Regularization

Deep Learning
CS 435/635

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AI Lab Coordinator @IIT Indore

Course Content

Module I: History of Deep Learning, Sigmoid Neurons, Perceptrons, and learning algorithms. Multilayer Perceptrons (MLPs), Representation Power of MLPs,.

Module II: Feedforward Neural Networks. Backpropagation. first and second-order training methods. NN Training tricks, **Regularization**

Module III: Introduction to Autoencoders and their characteristics, relation to PCA, Regularization in autoencoders, and Types of autoencoders.

Module IV: Architecture of Convolutional Neural Networks (CNN), types of CNNs.

Module V: Architecture of Recurrent Neural Networks (RNN), Backpropagation through time. Encoder-Decoder Models, Attention Mechanism. Advanced Topics: Transformers and BERT.

Acknowledgement

- Neural Networks and Deep Learning course by Danna Gurari University of Colorado Boulder

Today’s Topics

- Regularization
- Parameter norm penalty
- Early stopping
- Dataset augmentation
- Dropout
- Batch normalization
- Programming tutorial

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What is Regularization?

“any modification we make to a learning algorithm that is intended to reduce its generalization error but not its training error.”

- Ch. 5.2 of Goodfellow book on Deep Learning

What are strategies for preferring one function over another?

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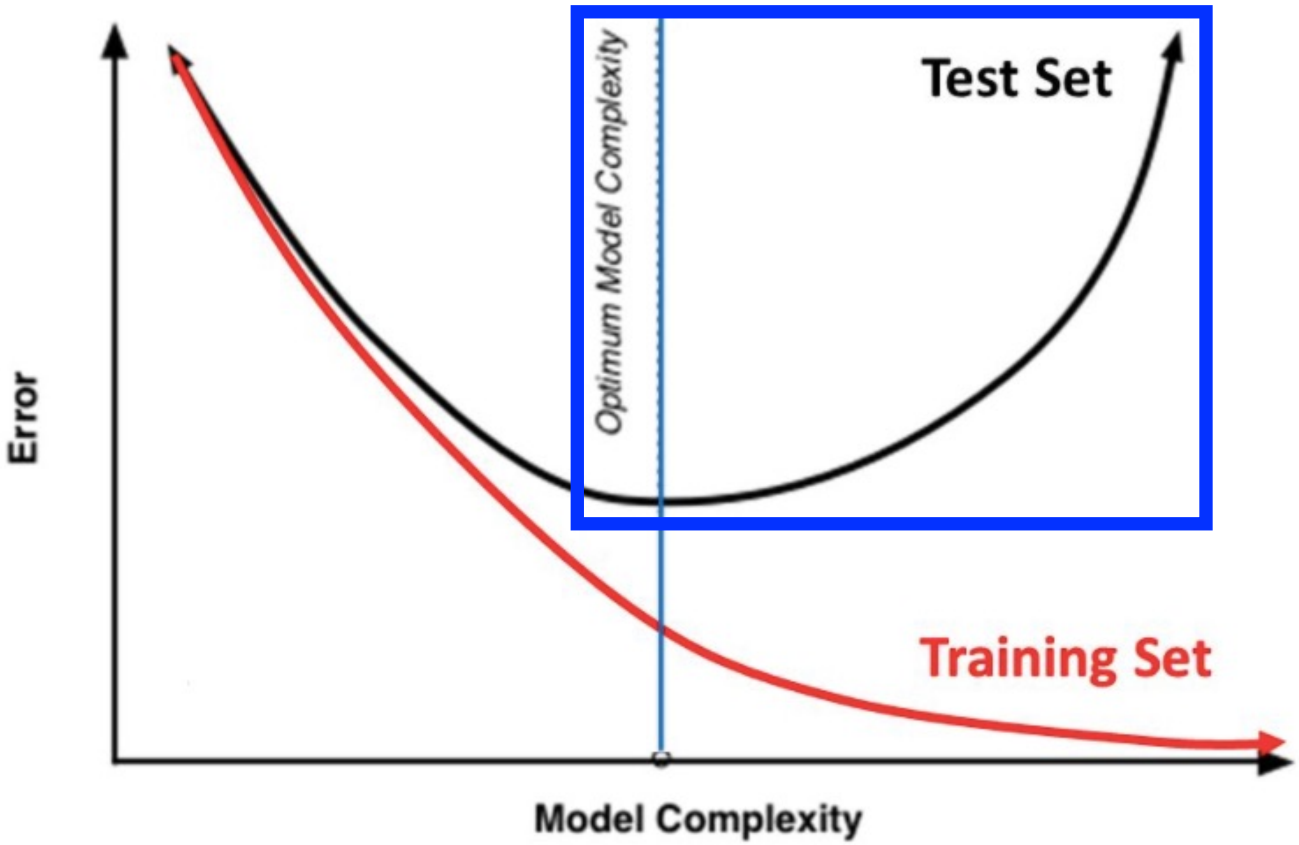
Goal

Rather than exclude functions from a hypothesis space, apply strategies that create a preference for one solution over another to reduce test error



https://cdn.analyticsvidhya.com/wp-content/uploads/2018/04/Screen-Shot-2018-04-04-at-2.43.37-PM.png

Goal

Rather than exclude functions from a hypothesis space, apply strategies that create a preference for one solution over another to reduce test error; e.g., regularize (c)

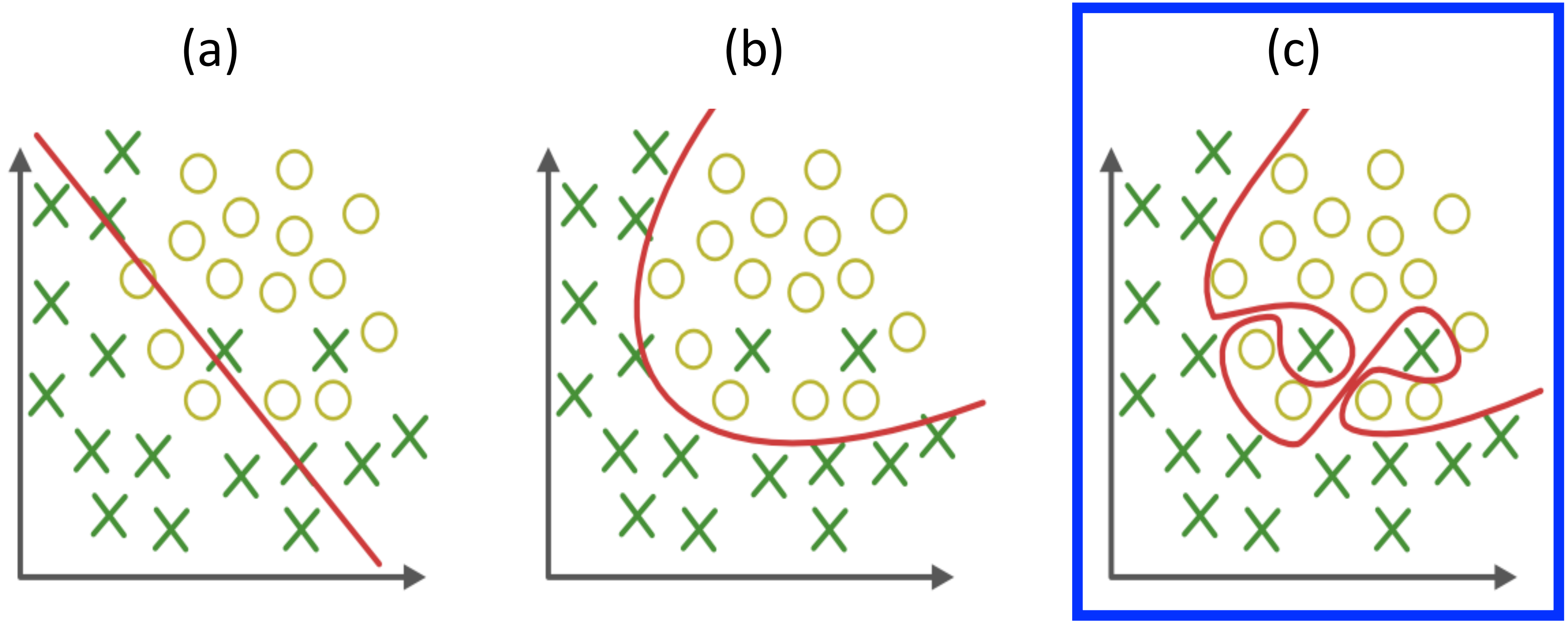
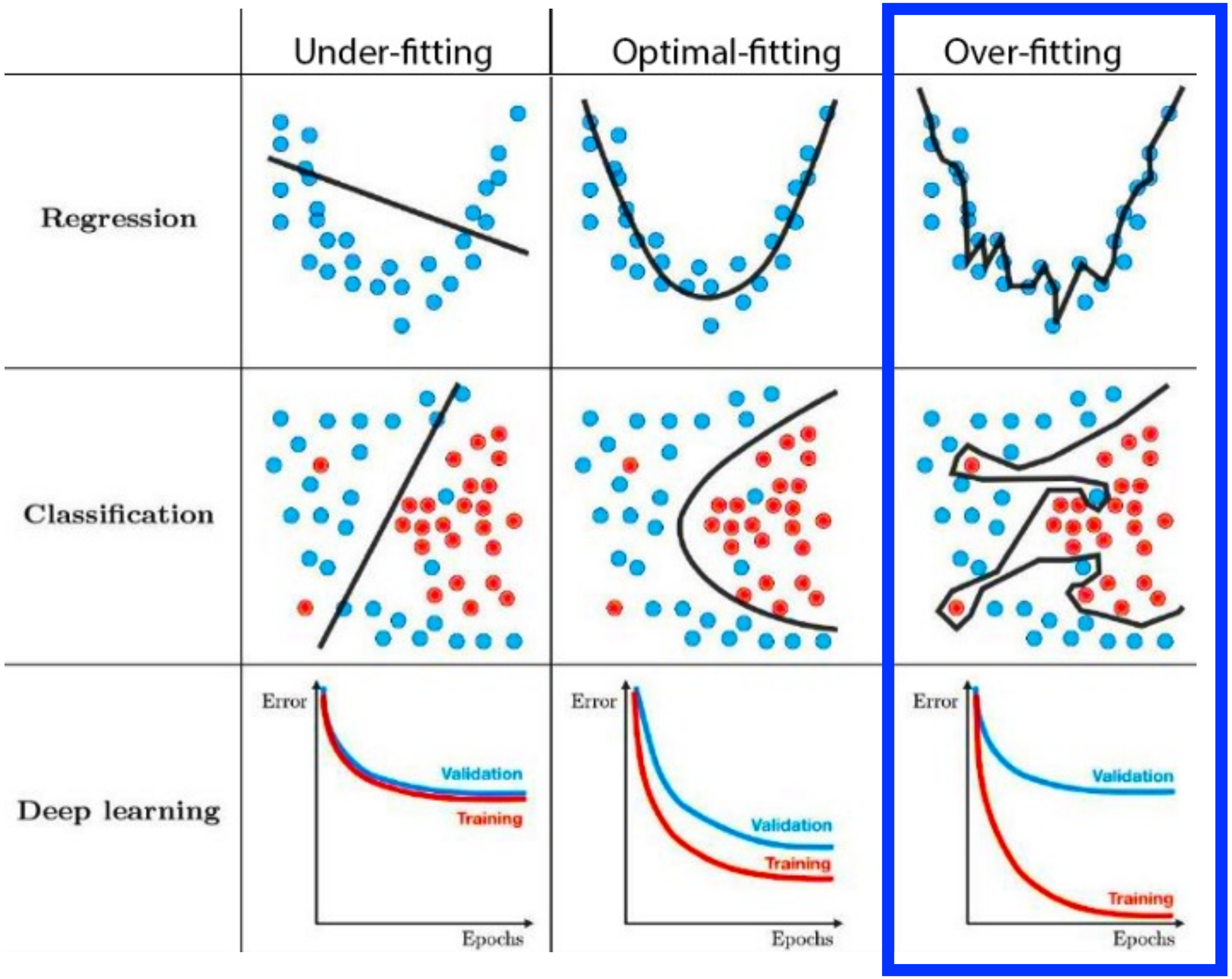


