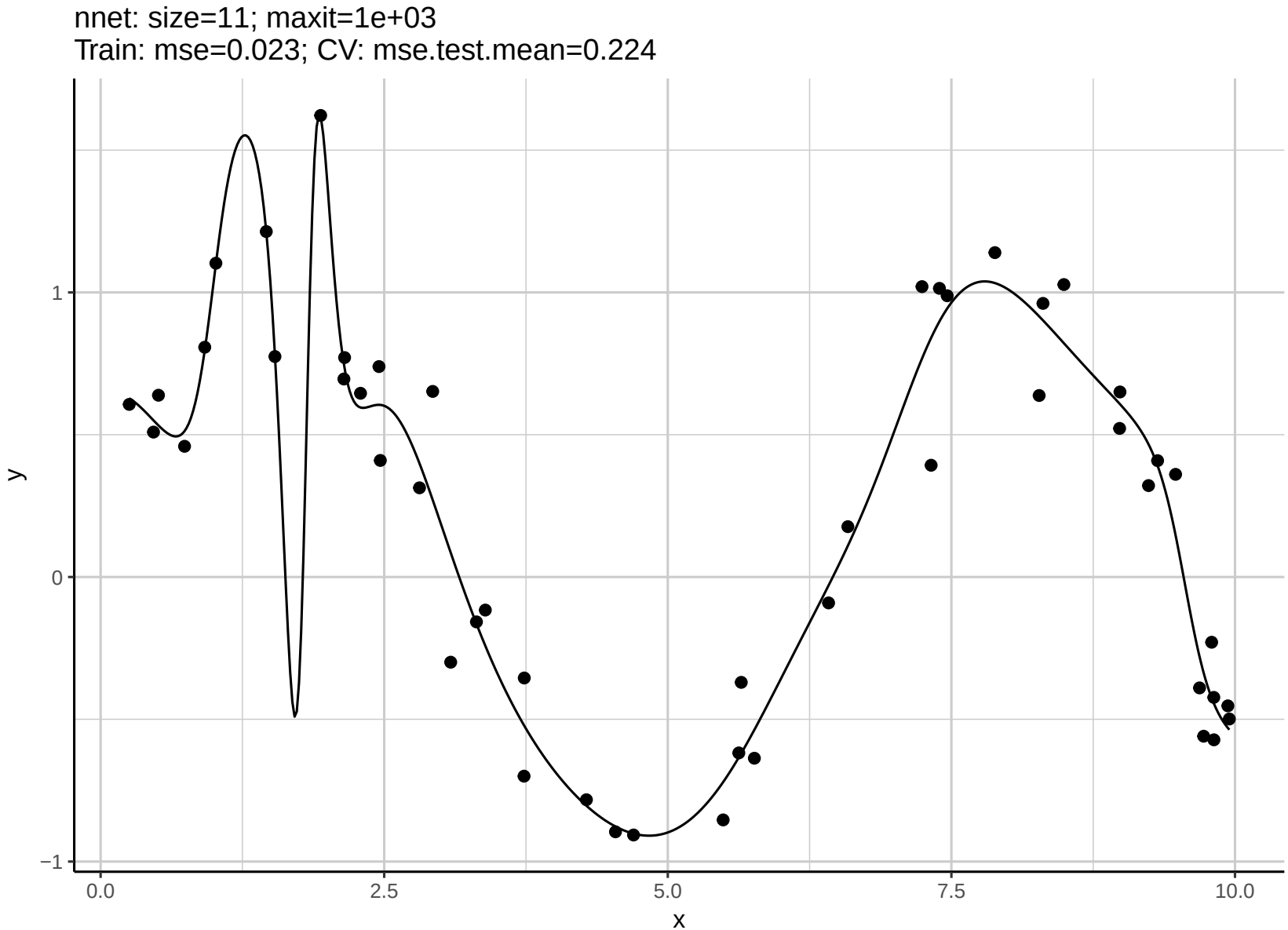
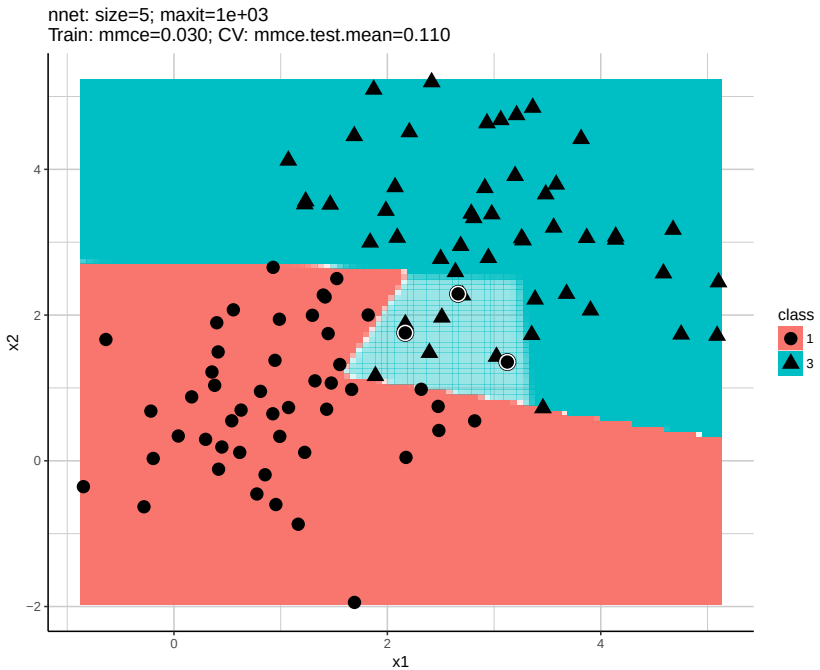


OVERFITTING IN REGRESSION



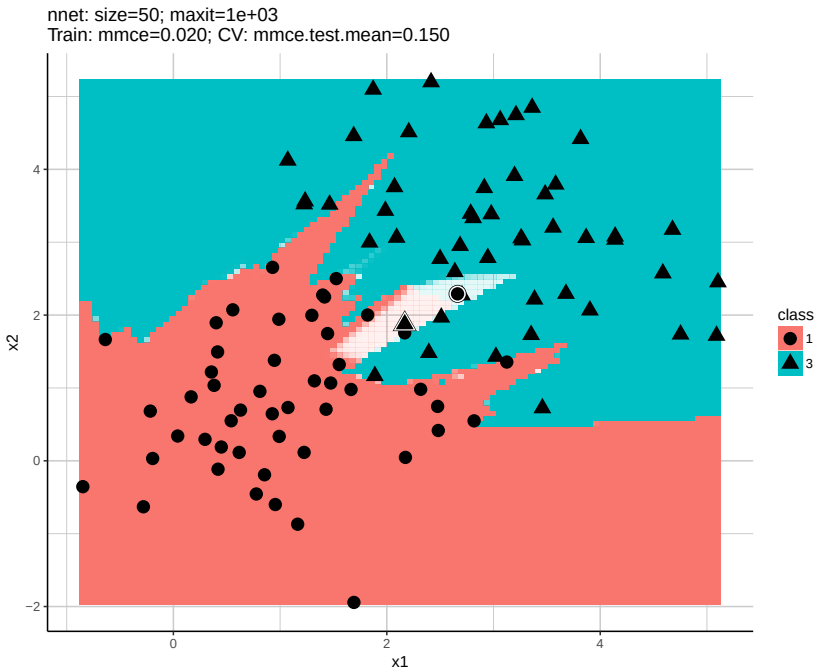
OVERFITTING IN CLASSIFICATION

- Non-overfitting model



Better test accuracy

- Overfitting model



Better training accuracy

PARAMETER NORM PENALTIES

- Norm penalization aims to limit the complexity of the model.

- Suppose we would like to regularize an objective function $R_{emp}(\theta|X, y)$, which generally is a loss function L(y, f(x)).
- By adding a parameter norm penalty term $\Omega(\theta)$, we obtain a regularized version of the objective function:

$$R_{reg}(\theta|X, y) = R_{emp}(\theta|X, y) + \lambda\Omega(\theta)$$

  with hyperparamater $\lambda \in [0, \infty)$, that weights the penalty term, relative to the unconstrained objective function $R_{emp}(\theta|X, y)$.

- Declaring $\lambda = 0$ obviously results in no penalization.
- We can choose between different parameter norm penalties $\Omega(\theta)$.

PARAMETER NORM PENALTIES

- Keep in mind, when penalizing a linear model, the parameters θ are the coefficients β.
- In neural networks, the parameters θ are the weights (e.g. w).
- In general, we do not penalize the bias.
  - Less data required for fitting the bias than for w.
  - A possible consequence of regularizing the bias is underfitting!

L2 REGULARIZATION (WEIGHT DECAY)

- Analogue to **ridge regression**: $\Omega(w) = \frac{1}{2}||w||_2^2$ such that

$$R_{reg}(w|X, y) = R_{emp}(w|X, y) + \frac{\lambda}{2} w^T w$$

with corresponding gradient:

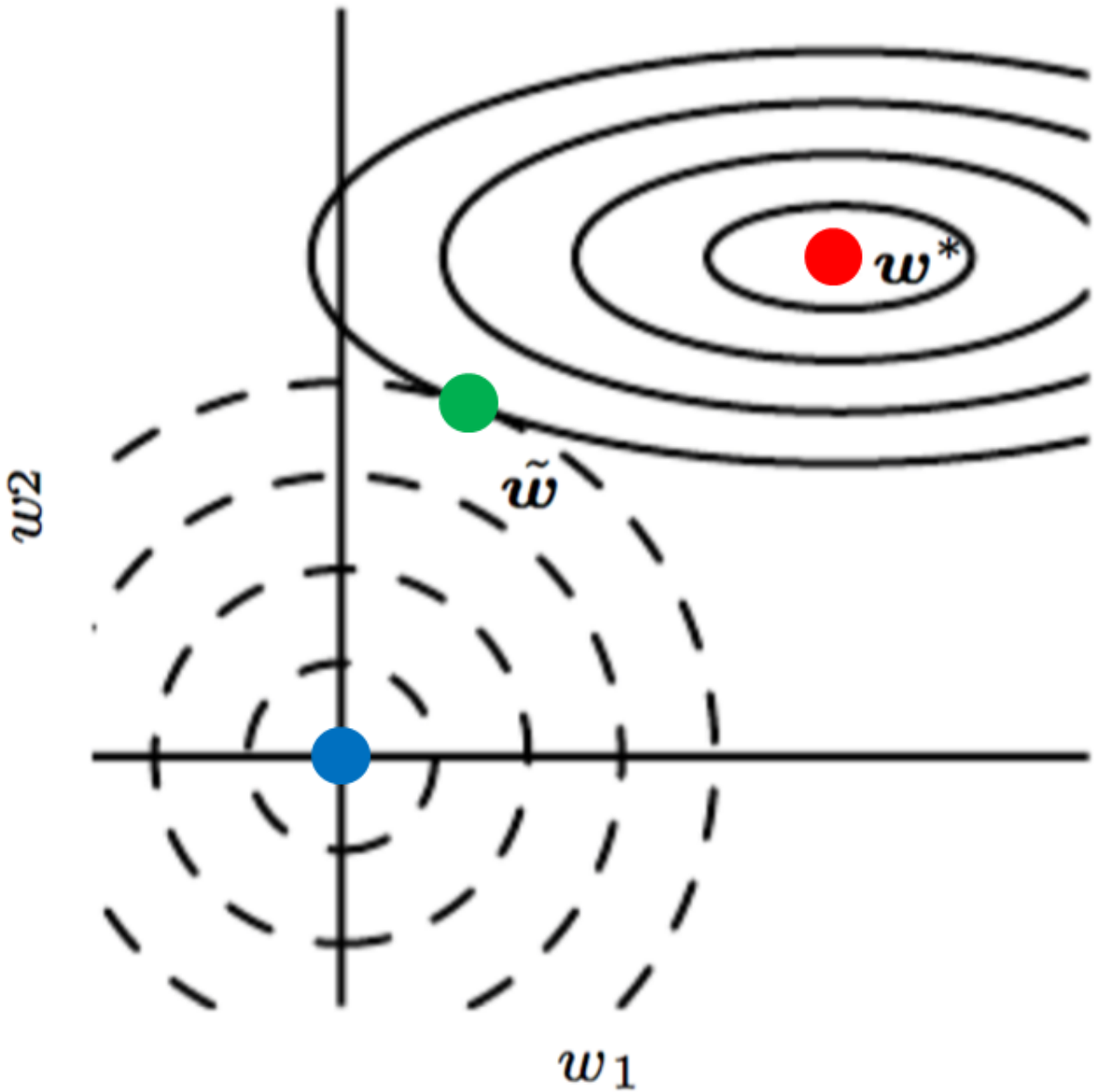
$$\nabla_w R_{reg}(w|X, y) = \nabla_w R_{emp}(w|X, y) + \lambda w$$

- One weight update using gradient descent is

$$\begin{aligned} w_{i+1} &= w_i - \alpha(\lambda w_i + \nabla_w R_{emp}(w_i|X, y)) \\ &= \underbrace{(1 - \alpha\lambda)}_{<1} w - \alpha \nabla_{w_i} R_{emp}(w_i|X, y)) \end{aligned}$$