Figure source: https://towardsdatascience.com/underfitting-and-overfitting-in-machine-learning-and-how-to-deal-with-it-6fe4a8a49dbf

Idea: Analogous to Wearing Belt on Big Pants

Observation: Sign of Overfitting is Large Weights

Very large positive weights get canceled by similarly large negative weights (i.e., due to correlated model parameters) in order to model noise



https://towardsdatascience.com/techniques-for-handling-underfitting-and-overfitting-in-machine-learning-348daa2380b9

Idea: Penalize Large Weights in Objective Function

e.g., objective is to *minimize* sum of squared errors over training examples

- L2 norm: penalize squared weight values

$$Error = \boxed{\sum_{i=1}^{n}(y^{(i)} - \widehat{y}^{(i)})^2} + \boxed{\alpha} \boxed{\sum_{j=1}^{m} w_j^2}$$

- L1 norm: penalize absolute weight values

$$Error = \boxed{\sum_{i=1}^{n}(y^{(i)} - \widehat{y}^{(i)})^2} + \boxed{\alpha} \boxed{\sum_{j=1}^{m} |w_j|}$$

- *Note: only weights are penalized, not bias terms (bias terms are fewer/less impactful)*

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- Hyperparameter determines contribution of norm penalty term (e.g., belt tightness)

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Intuitively, larger alpha values prioritizes having weights closer to 0 instead of minimizing sum of squared errors

- Hyperparameter determines contribution of norm penalty term (e.g., belt tightness)

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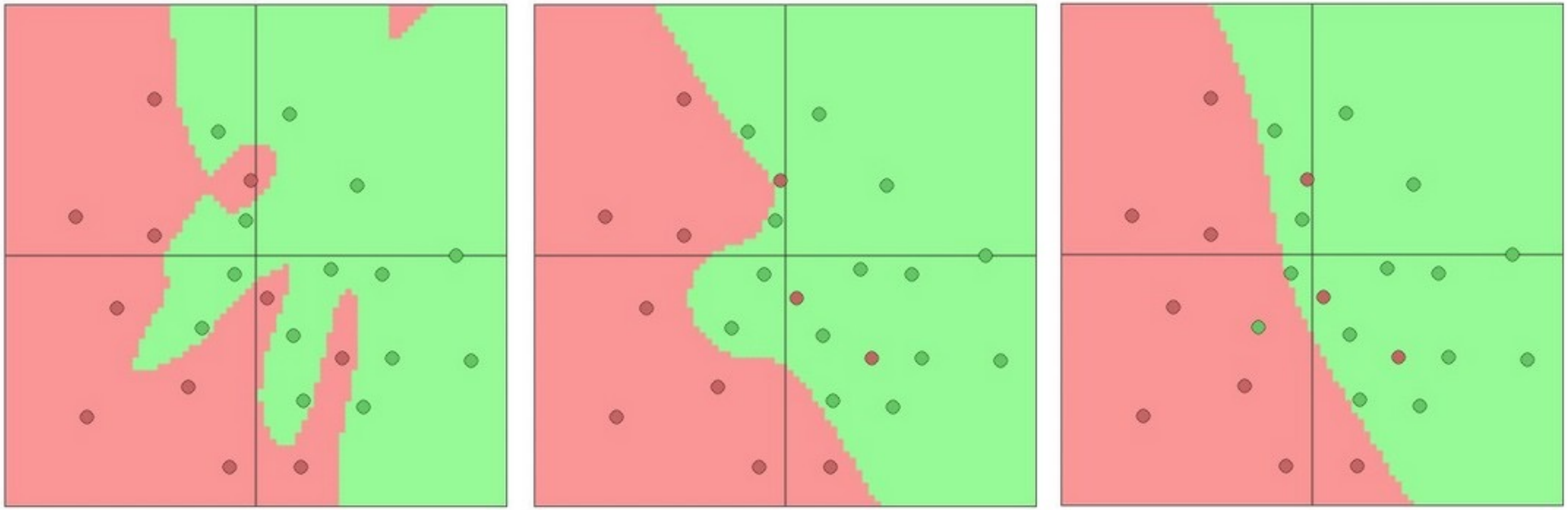
- Gradient derivation for learning with norm penalties found in assigned readings

How to Set Alpha?

Shown is the same neural network with different levels of regularization. Which model has the largest value for alpha (i.e., largest norm penalty contribution)?

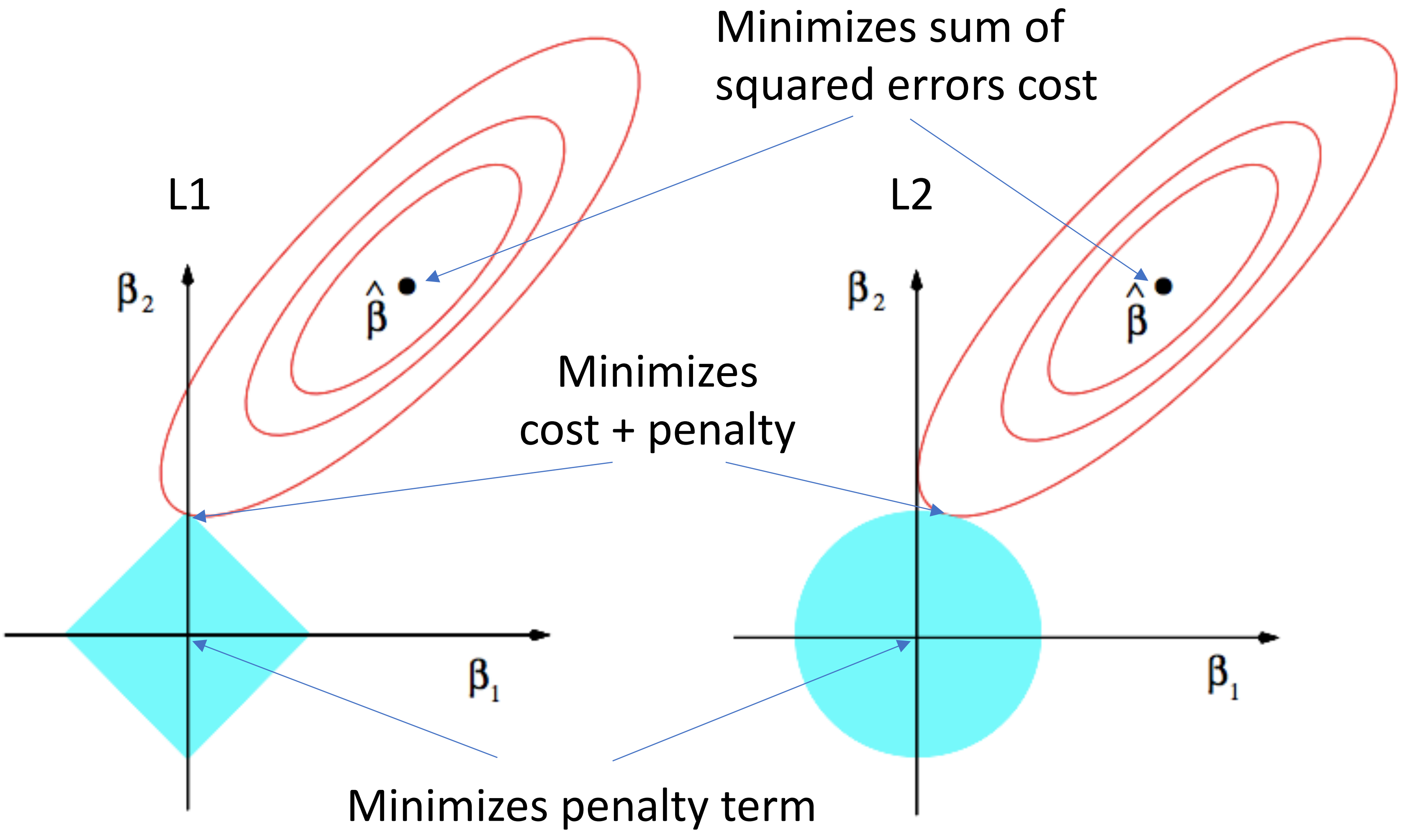
(a) (b) (c)



https://cs231n.github.io/neural-networks-1/

Geometric Interpretation in 2D

Note: L2 commonly used in practice



$|\beta_1| + |\beta_2| \leq t$ $\beta_1^2 + \beta_2^2 \leq t^2$

Contour of least square error function

Contour of regularization constraint functions shown below both plots

https://web.stanford.edu/~hastie/Papers/ESLII.pdf

Implementation Detail: Can Penalize Weights Globally as Well As Per Layer

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Recall: Overfitting Solution is Early Stopping