- Therefore termed **weight decay** in neural net applications

L2 REGULARIZATION (WEIGHT DECAY)



minimize empirical risk

minimize regularized risk

minimize penalty

WEIGHT DECAY EXAMPLE

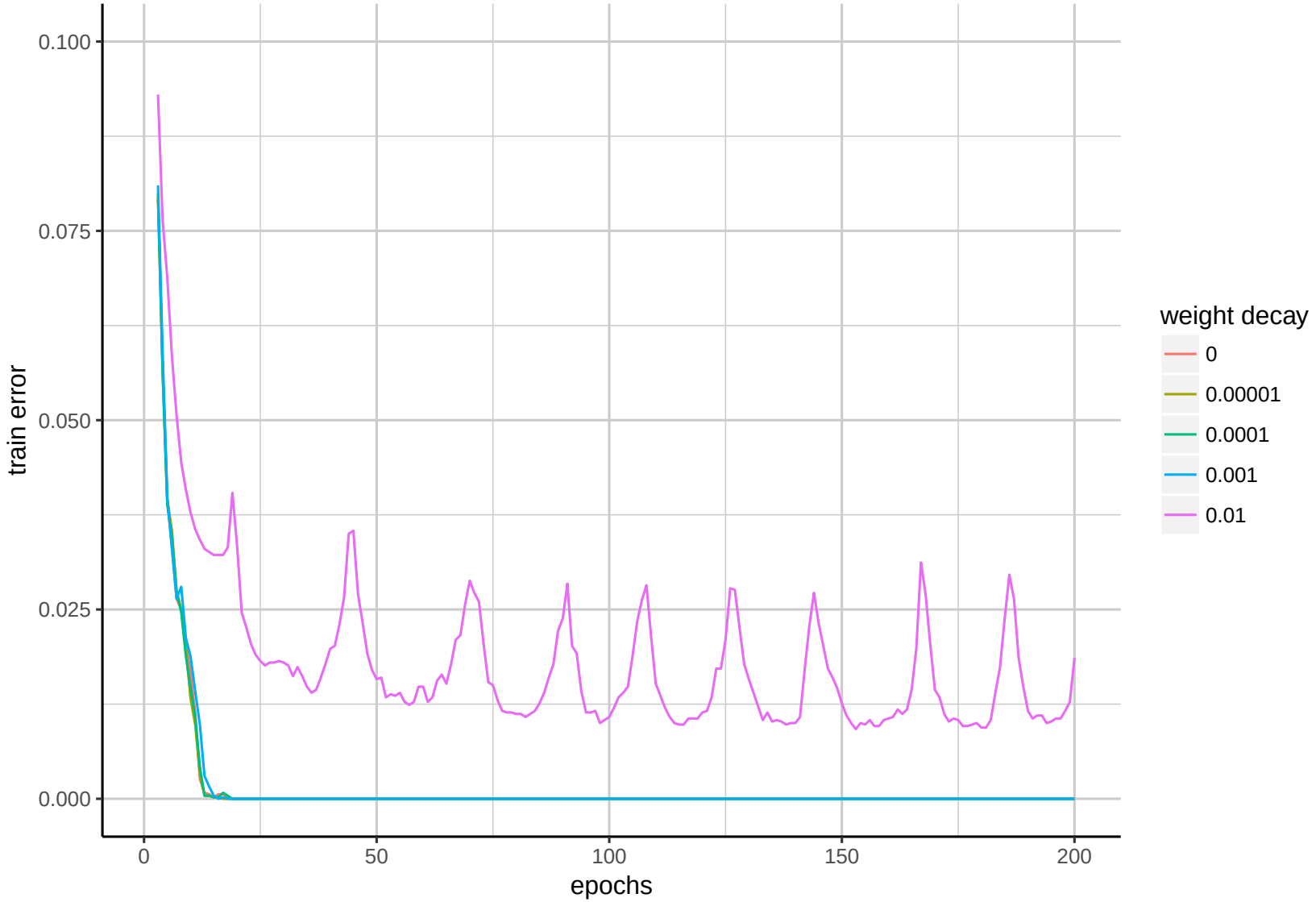
- Let's fit the following huge neural network on a smaller fraction of the mnist data:

```
layer1 = mx.symbol.FullyConnected(data, num_hidden = 512L)
activation1 = mx.symbol.Activation(layer1, act_type = "relu")
layer2 = mx.symbol.FullyConnected(activation1, num_hidden = 512L)
activation2 = mx.symbol.Activation(layer2, act_type = "relu")
layer3 = mx.symbol.FullyConnected(activation2, num_hidden = 512L)
activation3 = mx.symbol.Activation(layer3, act_type = "relu")
layer4 = mx.symbol.FullyConnected(activation3, num_hidden = 10L)
softmax = mx.symbol.SoftmaxOutput(layer4, name = "softmax")
```

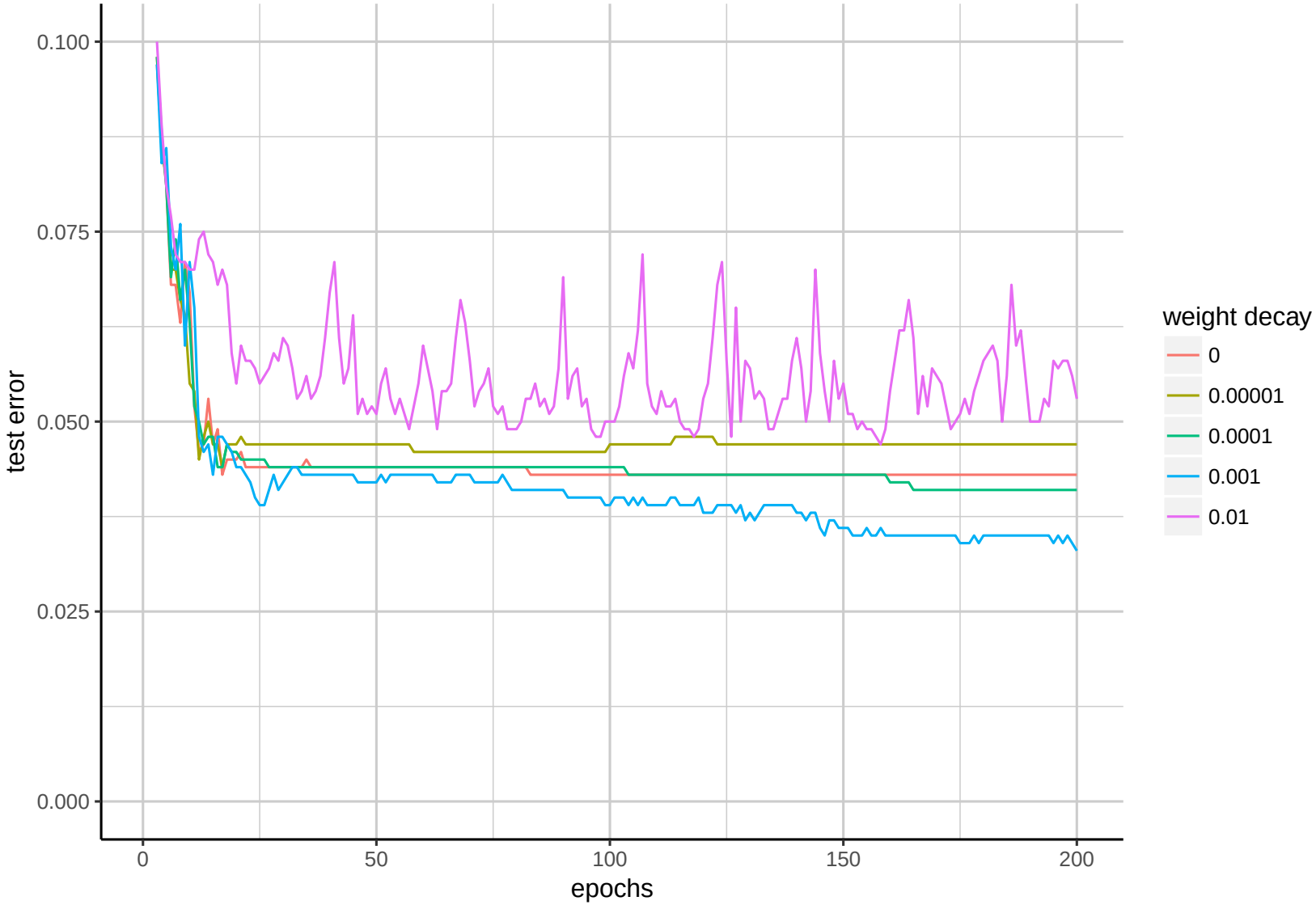
- That is to say 5000 training and 1000 testing samples with evenly distributed class labels.
- We try out different values of weight decay:

$$\alpha \in (0.01, 0.001, 0.0001, 0.00001, 0)$$

WEIGHT DECAY EXAMPLE



WEIGHT DECAY EXAMPLE



WEIGHT DECAY EXAMPLE

- The misclassification accuracy of a neural network can still improve even if we reach 100% training accuracy.
- Consider a binary classification problem with labels 0 and 1.
  - Assume a training sample with label 0 is assigned output probabilities $[0.75, 0.25]$ by the neural net.
  - Thus, the training error with respect to this point it 0, because the predicted label is 0.
  - Applying the negative log-likelihood (cross entropy) as loss function may still lead to improvements in the neural networks "confidence", even after training error reaches 0% (i.e.$[0.9, 0.1]$).
- Note that this is a theoretical concept and in practice we will almost always overfit by the time we reach 100% training accuracy.

EARLY STOPPING

- Goal: find optimal number of epochs.
- Stop algorithm early, before generalization error increases.

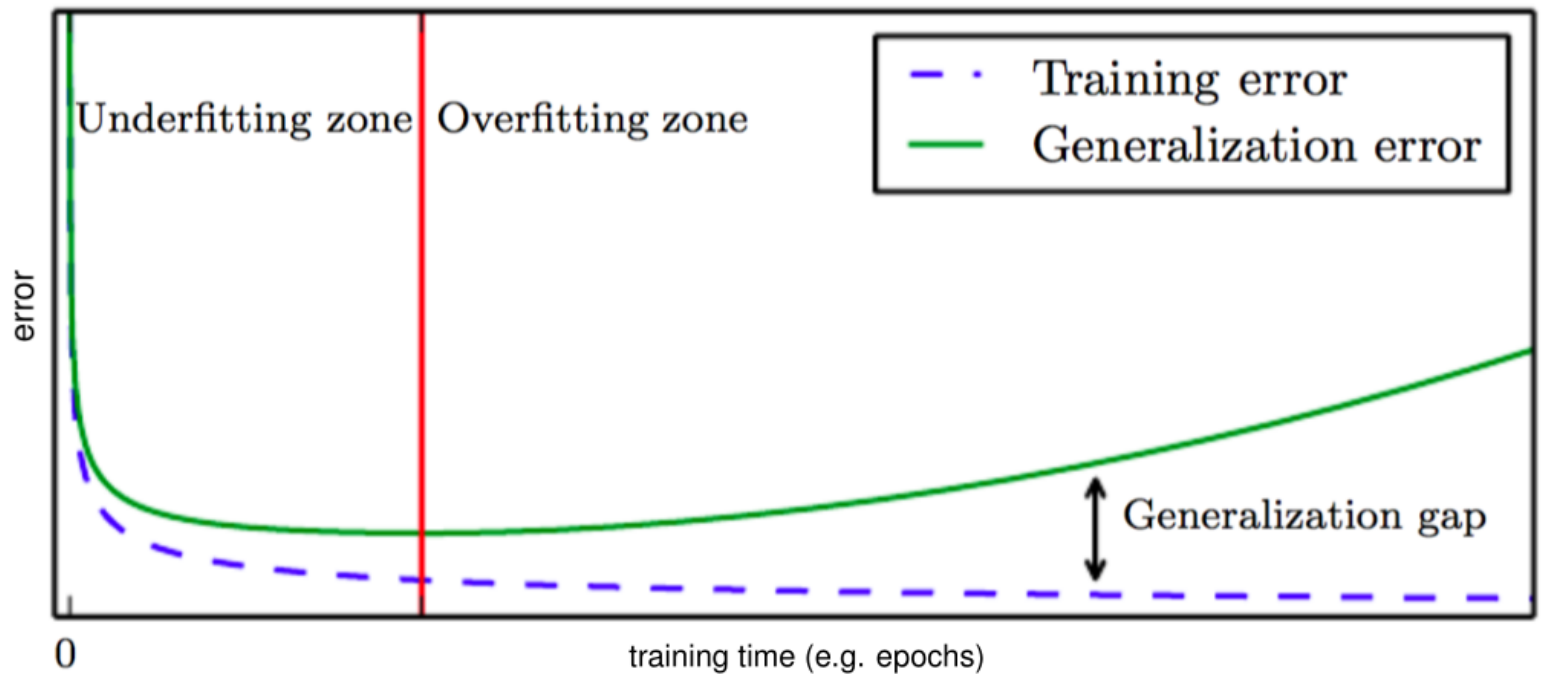


Figure: Underfitting vs. overfitting (Goodfellow et al. (2016))

EARLY STOPPING

How early stopping works:

1. Split training data $(X^{(train)}, y^{(train)})$ into $(X^{(subtrain)}, y^{(subtrain)})$ and $(X^{(validation)}, y^{(validation)})$ (e.g. with a ratio of 2:1).
2. Use $(X^{(subtrain)}, y^{(subtrain)})$ and evaluate model using the $(X^{(validation)}, y^{(validation)})$.
3. Stop training when validation error stops decreasing (after a range of “patience” steps).
4. Use parameters of the previous step for the actual model.

More sophisticated forms also apply cross-validation.

EARLY STOPPING

Strengths	Weaknesses
Effective and simple	Periodical evaluation of validation error
Applicable to almost any model without adjustment	Temporary copy of θ^* (we have to save the whole model at each iteration).
Combinable with other regularization methods	Less data for training $\rightarrow$ include $(X^{(validation)}, y^{(validation)})$ afterwards

- Relation between optimal early stopping iteration m and weight decay penalization parameter λ (see Goodfellow et al. (2016) page 251-252 for proof):

$$\begin{aligned} m &\approx \frac{1}{\alpha\lambda} \\ &\Leftrightarrow \quad \lambda \approx \frac{1}{m\alpha} \end{aligned}$$

- Small λ (low penalization) $\Rightarrow$ high m (deep model/lots of updates)

EARLY STOPPING

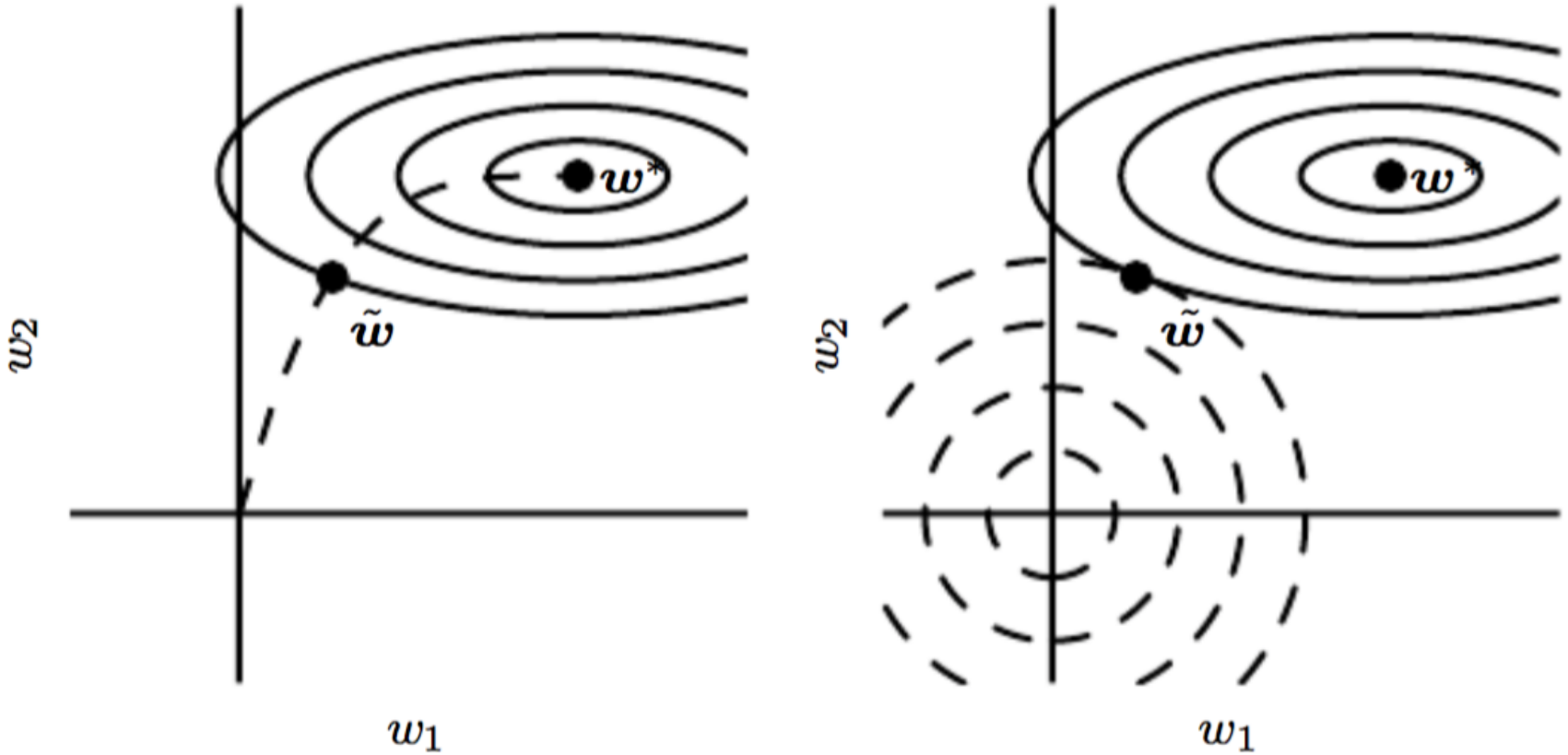
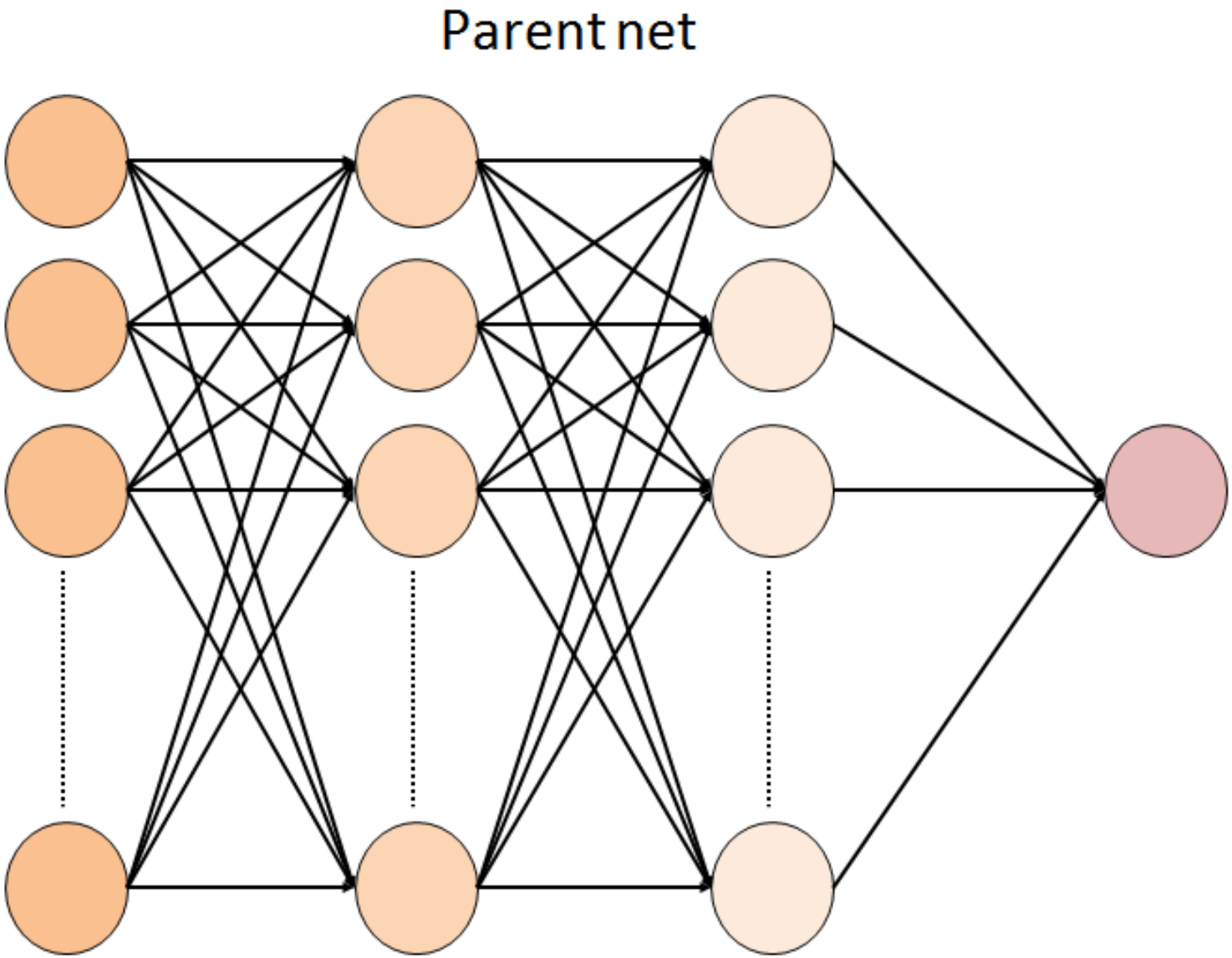


Figure: Optimization path of early stopping (left) and weight decay (right) (Goodfellow et al. (2016))

DROPOUT

- Idea: constrain the networks adaptation to the training data to avoid becoming “too smart” in learning the input data.
  - Dropout can be thought of as making bagging practical for ensembles of many large neural networks!
  - In ensemble learning we take a number of weaker classifiers, train them separately and finally average them.
  - Since each classifier has been trained independently, it has learned different “aspects” of the data.
  - Combining them helps to produce an stronger classifier, which is less prone to overfitting (e.g. random forests)
- So how does dropout actually work?

DROPOUT



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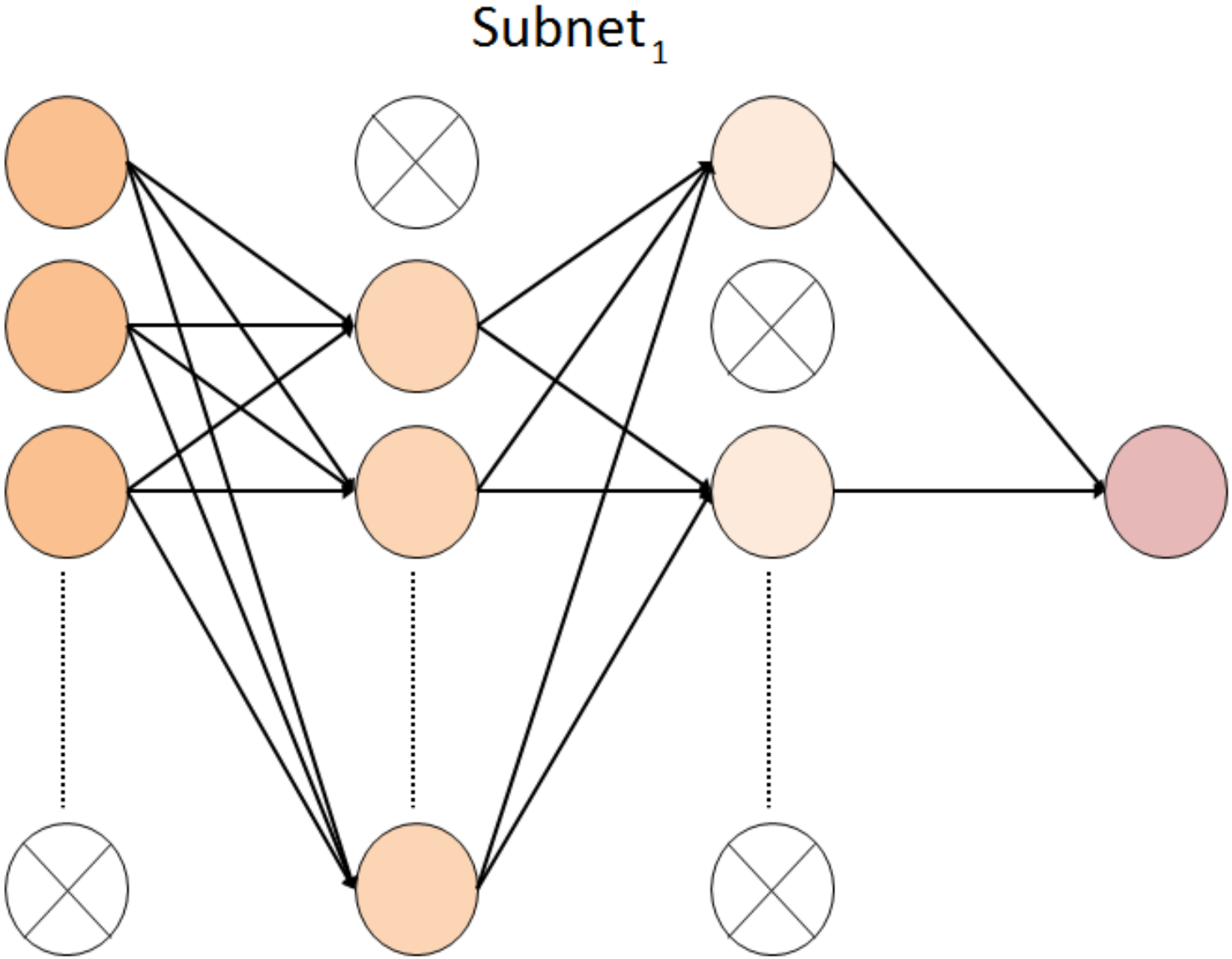

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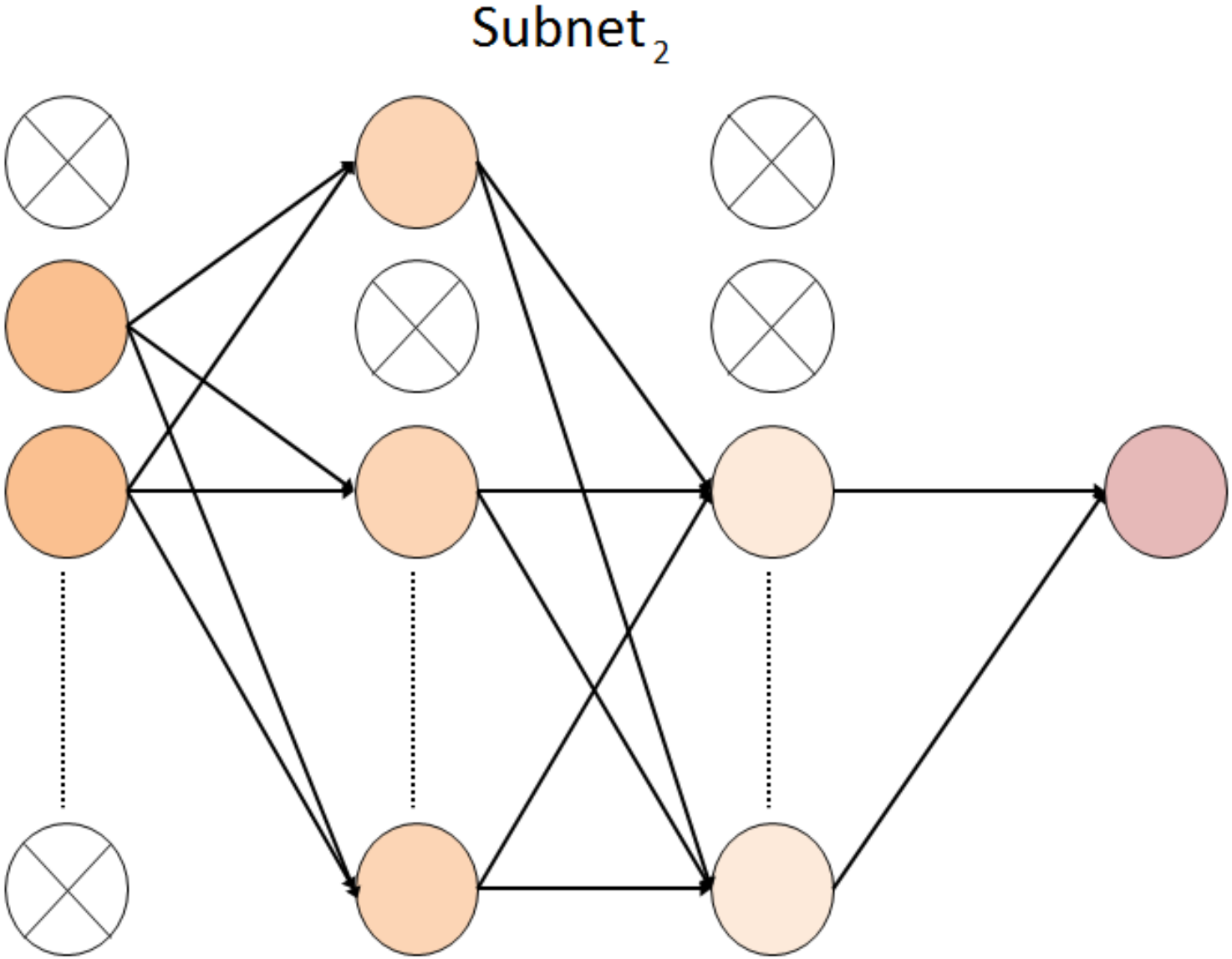