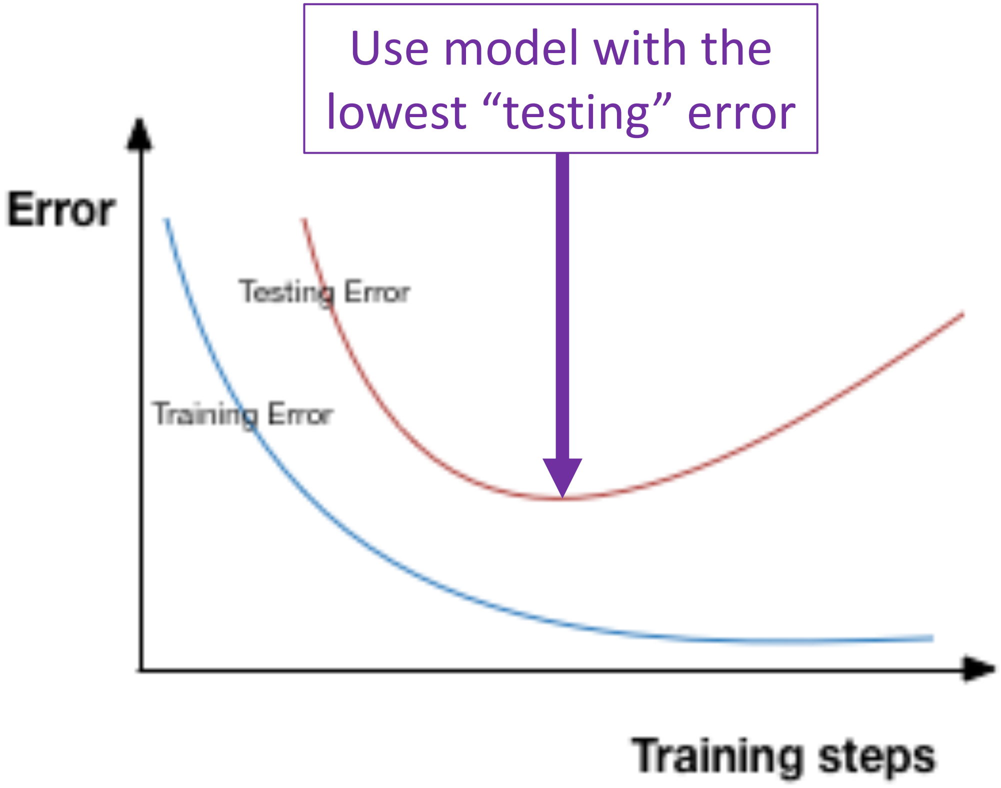
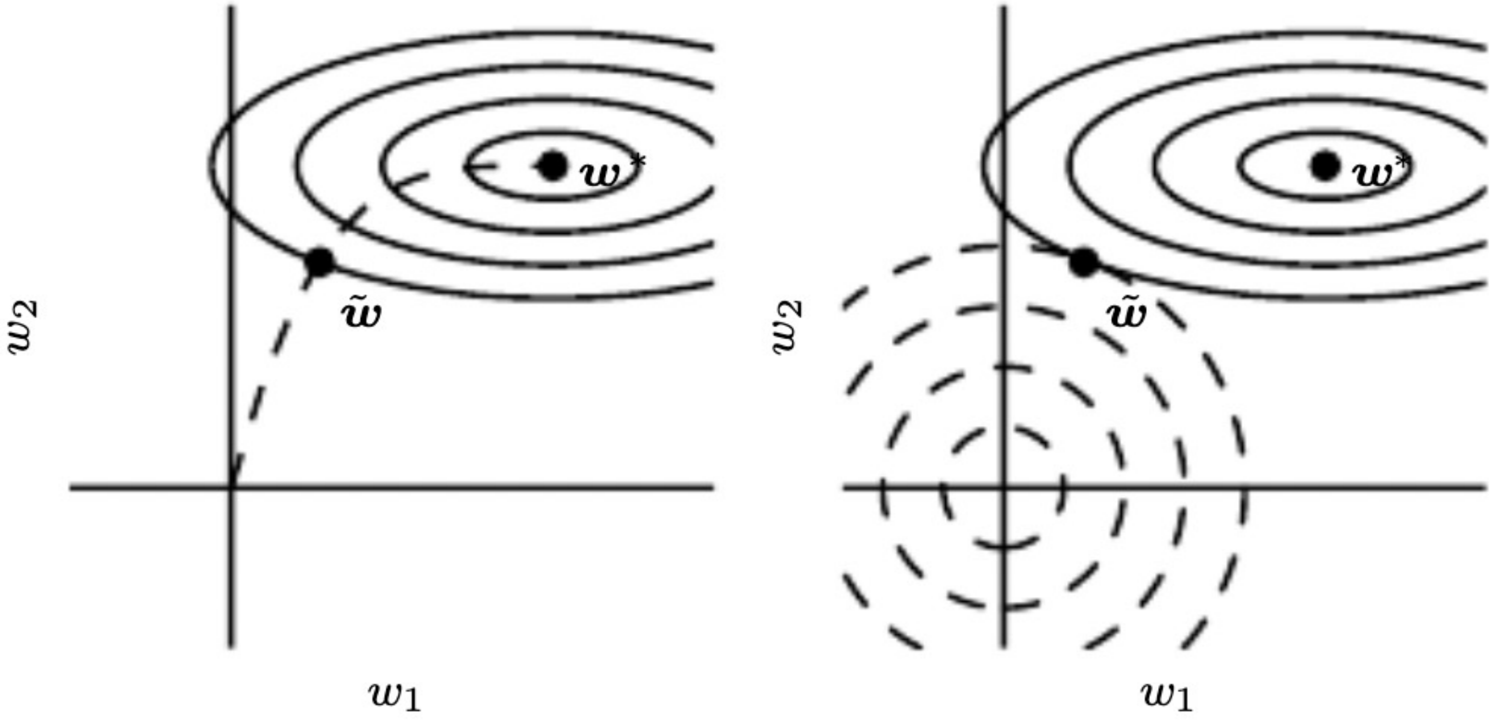


Image Source: https://chatbotslife.com/regularization-in-deep-learning-f649a45d6e0

Why Early Stopping Acts As a Regularizer

With parameters initialized around the origin, early stopping can behave like a parameter norm penalty (e.g., L2, without having a hyperparameter to tune) since weight values have an insufficient training duration to grow too large; e.g.,



https://www.deeplearningbook.org/contents/regularization.html

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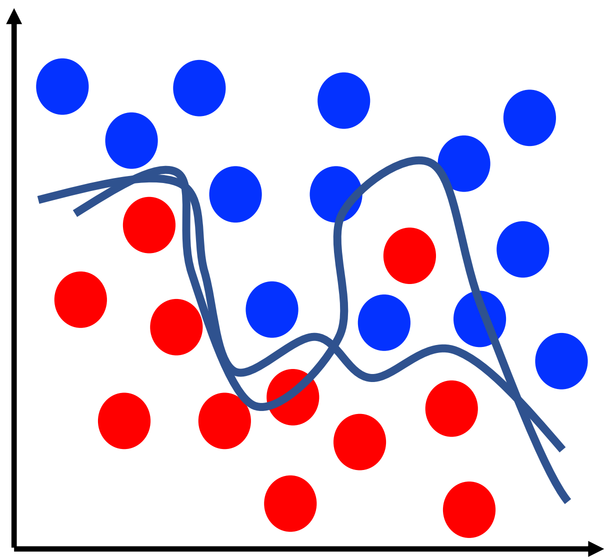
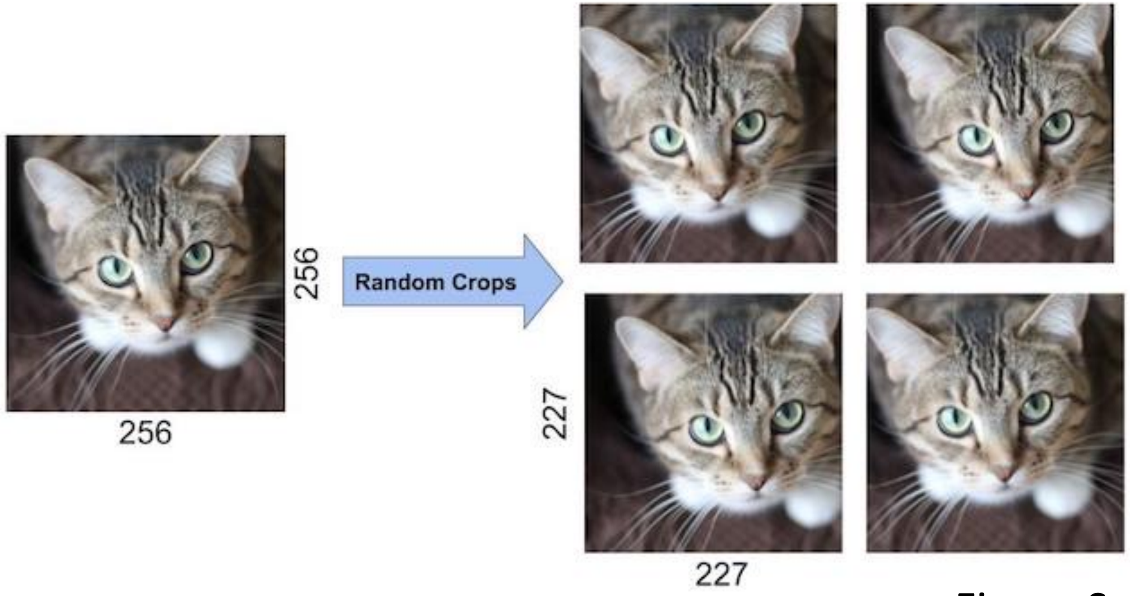
Recall: Overfitting Solution is to Add Data

Adding training data



AlexNet's Data Augmentation Strategy

- Recall overfitting is risk for models with larger representational capacity, and AlexNet has 60 million parameters!
- Data augmentation strategy
    1. Random patches and their mirror images (2048x more data)
    2. Adjust RGB channels (using PCA to add multiples of principal components)