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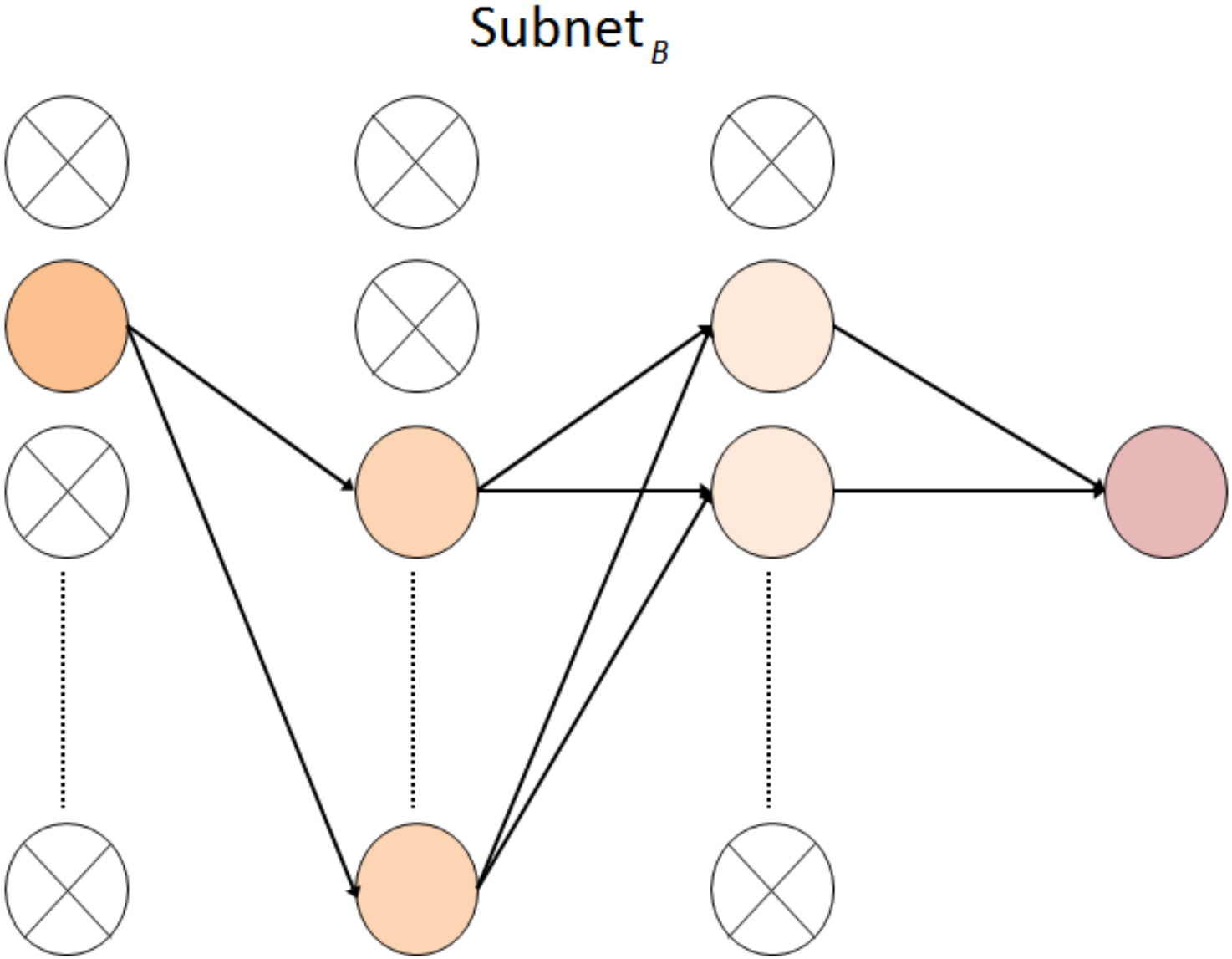
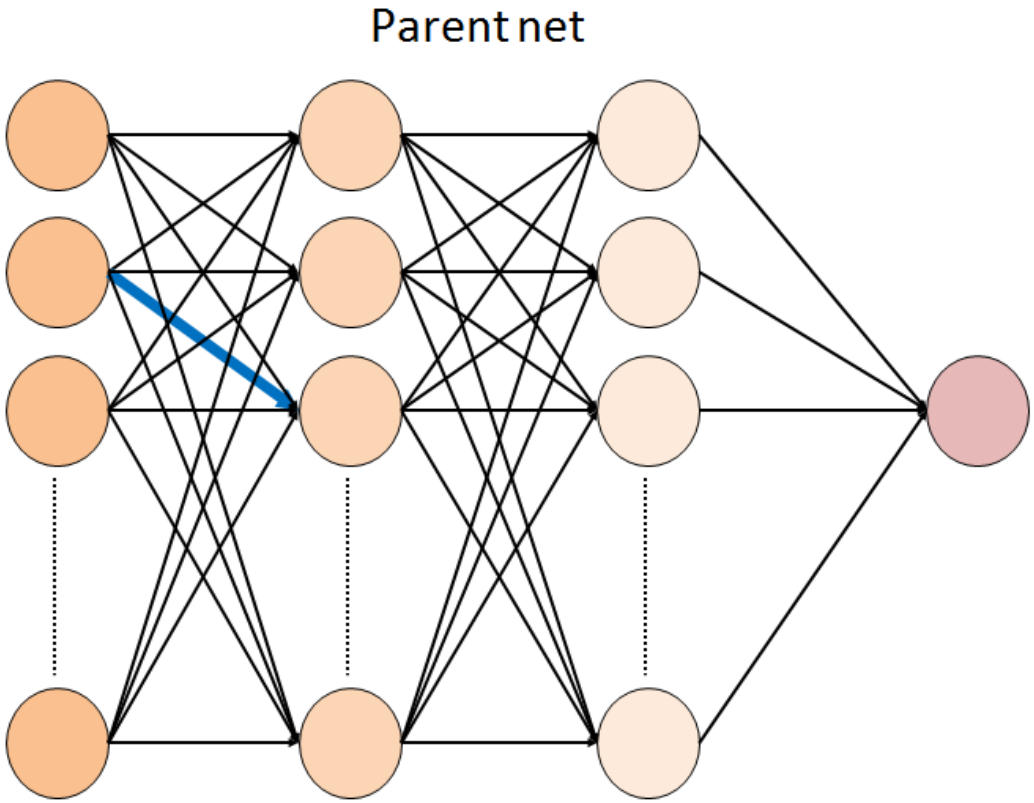


DROPOUT

- Bagging: all models are independent.
- Dropout: models not independent as they share parameters!
  - Each subnets archtitecture is defined by a "mask" μ. The mask μ randomly determines the in-or exclusion of units (neurons) and is trained on one randomly sampled training data point (x, y) (or mini batch).
  - The mask μ is a vector of length d (total number of units (neurons) in the network) with $\mu = (\mu_1, \mu_2, \ldots, \mu_d),\ \mu_i = \{0, 1\}$ and $P(\mu_i = 1) = p$.
  - Thus, each subnet inherits a different subset of parameters from the parent neural network.
  - Parameter sharing makes it possible to represent huge number of of models with particular amount of memory (hardware limitation!).

PARAMETER SHARING

- Parameter sharing:
  - In the case of bagging, the models are all independent.
  - In dropout on the other hand, all models share parameters. That means each model inherits a different subset of parameters from the parent neural network.



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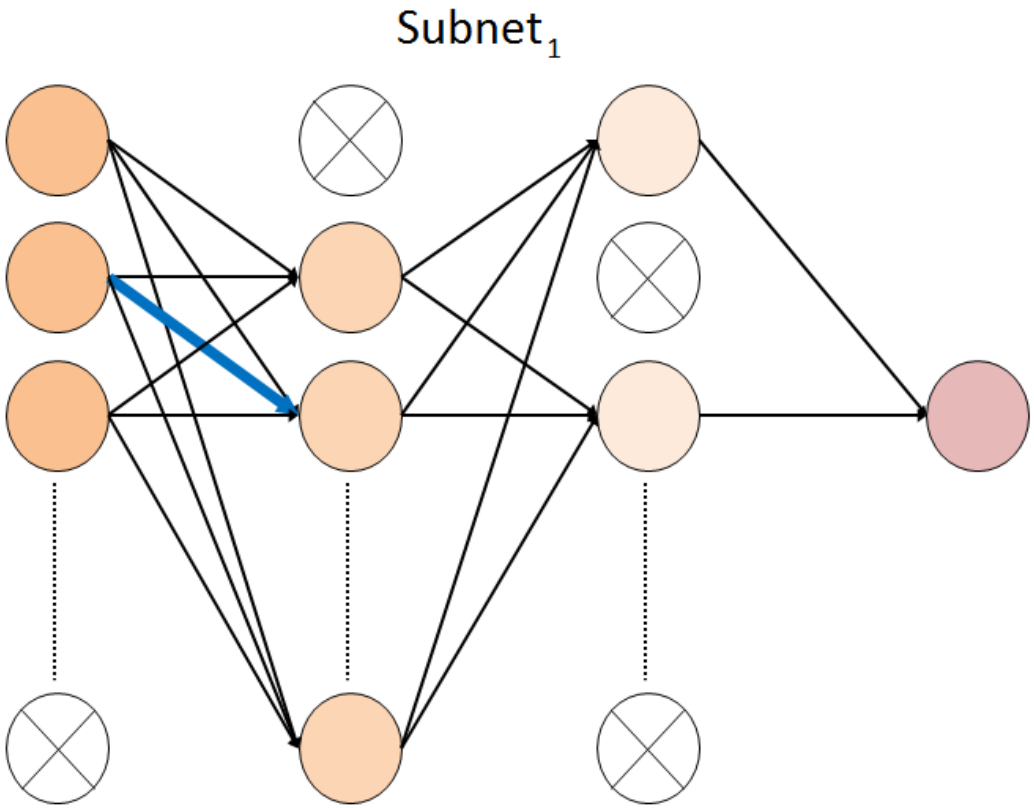

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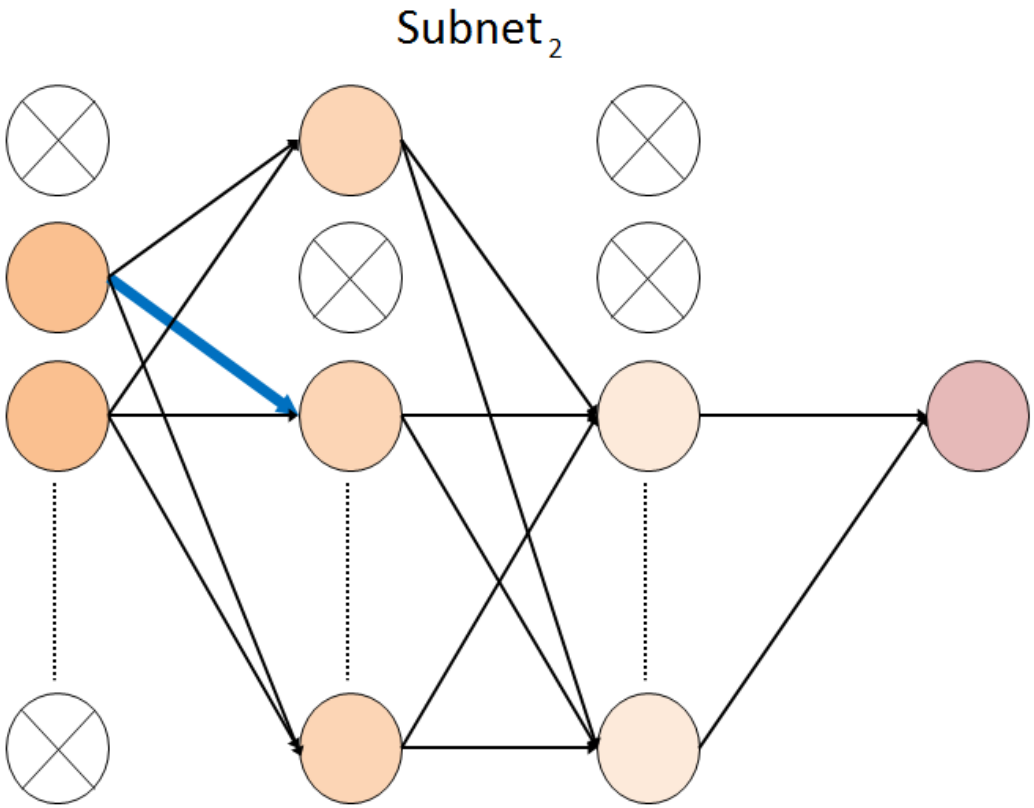

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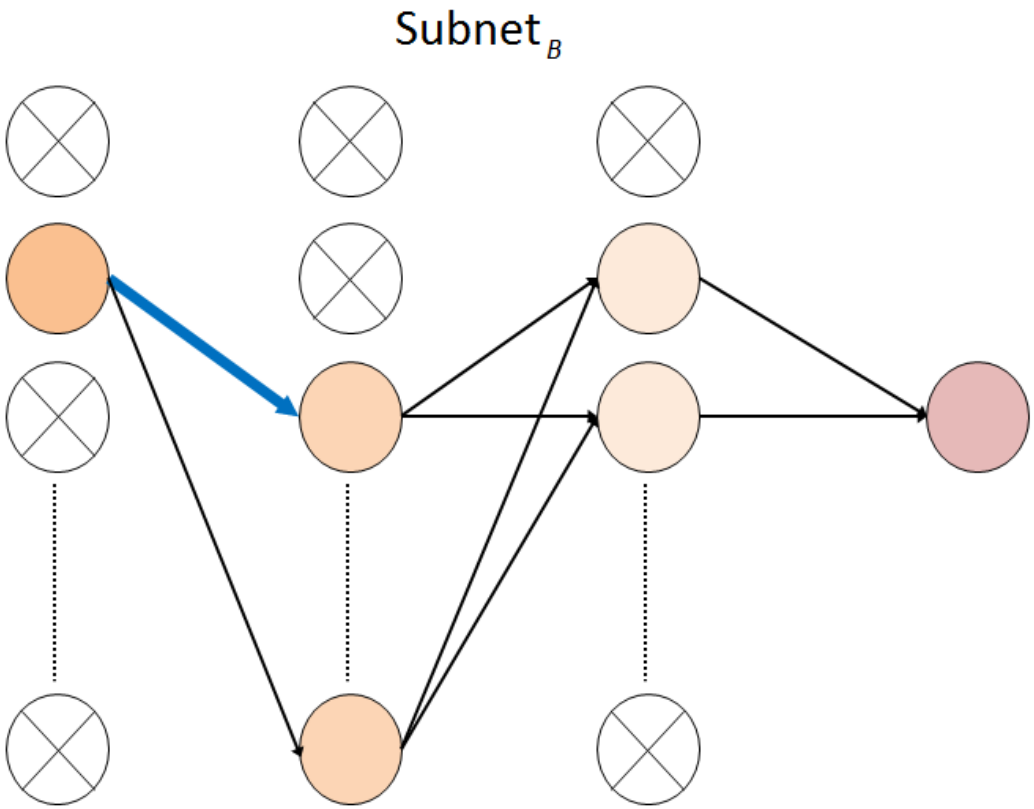

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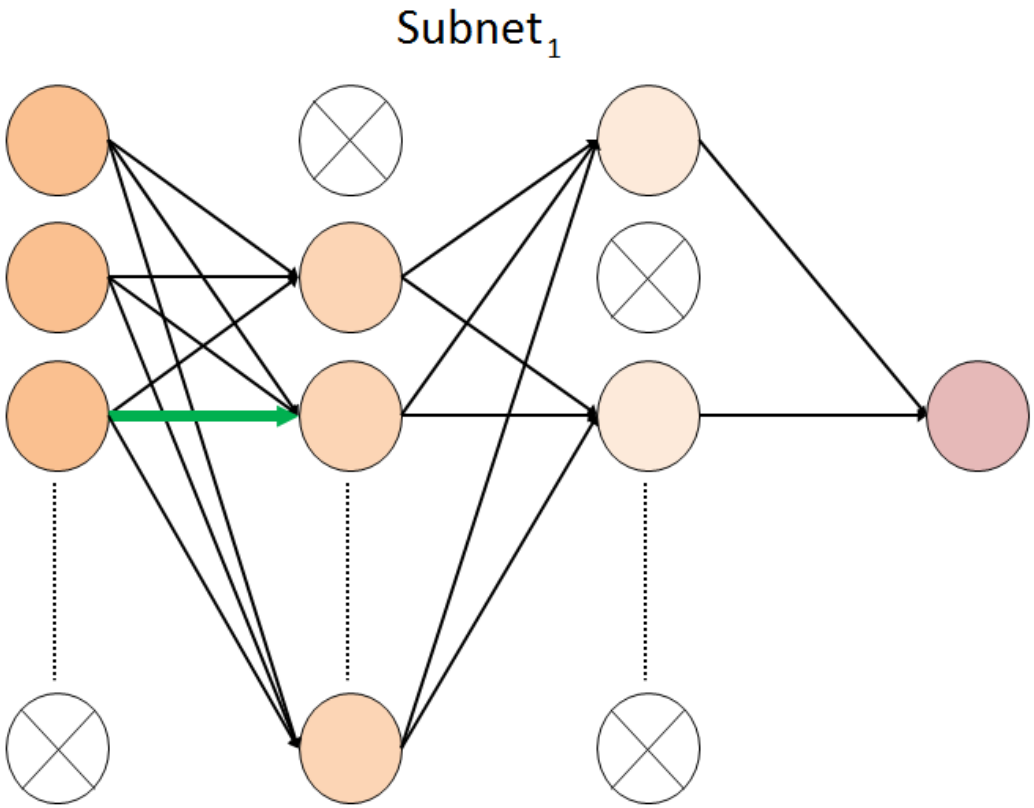

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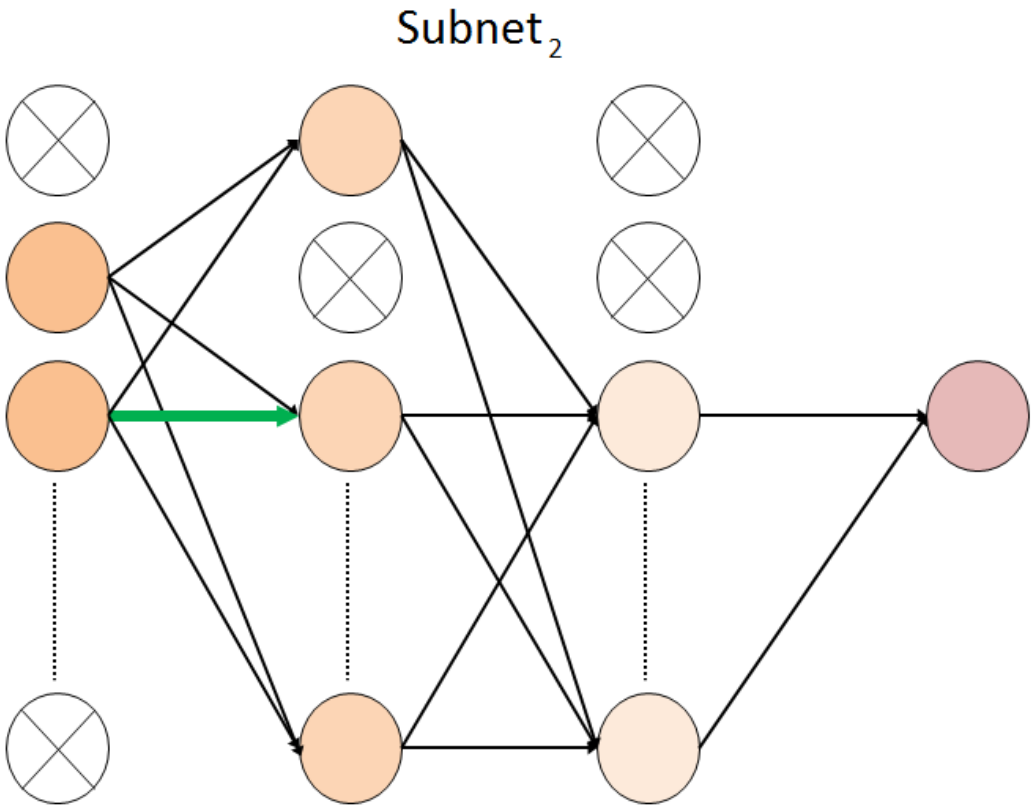

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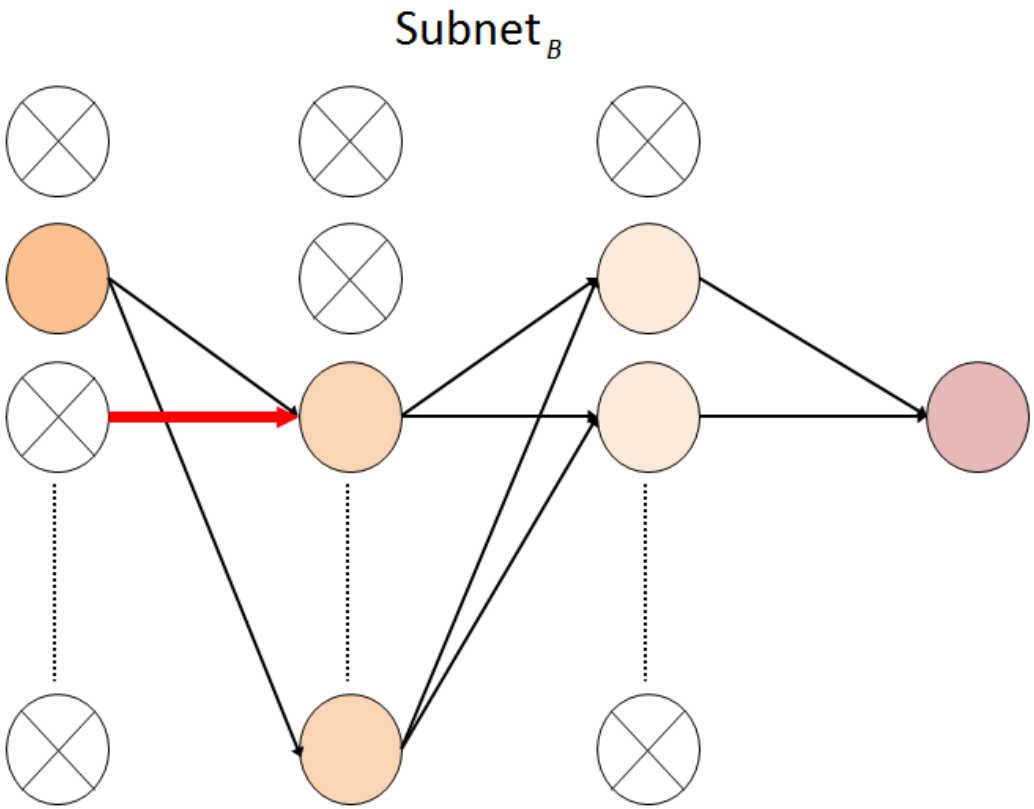


- Models output **probability distributions**: $p(y = y_j|x, \mu)$
- Bagging: arithmetic mean:

$$\tilde{p}_{ensemble}(y = y_k|x) = \frac{1}{B}\sum_{i=1}^{B} p^{(i)}(y = y_k|x)$$

- Dropout: more robust weighting via geometric mean:

$$\tilde{p}_{ensemble}(y = y_k|x) = \sqrt[2^B]{\prod_{\mu} p(y = y_k|x, \mu)}$$

and normalized for prediction:

$$p_{ensemble}(y = y_k|x) = \frac{\tilde{p}_{ensemble}(y = y_k|x)}{\sum_j \tilde{p}_{ensemble}(y = y_k|x)}$$

ILLUSTRATION GEOMETRIC MEAN IN DROPOUT

	$P(y = y_1 \mid x)$	$P(y = y_2 \mid x)$	$P(y = y_3 \mid x)$	$\sum$
Model 1	0.20	0.70	0.10	1.00
Model 2	0.10	0.80	0.10	1.00
Model 3	0.05	0.90	0.05	1.00
Model 4	0.05	0.90	0.05	1.00
Model 5	**0.80**	**0.10**	**0.10**	**1.00**
Arithmetic mean	0.24	0.68	0.08	1.00
Geometric mean	0.13	0.54	0.08	0.75
Re-normalized	0.18	0.72	0.10	1.00

$$mean_{arithmetic}(x_1, ..., x_n) = \frac{1}{n} \sum_{i=1}^{n} x_i$$

$$mean_{geometric}(x_1, ..., x_n) = \sqrt[n]{\prod_{i=1}^{n} x_i} \text{ with } x_i > 0 \forall i = 1, .., n$$

DROPOUT

	Bagging	Dropout
Basic Idea	model averaging	
# models	B	up to 2^B
Prediction	atrithmetic mean	geometric mean
Parameters	B independent models	parameter sharing
Train method	each model to convergence	each sub-net trained on mini batch restricted by μ

DROPOUT: THEORY VS PRACTICE

- Computing the complete ensemble is to expensive in practice!
- Instead we approximate it.

Algorithm 1 Training a neural network with dropout

1: Define parent network and initialize weights
2: **for** each training sample: **do**
3: Draw mask μ
4: Compute forward pass for $network_\mu$
5: Update the weights of $network_\mu$, e.g. by performing a gradient step with weight decay
6: **end for**

- For prediction: use weight scaling rule.

DROPOUT

- Weight scaling rule (Hinton et al. (2012)):
  - Approximate $p_{ensemble}$ by inspection of the **complete model**
  - Multiply shared weights of the trained model coming out of unit (neuron) *i* by *p*

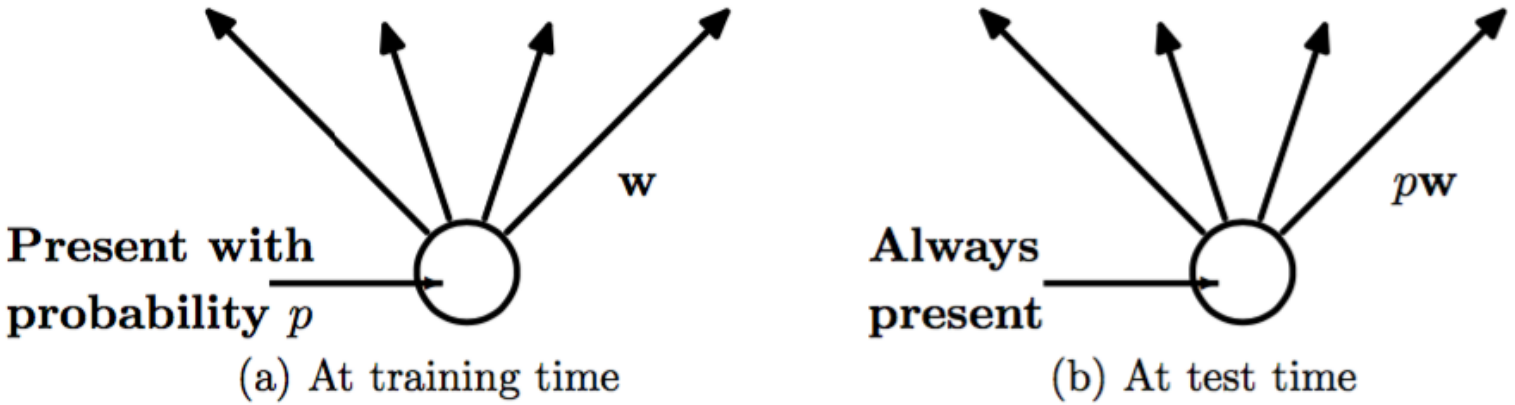


Figure: (Goodfellow et al. (2016))