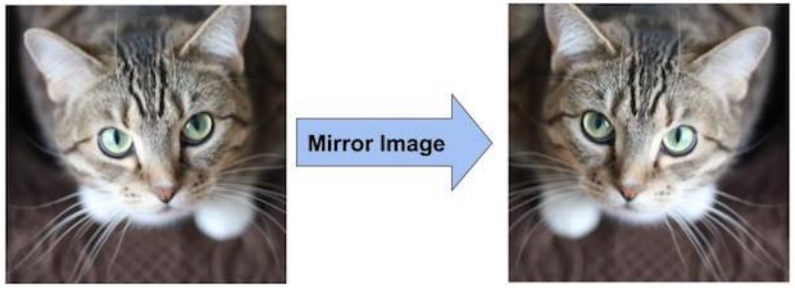
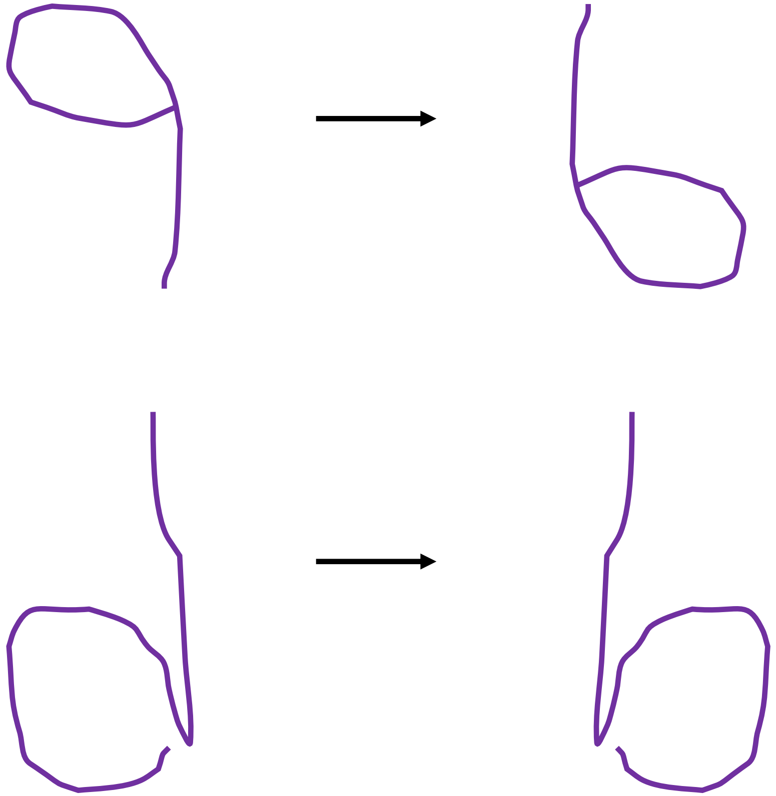


Figure Source: https://learnopencv.com/understanding-alexnet/

Caution: Match Augmentation Scheme to Data

- e.g., image mirroring and flipping could be poor choices for character recognition



Class Discussion

1. When/why are random patches a good/poor choice for data augmentation?

2. How else can you augment data for learning image classification models?

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Idea: Use Wisdom of the Crowds

More than 1: Ensemble

Why Choose Ensemble vs One Predictor?

- Reduces probability for making a wrong prediction
- Suppose:
  - n classifiers for binary classification task
  - Each classifier has same error rate ε
  - Classifiers are independent (not true in practice!)
  - Probability mass function indicates the probability of error from an ensemble:

Number of classifiers

Classifier error rate

$$P(y \ge k) = \sum_{k}^{\boxed{n}} \boxed{\binom{n}{k}} \varepsilon^k (1 - \boxed{\varepsilon})^{n-k} = \boxed{\varepsilon_{ensemble}}$$

Error probability

ways to choose *k* subsets from set of size *n*

  - e.g., n = 11, ε = 0.25; k = 6: probability of error is ~0.034 which is much lower than probability of error from a single algorithm (0.25)

How to Produce an Ensemble? - Bagging

Bootstrap Aggregation (1994)

Train algorithm repeatedly on different random subsets of the training set

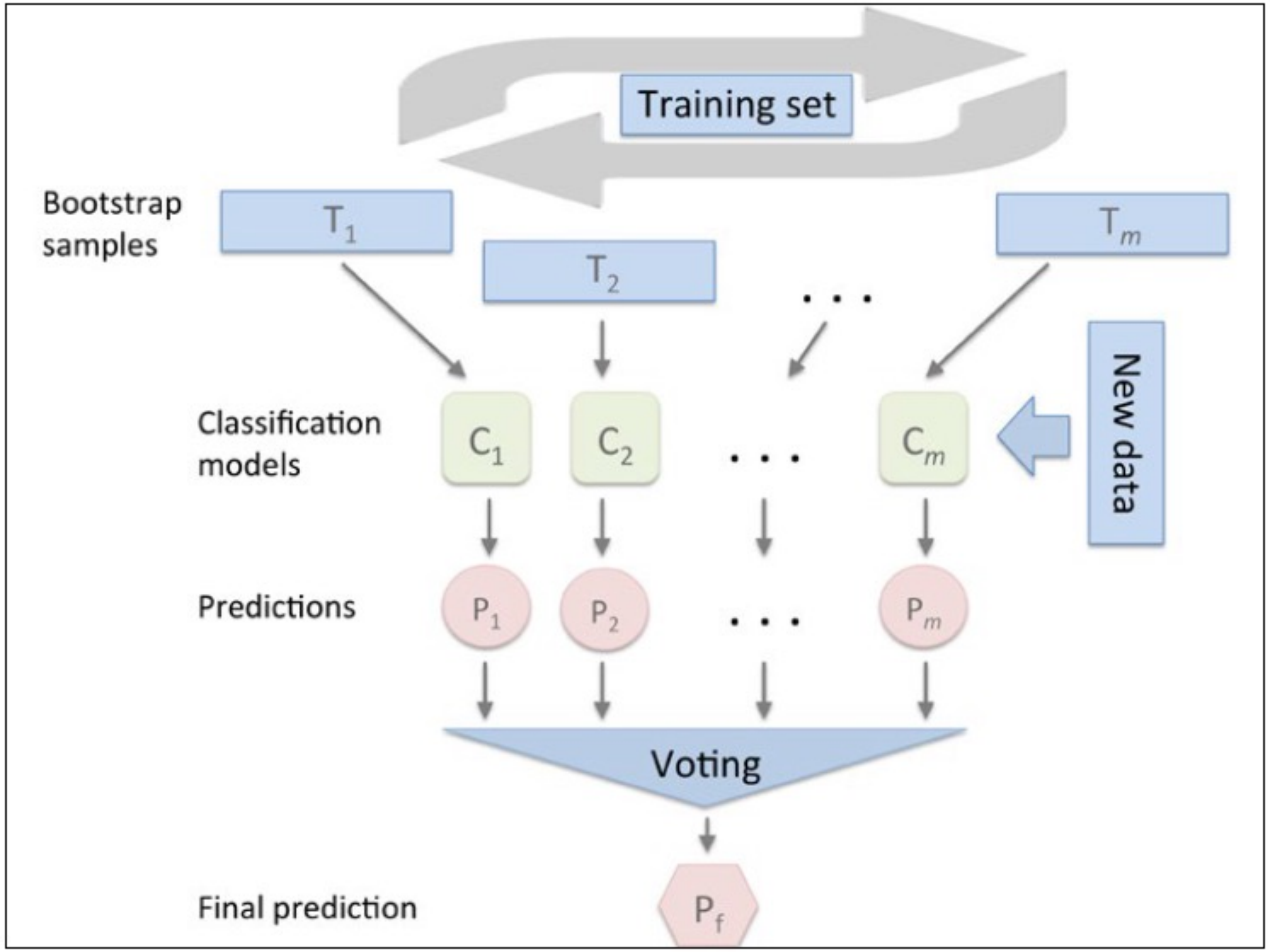


Figure Credit: Raschka & Mirjalili, Python Machine Learning.

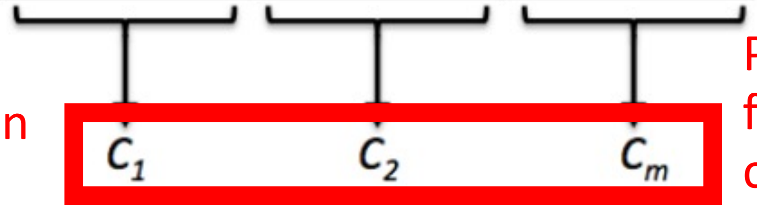
How to Produce an Ensemble? - Bagging

- Build ensemble from "bootstrap samples" drawn with replacement
- e.g.,

Sample indices	Bagging round 1	Bagging round 2	...
1	2	7	...
2	2	3	...
3	1	2	...
4	3	1	...
5	7	1	...
6	2	7	...
7	4	7	...

Duplicate data can occur for training

Some examples missing from training data; e.g., round 1



Each classifier trained on different subset of data

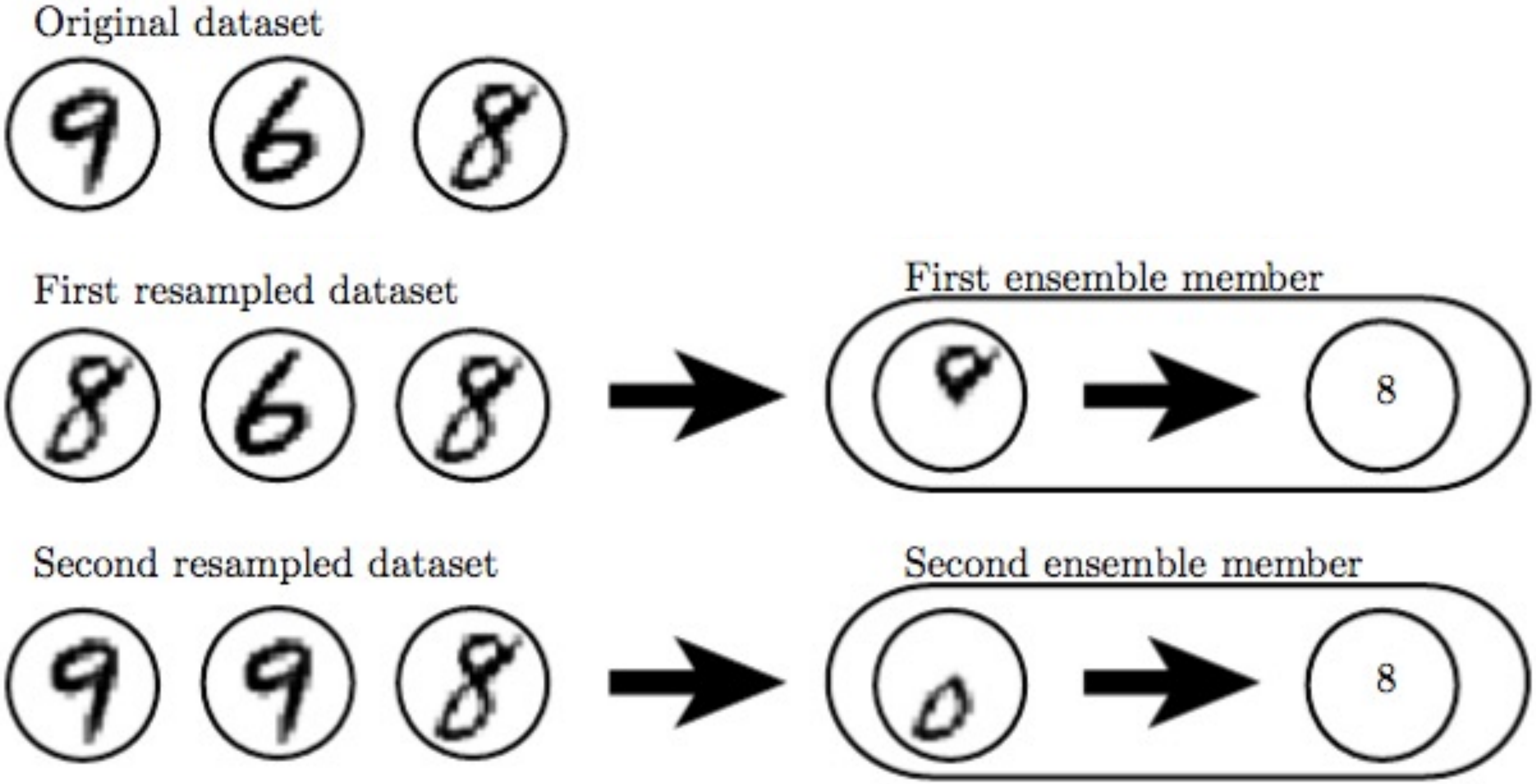
Predictions made from votes by classifiers

Breiman, Bagging Predictors, 1994.