DROPOUT - EXAMPLE

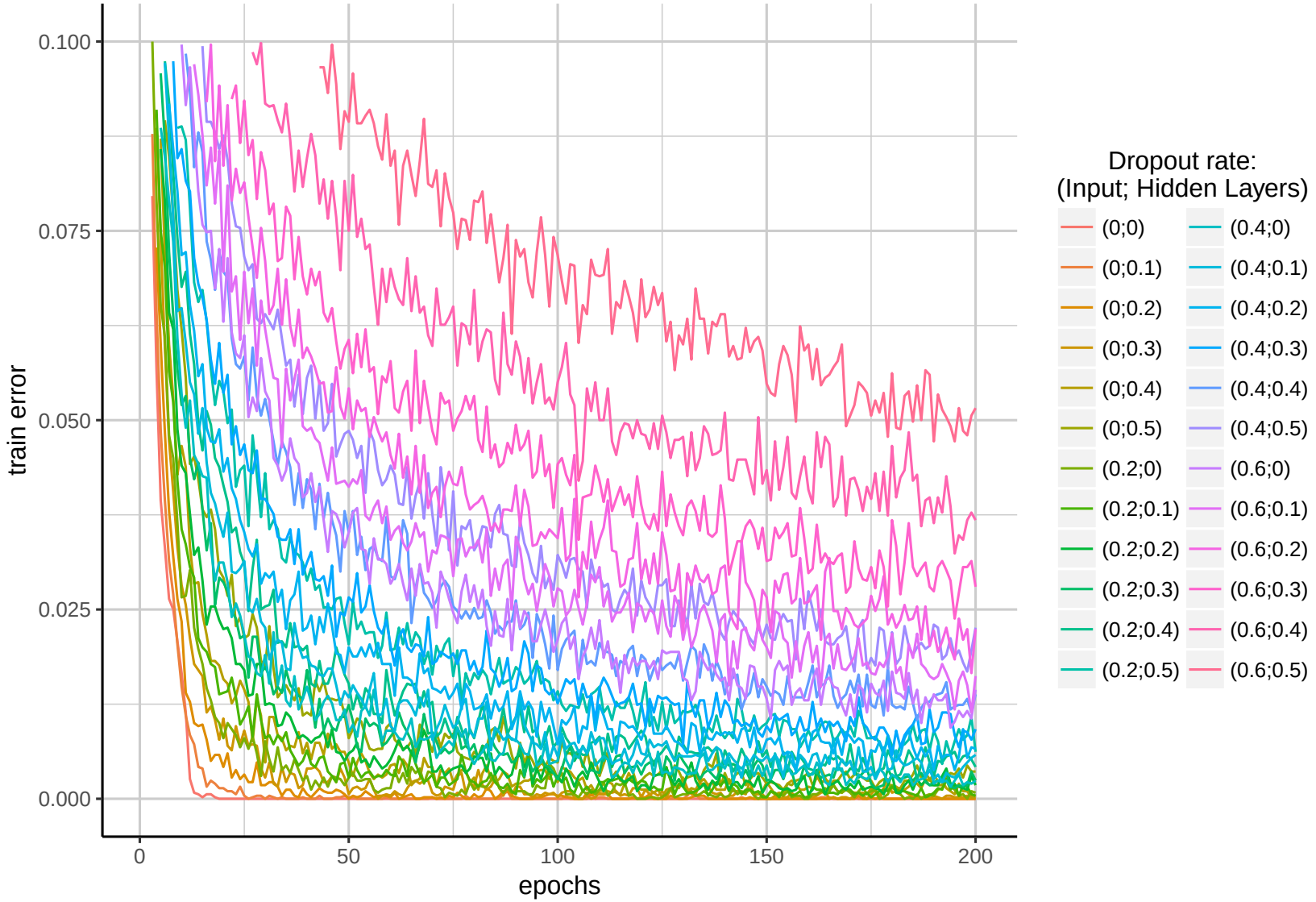
- To demonstrate how dropout can easily improve generalization we compute various models

```
drop0 = mx.symbol.Dropout(data, p = dropoutInputValues)
fc1 = mx.symbol.FullyConnected(drop0, name = "fc1", num_hidden = 512)
act1 = mx.symbol.Activation(fc1, name = "relu1", act_type = "relu")
drop1 = mx.symbol.Dropout(act1, p = dropoutLayerValues)
fc2 = mx.symbol.FullyConnected(drop1, name = "fc2", num_hidden = 512)
act2 = mx.symbol.Activation(fc2, name = "relu2", act_type = "relu")
drop2 = mx.symbol.Dropout(act2, p = dropoutLayerValues)
fc3 = mx.symbol.FullyConnected(drop2, name = "fc3", num_hidden = 512)
act3 = mx.symbol.Activation(fc3, name = "relu3", act_type = "relu")
drop3 = mx.symbol.Dropout(act3, p = dropoutLayerValues)
fc4 = mx.symbol.FullyConnected(drop3, name = "fc4", num_hidden = 10)
softmax = mx.symbol.SoftmaxOutput(fc4, name = "sm")
```

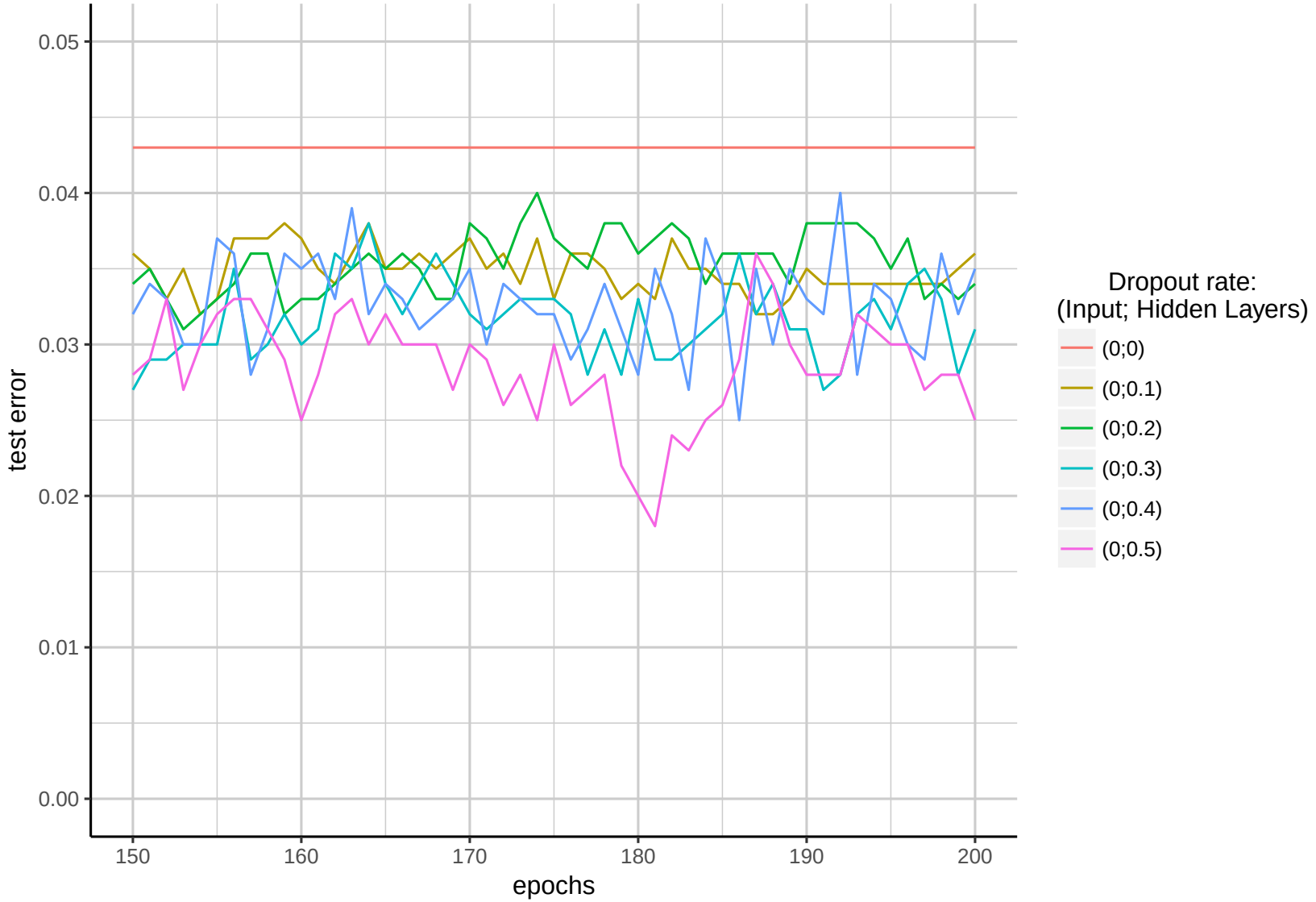
- We compute all models of the Cartesian product between the variables dropoutInputValues and dropoutLayerValues. That is