Ho, Random Decision Forests, 1995.

Figure Credit: Raschka & Mirjalili, Python Machine Learning.

Intuition of Bagging (Train an 8 detector)



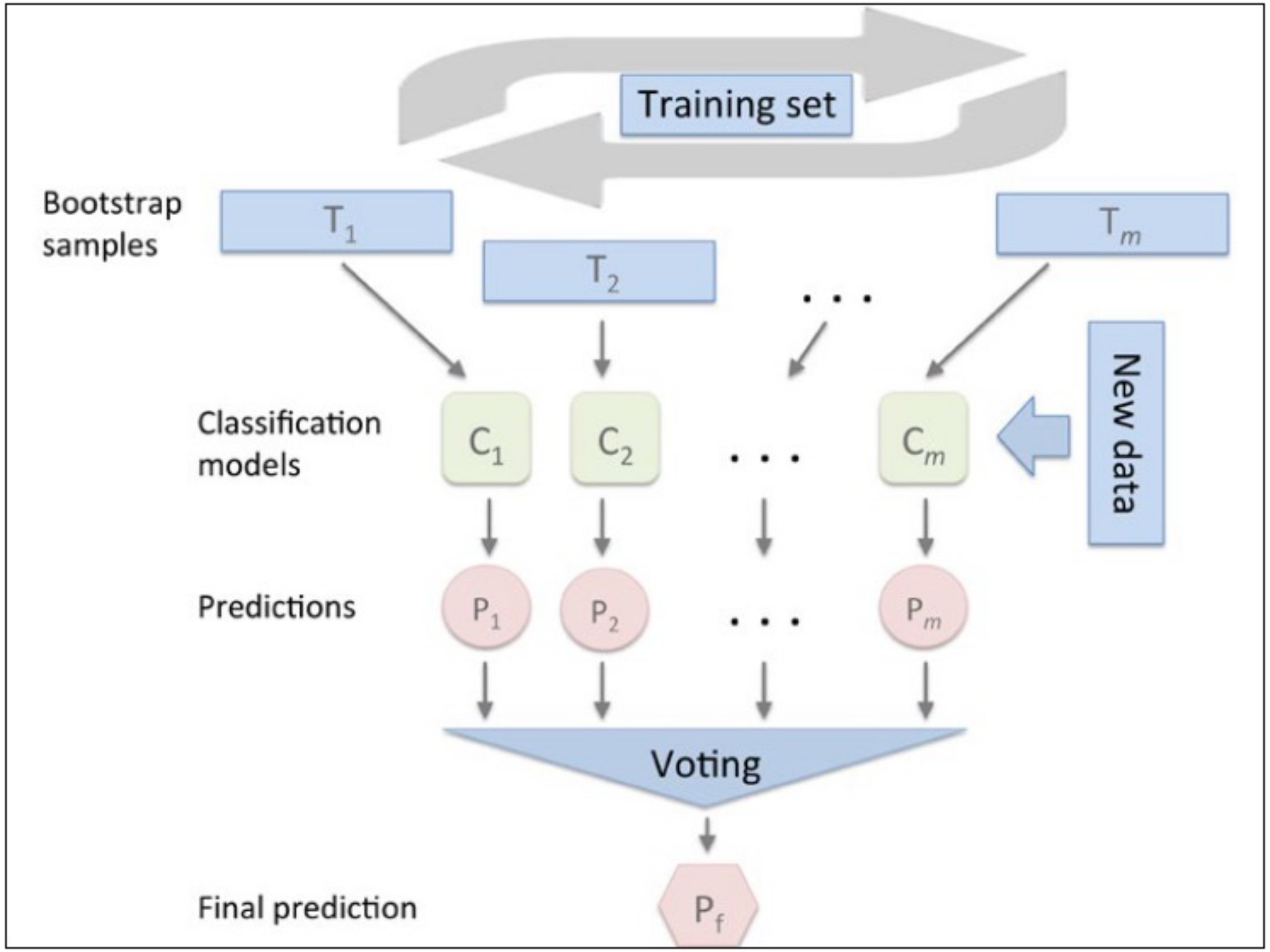
Goodfellow et al., Deep Learning (chapter 7), 2016.

Bagging Limitations

Train algorithm repeatedly on different random subsets of the training set

Why is bagging a poor approach for neural networks?

- Finding optimal hyperparameters for each architecture is time-consuming
- Applying multiple neural networks is often infeasible since the models require lots of memory and are computationally expensive to run



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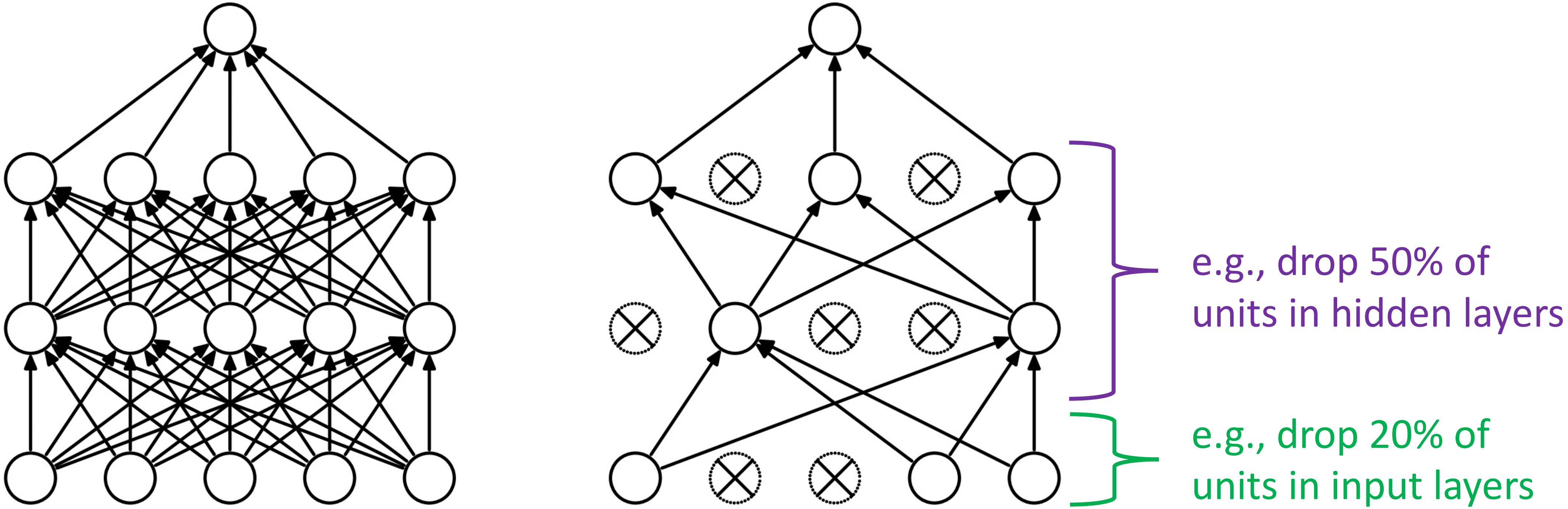
How to Produce an Ensemble?

- Idea: approximate bagging with dropout during training so different sub-models in the network are trained with different training data



(a) Standard Neural Net (b) After applying dropout.

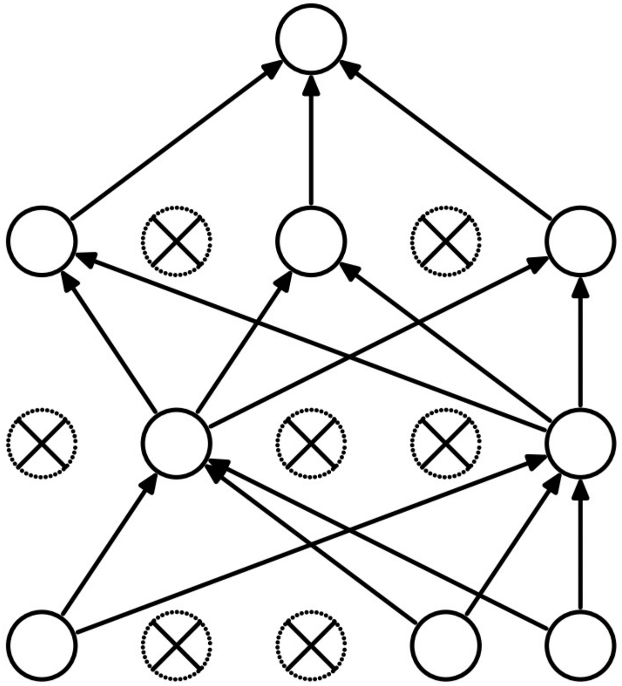
Srivastava et al. Dropout: A Simple Way to Prevent Neural Networks from Overfitting. Journal of Machine Learning Research. 2014

How to Produce an Ensemble?

- Idea: approximate bagging with dropout during training so different sub-models in the network are trained with different training data

For training, the forward pass and backpropagation run only through the sub-network (with a different dropout per minibatch).

Note dropout can lead to bouncier loss curves since the underlying network continuously changes.



(b) After applying dropout.

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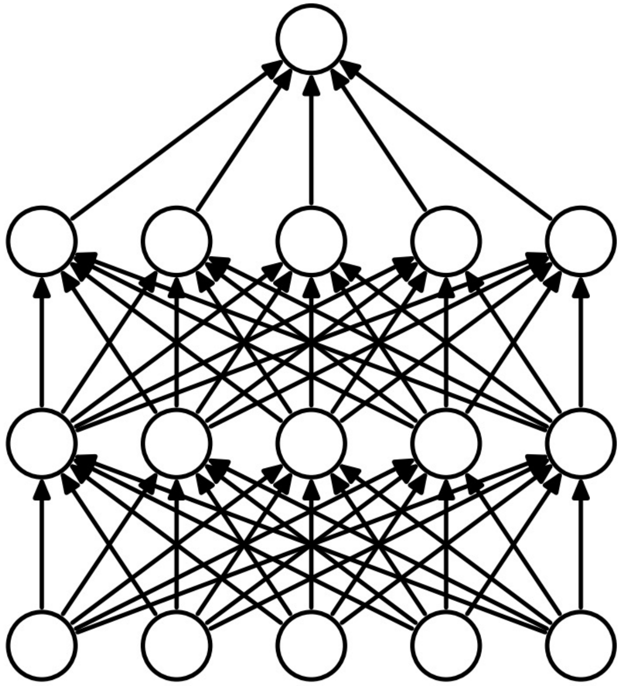
How to Produce an Ensemble?

- Idea: approximate bagging with dropout during training so different sub-models in the network are trained with different training data

An ensemble is emulated at test time by applying the network without dropout.

To reflect the network's expectation for a smaller activation signal than observed at test time (e.g., input from 2 versus 5 units), each unit's outgoing weights should be multiplied by the probability it was dropped at training.

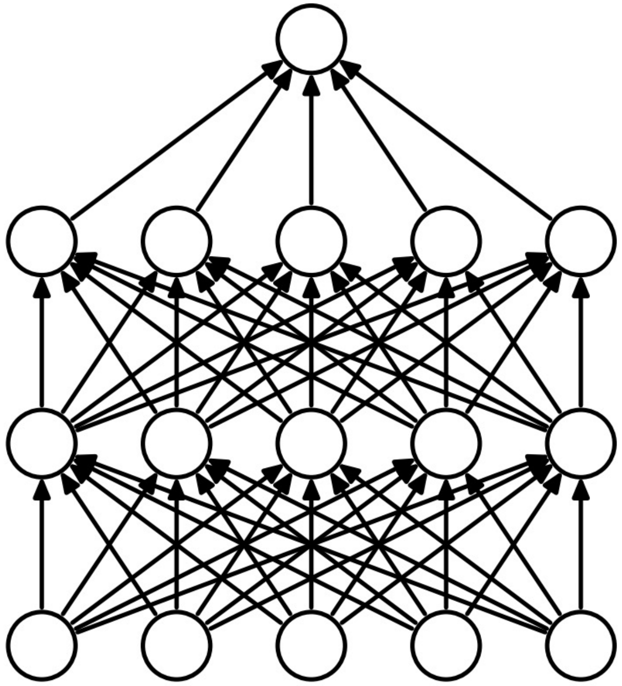


(b) After applying dropout.

Srivastava et al. Dropout: A Simple Way to Prevent Neural Networks from Overfitting. Journal of Machine Learning Research. 2014

Dropout vs Bagging

- Dropout approximates bagging with many models inexpensively
  - Trains algorithm repeatedly on different random subsets of the training set
- Dropout differences are that subnetworks are not:
  - Trained to convergence (instead, trained for one step)
  - Independent (instead, they all share parameters)



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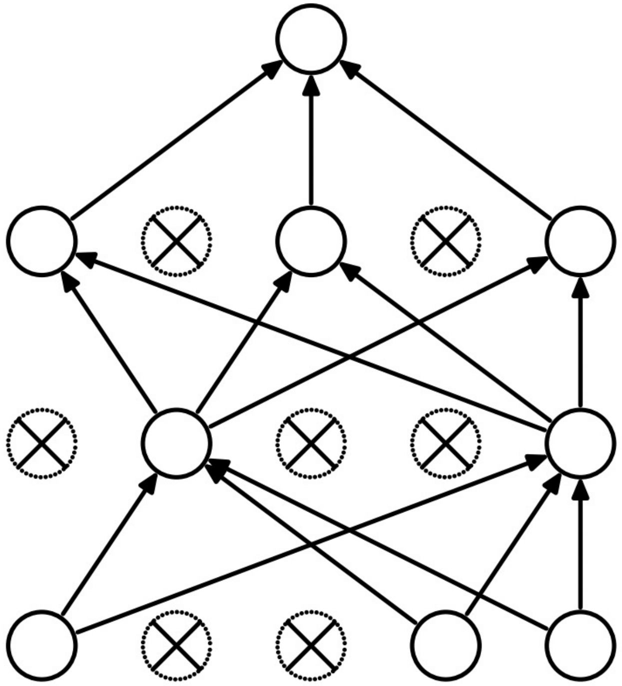
Motivation for Dropout

This approach was motivated by the role of sex in evolution. "… the role of sexual reproduction is not just to allow useful new genes to spread throughout the population, but also to facilitate this process by reducing complex co-adaptations that would reduce the chance of a new gene improving the fitness of an individual."



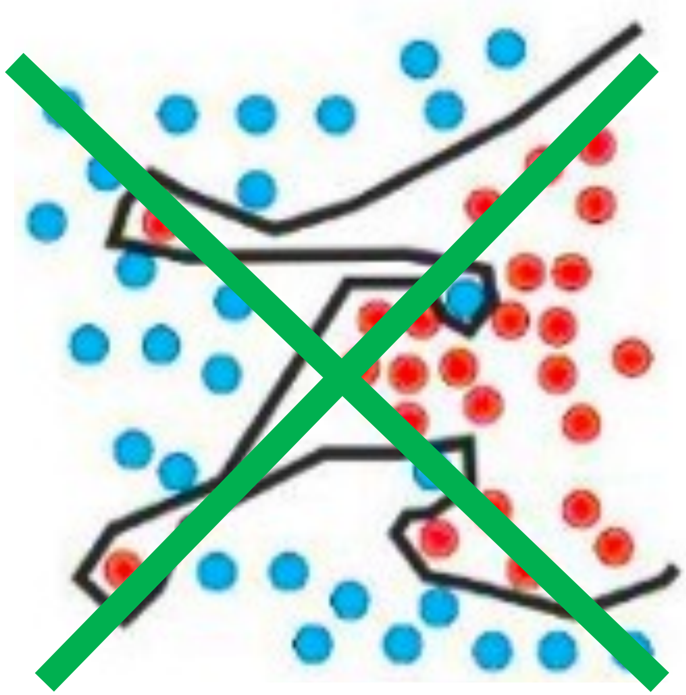
(b) After applying dropout.

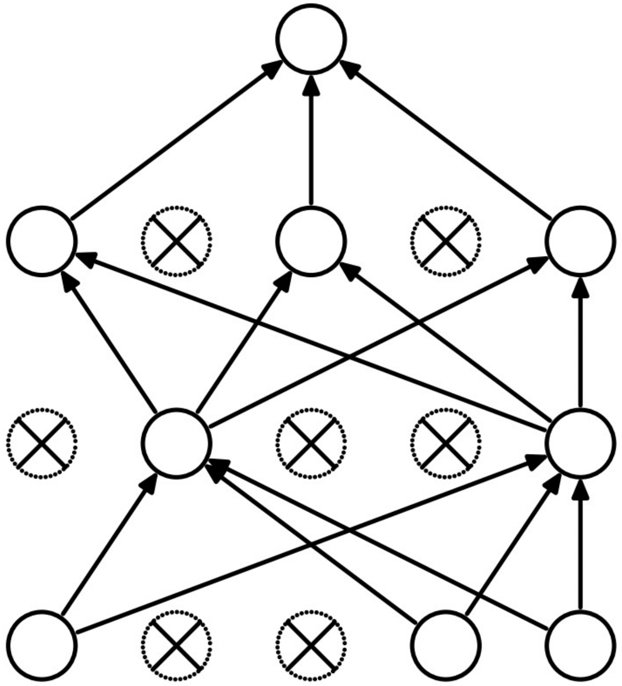
"Similarly, each hidden unit in a neural network trained with dropout must learn to work with a randomly chosen sample of other units. This should make each hidden unit more robust and drive it towards creating useful features on its own without relying on other hidden units to correct its mistakes."

Srivastava et al. Dropout: A Simple Way to Prevent Neural Networks from Overfitting. Journal of Machine Learning Research. 2014

Motivation for Dropout

Units in the network learn to be useful with many different subsets of other units rather than in conjunction with other units; e.g., mitigates the situation where large positive weights cancel similarly large negative weights, a sign of overfitting.





(b) After applying dropout.

https://towardsdatascience.com/techniques-for-handling-underfitting-and-overfitting-in-machine-learning-348daa2380b9
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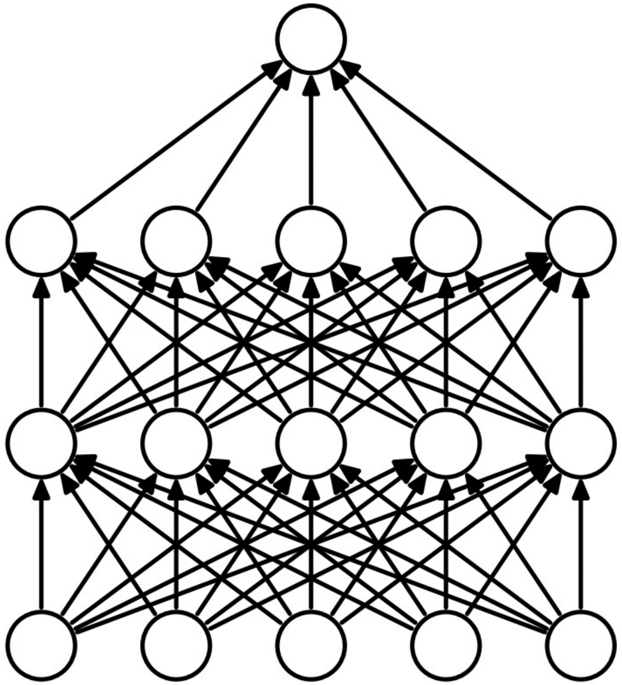
How to Produce an Ensemble?

A generalization of zeroing units out is to instead multiply units by noise; this is common for convolutional layers



(b) After applying dropout.

Relevant articles:
*https://towardsdatascience.com/dropout-on-convolutional-layers-is-weird-5c6ab14f19b2
*Wu and Gu. "Towards dropout training for convolutional neural networks." Neural Networks, 2015.