$$(0, 0.2, 0.4, 0.6) \times (0, 0.1, 0.2, 0.3, 0.4, 0.5)$$

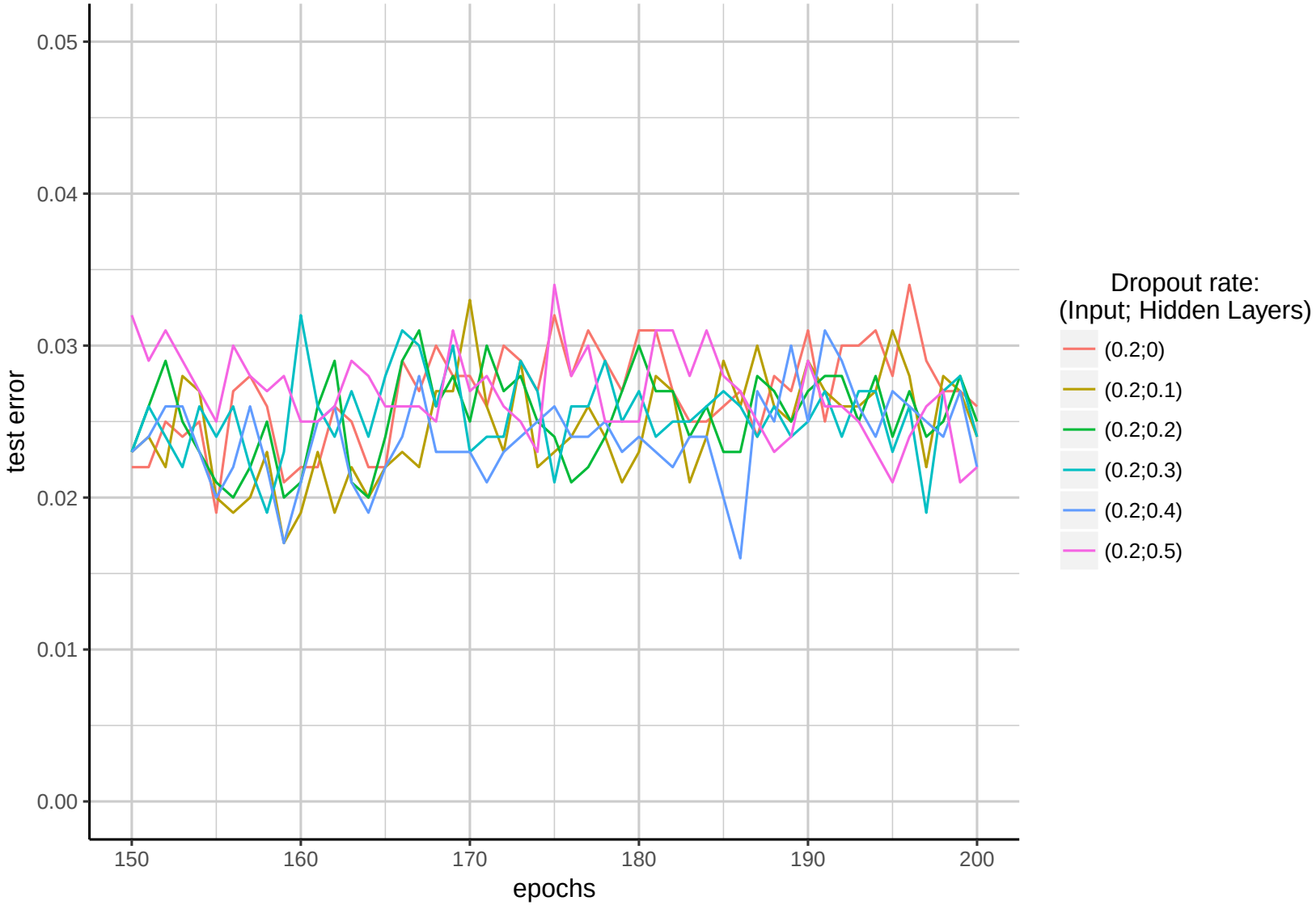
DROPOUT - EXAMPLE



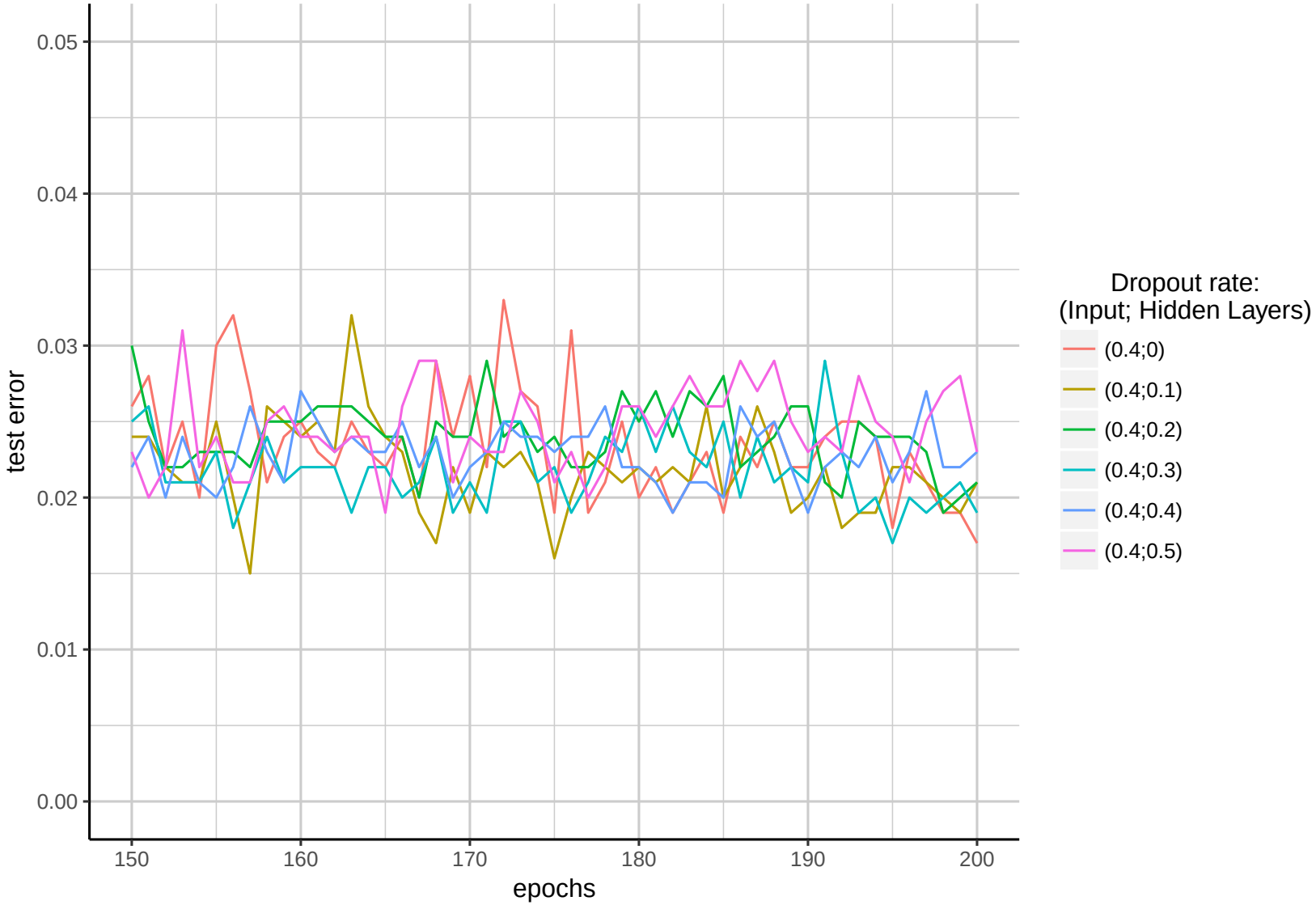
DROPOUT - EXAMPLE



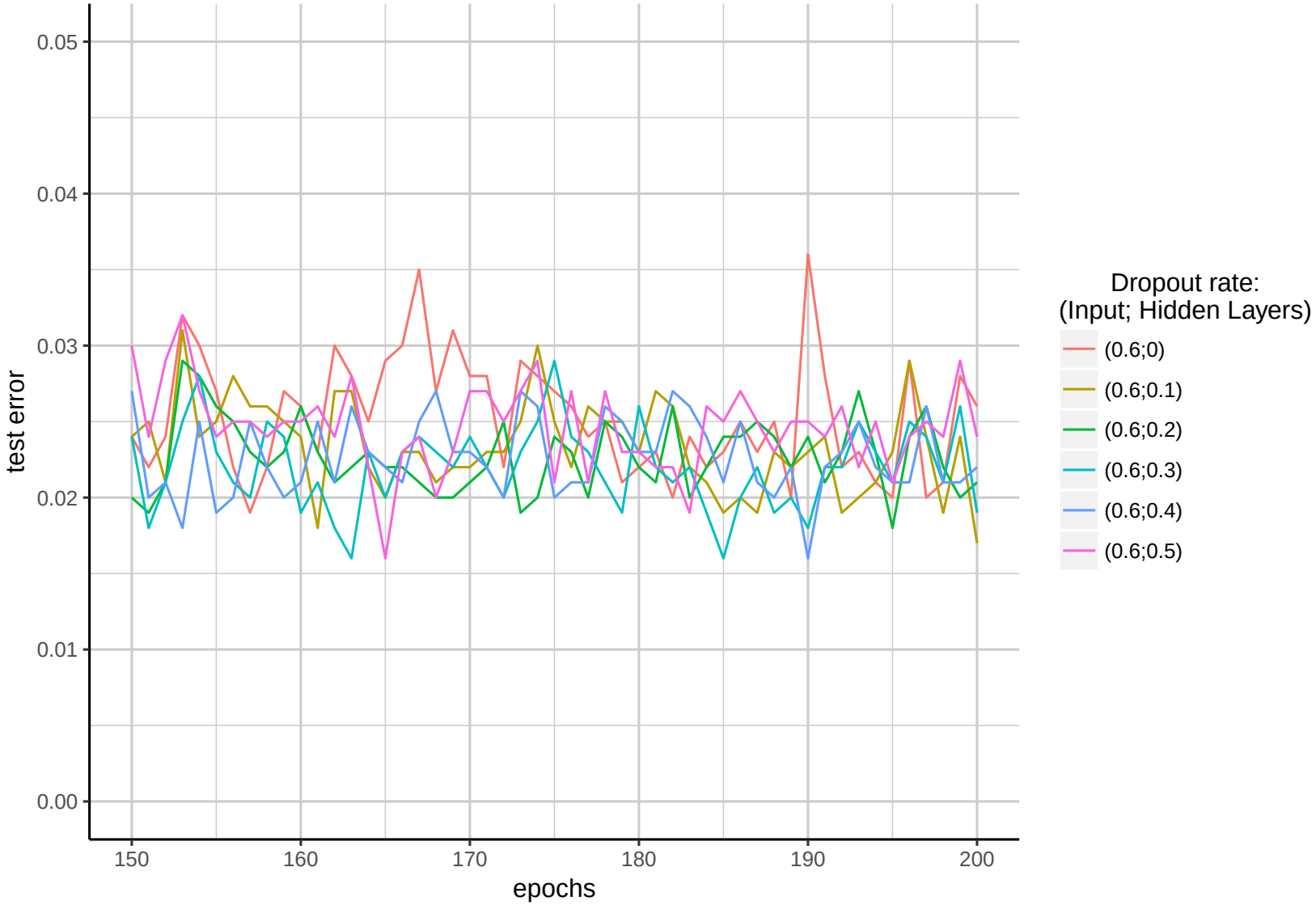
DROPOUT - EXAMPLE



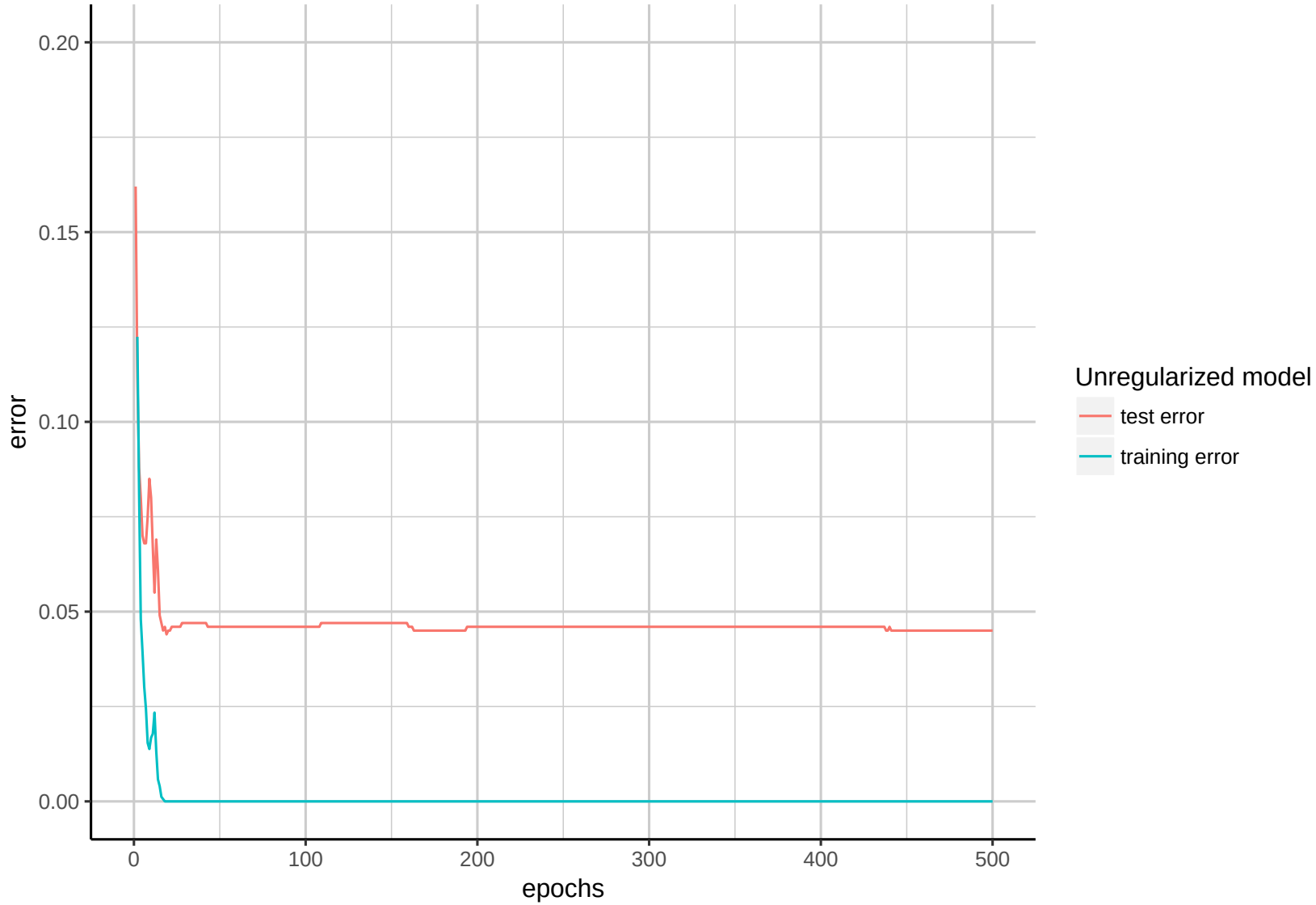
DROPOUT - EXAMPLE



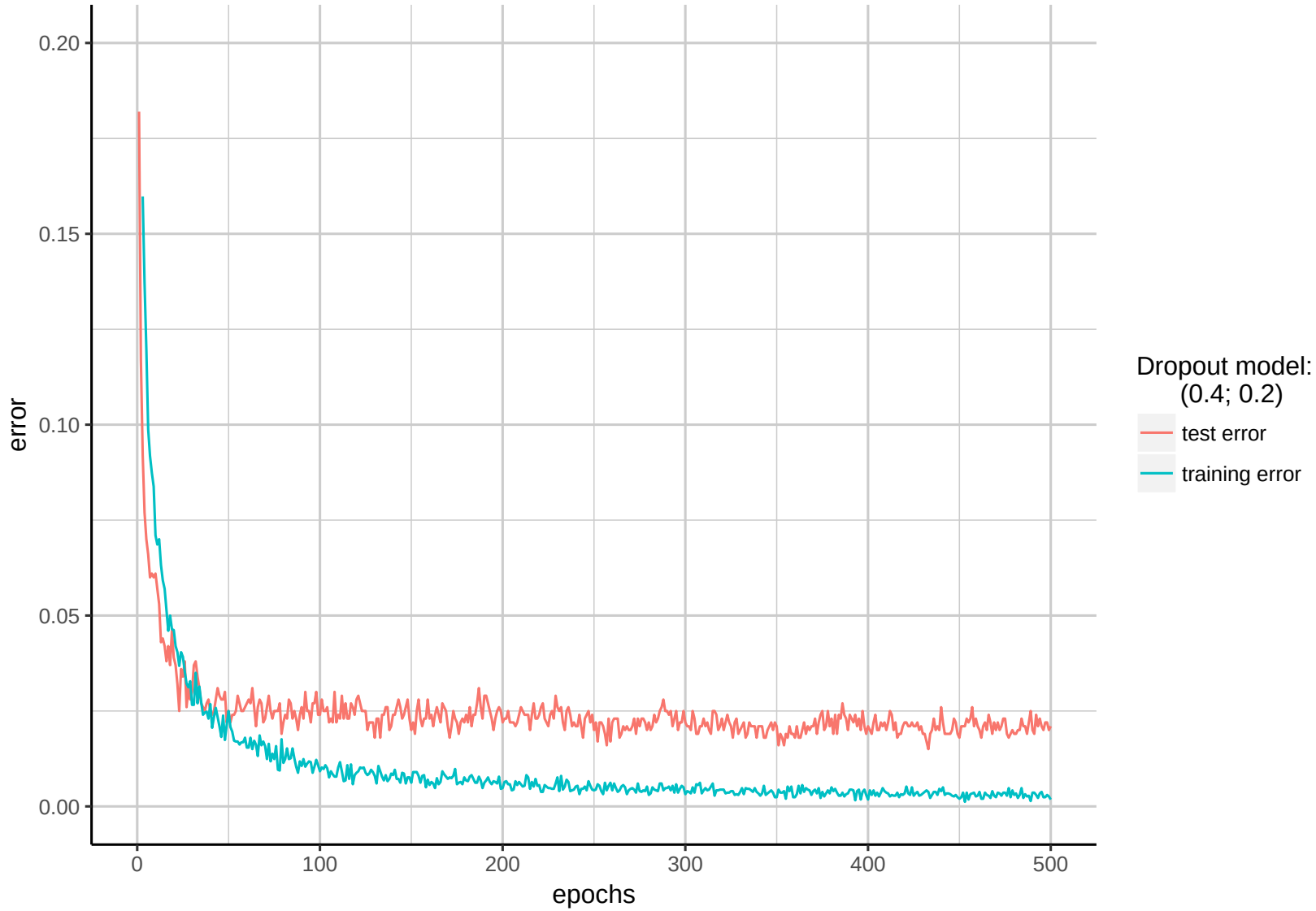
DROPOUT - EXAMPLE



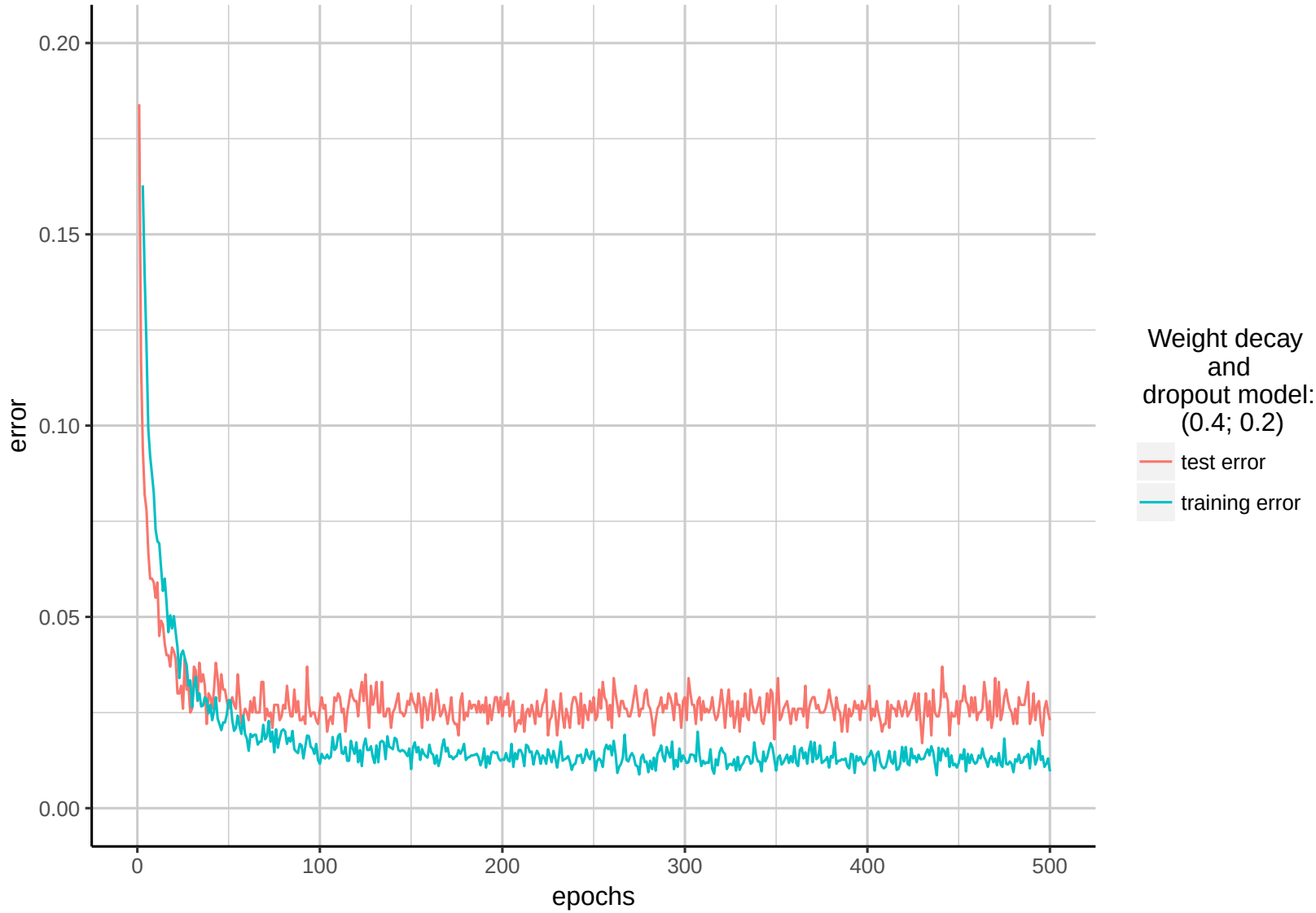
DROPOUT, WEIGHT DECAY OR BOTH?



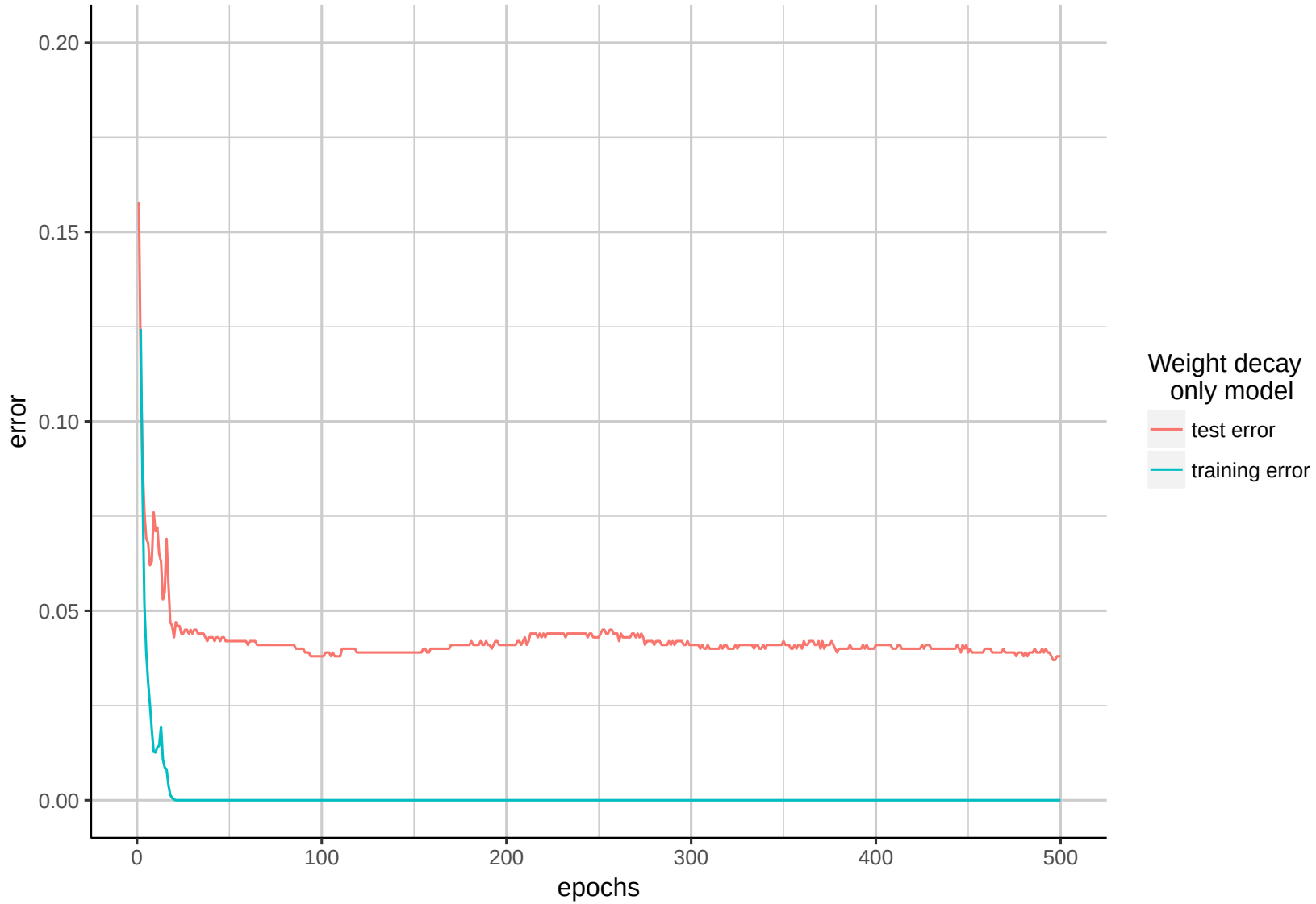
DROPOUT, WEIGHT DECAY OR BOTH?



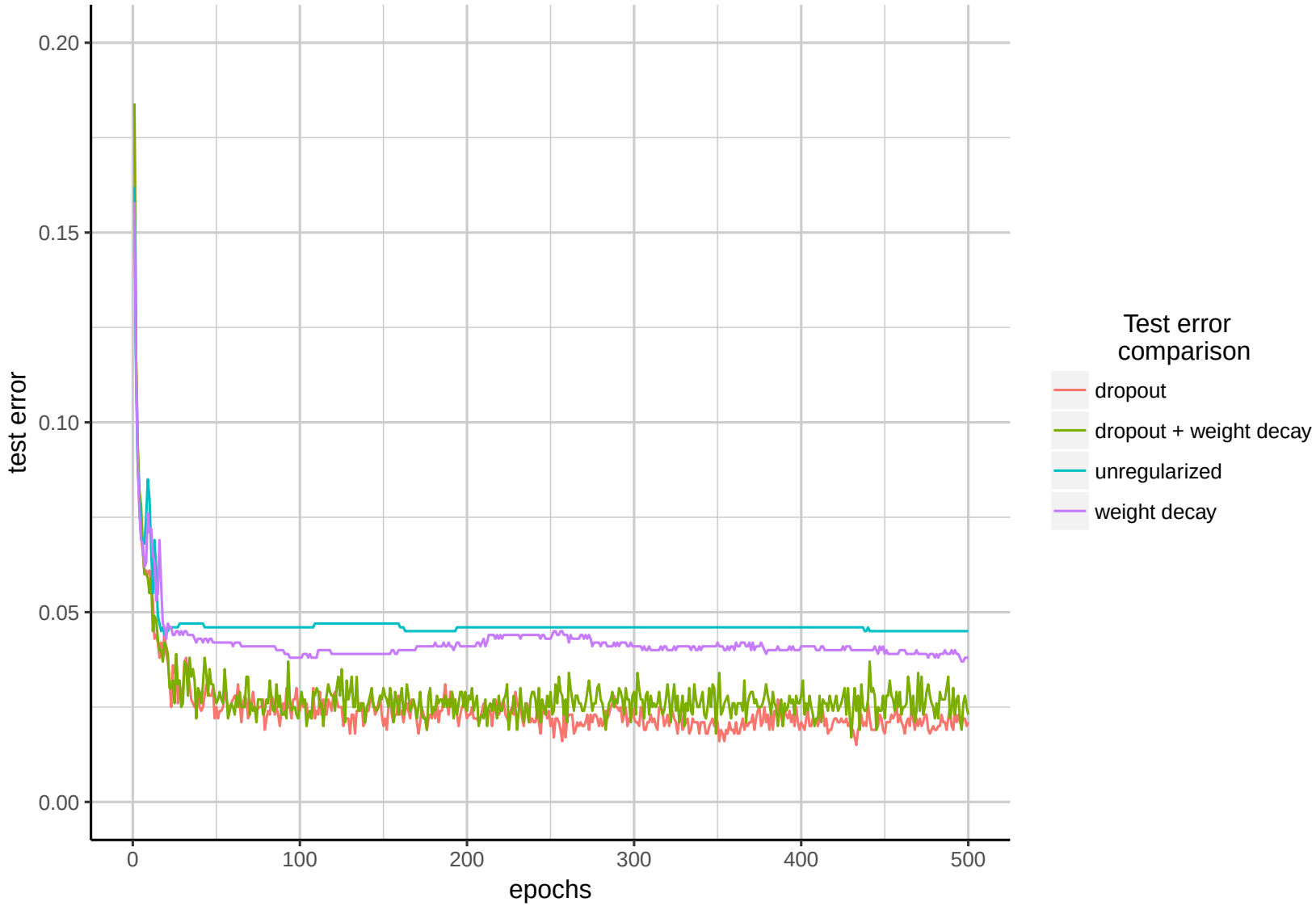
DROPOUT, WEIGHT DECAY OR BOTH?



DROPOUT, WEIGHT DECAY OR BOTH?



DROPOUT, WEIGHT DECAY OR BOTH?



DATASET AUGMENTATION

- Problem: low generalization because high ratio of

$$\frac{\text{complexity of the model}}{\text{\#train data}}$$

- Idea: artificially increase the train data.
  - Limited data supply $\rightarrow$ create “fake data”!
- Increase variation in inputs **without** changing the labels.
- Application:
  - Image and Object recognition (rotation, scaling, pixel translation, flipping, noise injection, vignetting, color casting, lens distortion, injection of random negatives)