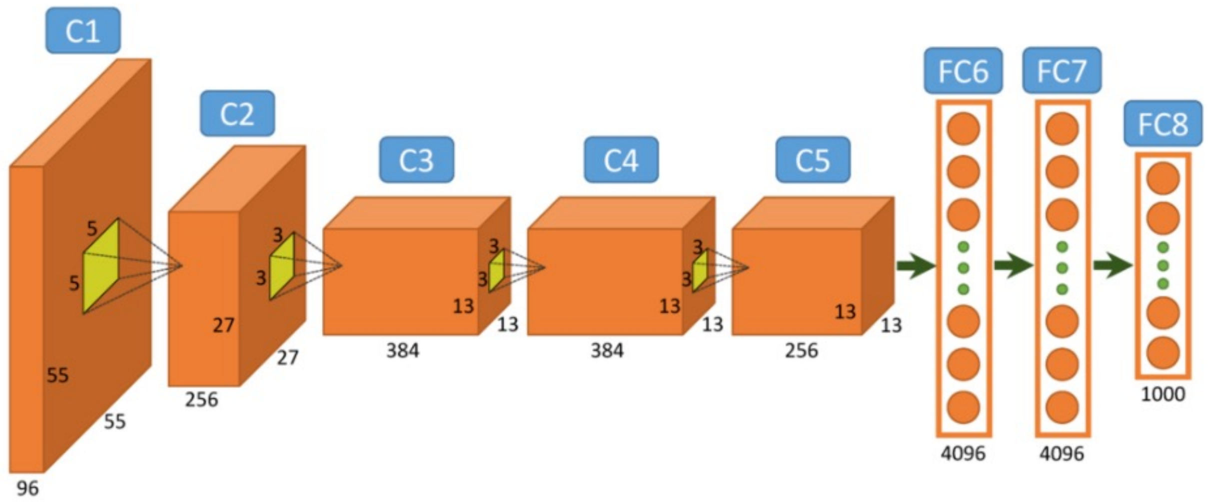
Srivastava et al. Dropout: A Simple Way to Prevent Neural Networks from Overfitting. Journal of Machine Learning Research. 2014

Dropout for CNNs

For image classification algorithms we discussed, dropout is used only in fully connected layers; why do you think it is typically not used in convolutional layers?

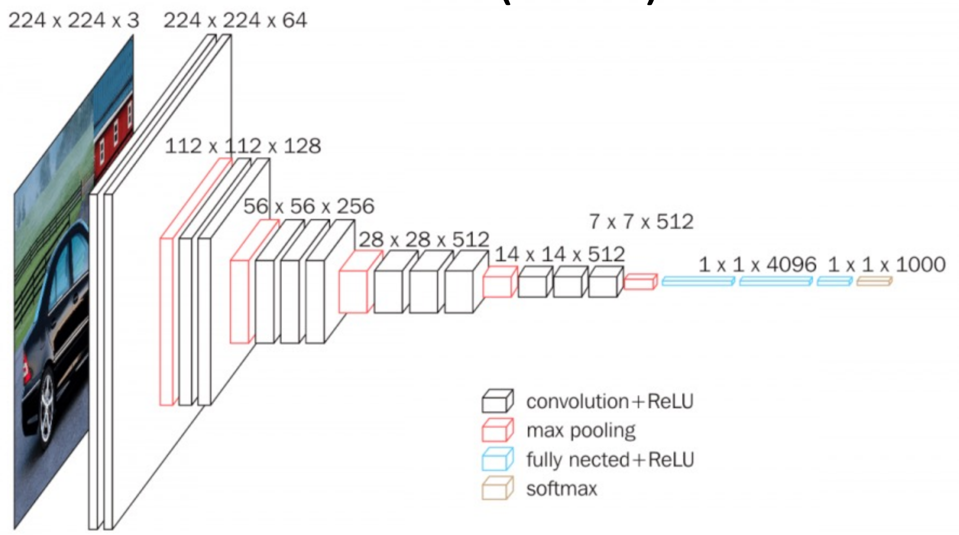
- Parameter tying reduces parameter count and so already offers regularization

AlexNet (2012)



https://www.researchgate.net/figure/Architecture-of-Alexnet-From-left-to-right-input-to-output-five-convolutional-layers_fig2_312303454

VGG (2014)



https://neurohive.io/en/popular-networks/vgg16/

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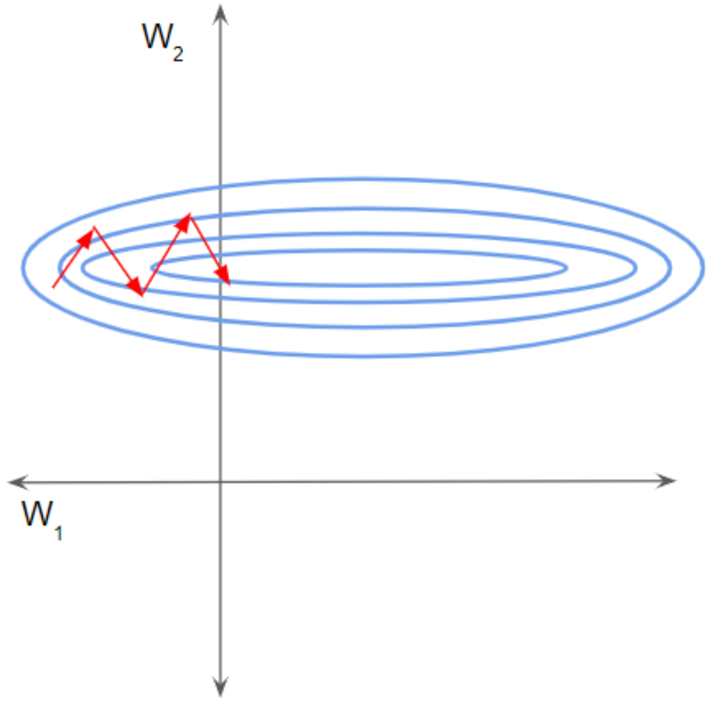
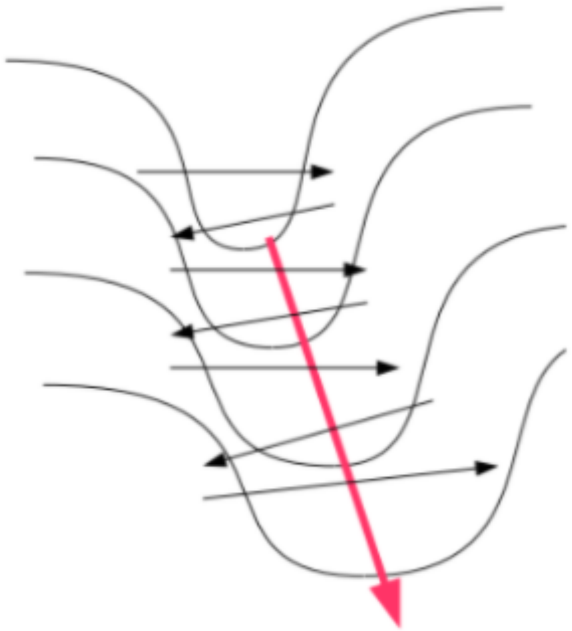
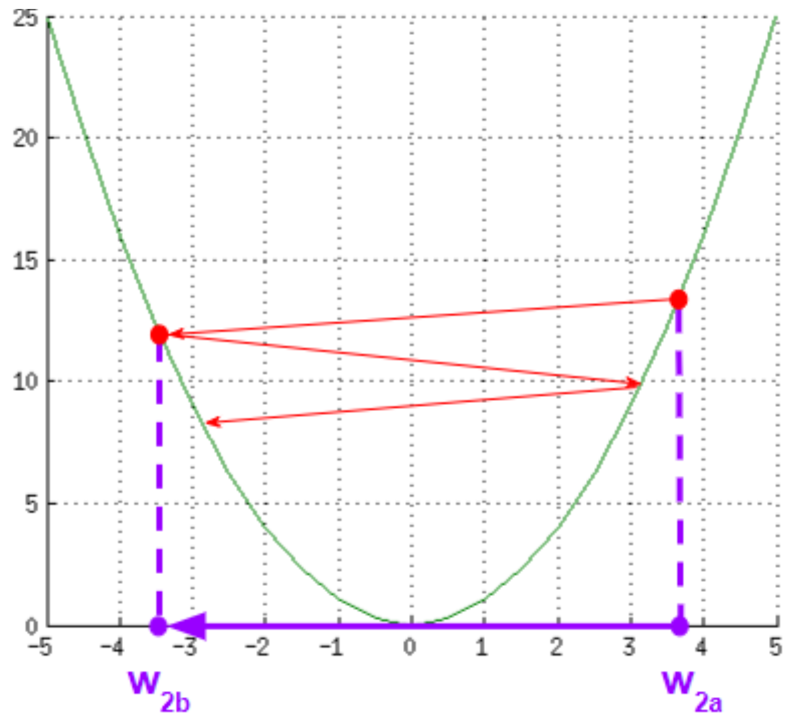
Motivation: Features On Different Scales Can Cause Learning To Be Slower and Poor Performance

e.g., 2D loss function:



Inefficient bouncing can occur during learning when larger updates are needed for some weights to minimize the loss during gradient descent



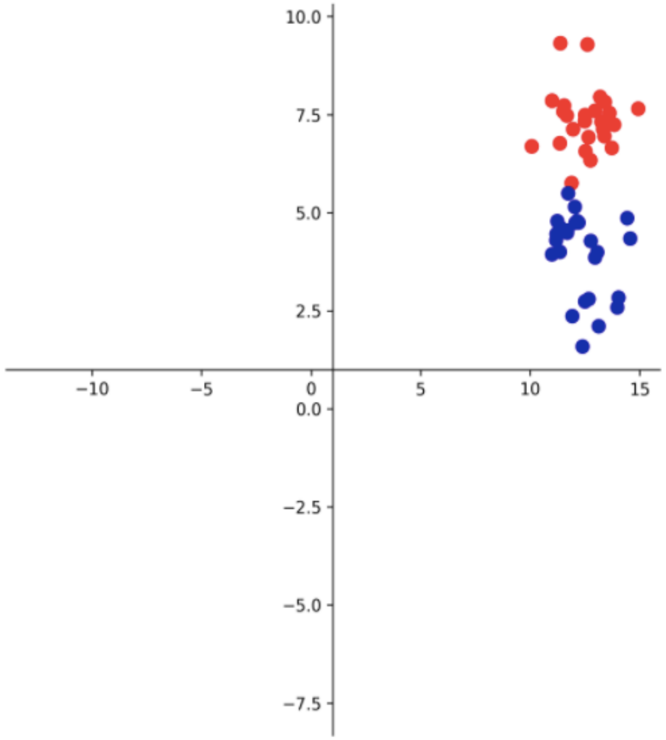


https://towardsdatascience.com/batch-norm-explained-visually-how-it-works-and-why-neural-networks-need-it-b18919692739