  - Speech recognition (speed augmentation, vocal tract perturbation)

DATASET AUGMENTATION

(a) Original (b) Color

(c) Rotate (d) Horizontal Stretch

Figure: (Wu et al. (2015))

DATASET AUGMENTATION

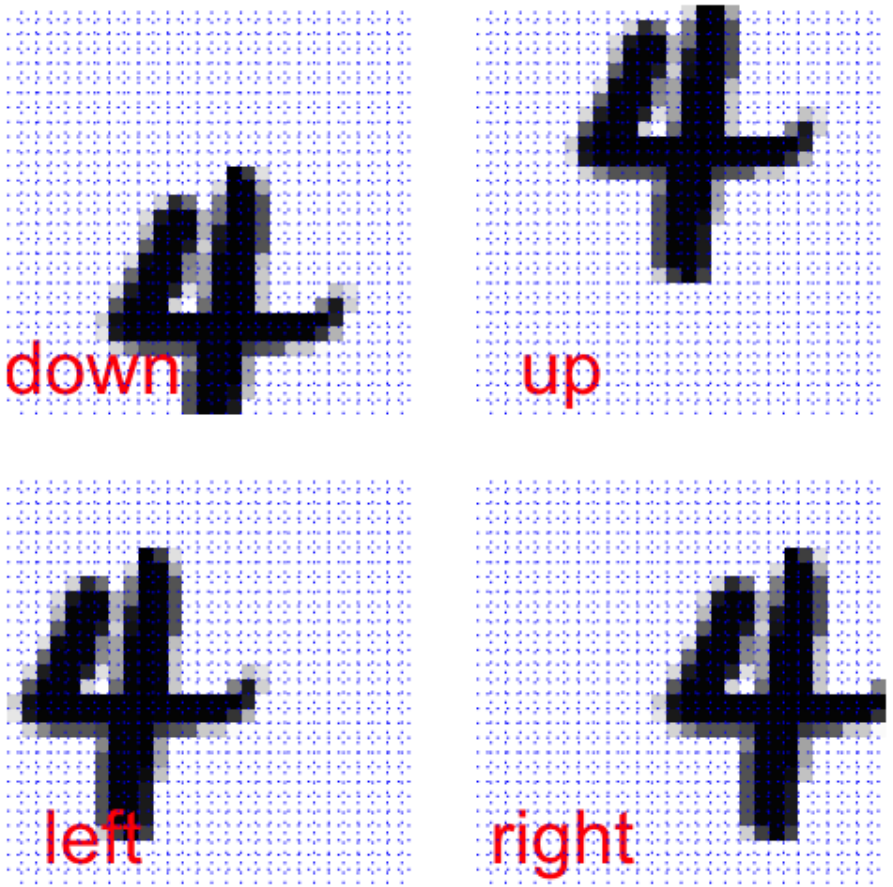


Figure: (Wu et al. (2015))

$\Rightarrow$ careful when rotating digits (6 will become 9 and vice versa)!

ARTIFICIAL NOISE

- Intentionally inject noise to the model, to make it more robust to small pertubations in the inputs.
- This method may force the model to “grow” weights in regions of flat minima.
  - Thus, the noisy model may not find perfect minima but its approximations lie in a flatter surrounding.
- Bishop (1995) shows that the injection of artifical noise has the same effect as norm penalization strategies.
- In practice, it is common to apply noise to the outputs.
  - This strategy is termed label smoothing as it incorporates a small noise term on the labels of the classification outputs. The intuition is to account for possible errors in the labeling process.

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