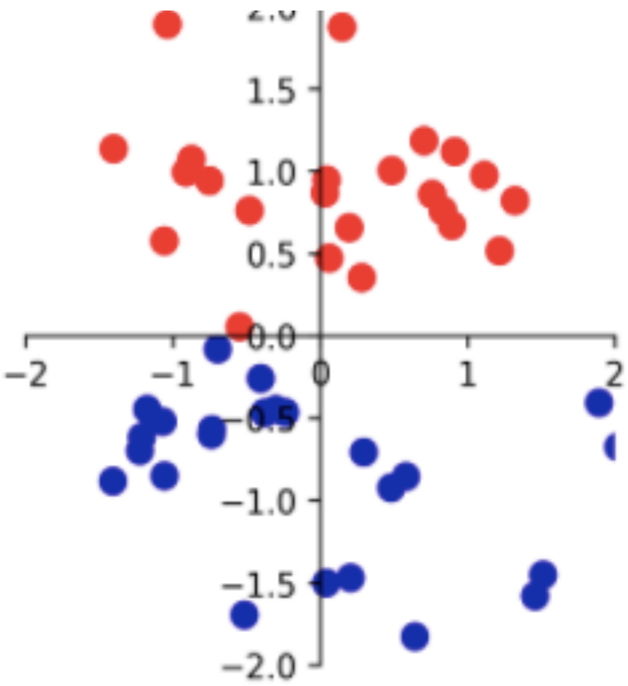
Recall: Basic Data Initialization Approach

* Simplify learning by standardizing input data so mean is 0 and standard deviation 1

Original data:



Standardized data:



https://github.com/amueller/introduction_to_ml_with_python/blob/master/03-unsupervised-learning.ipynb

Recall: Basic Data Initialization Approach

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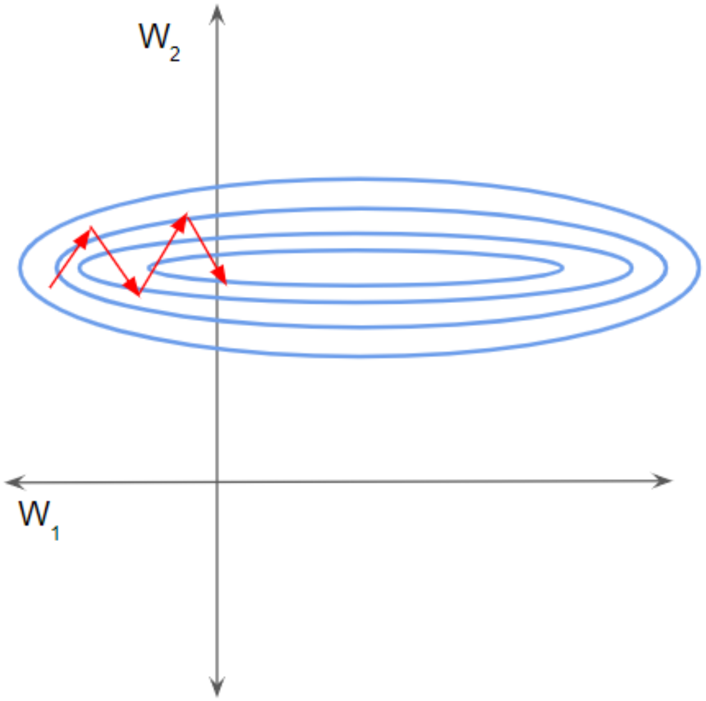
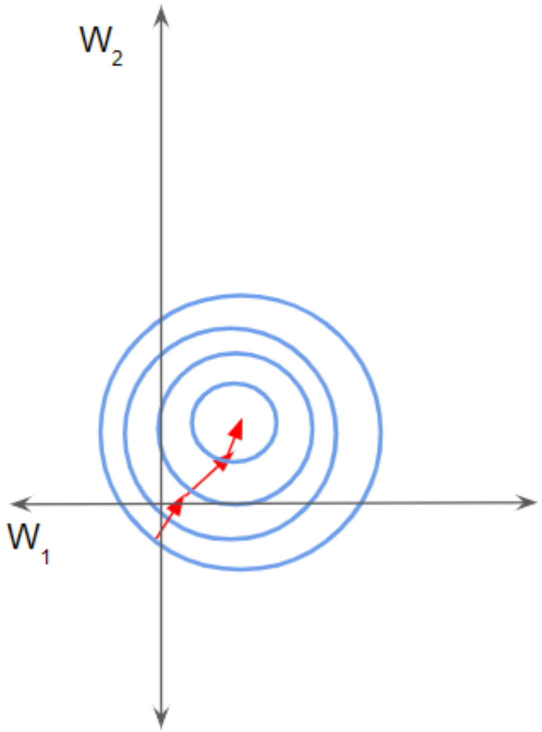


Standardization changes the loss function so gradient descent can more smoothly arrive at the minimum!



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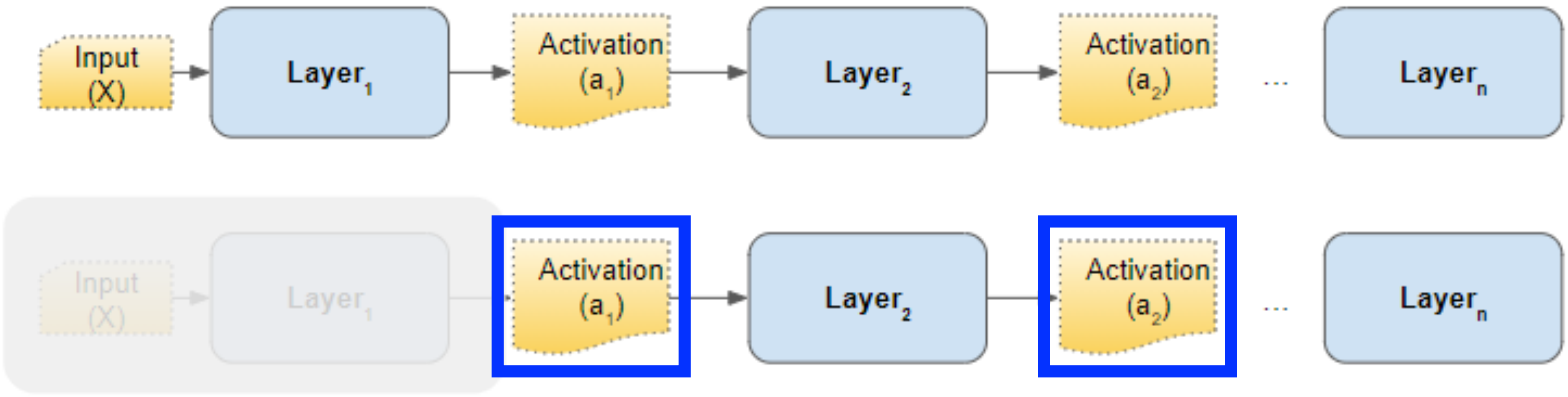
Idea: Further Simplify Learning by Transforming Input to Hidden Layer(s)



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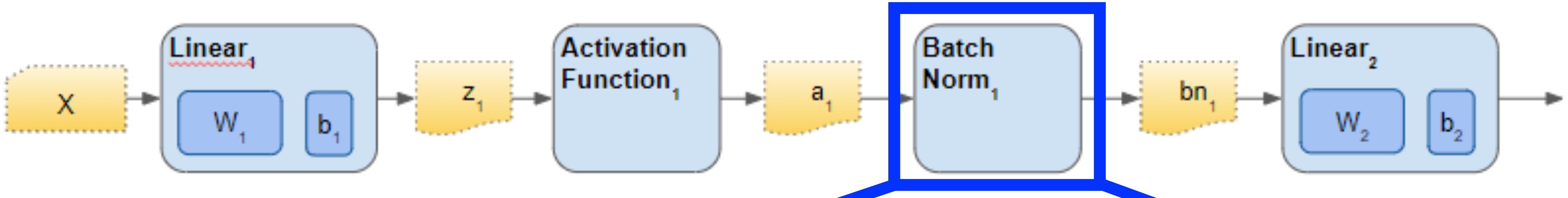
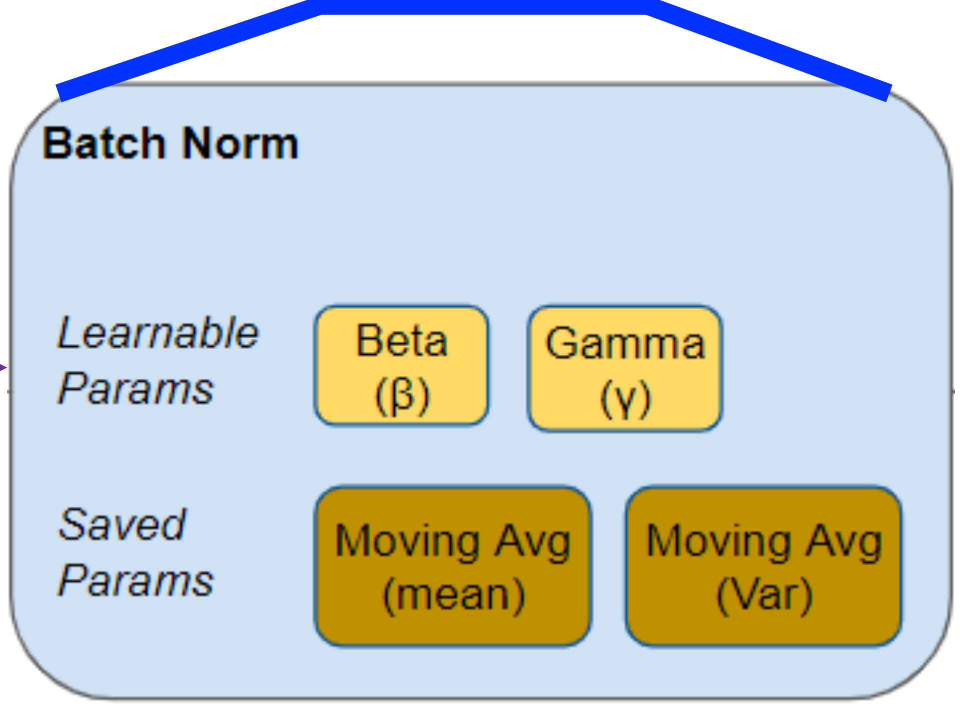
Batch Normalization Layer



Parameters per layer:

Offers flexibility for each layer to shift and scale a minibatch's activation values to a *learned* mean and variance that improves learning



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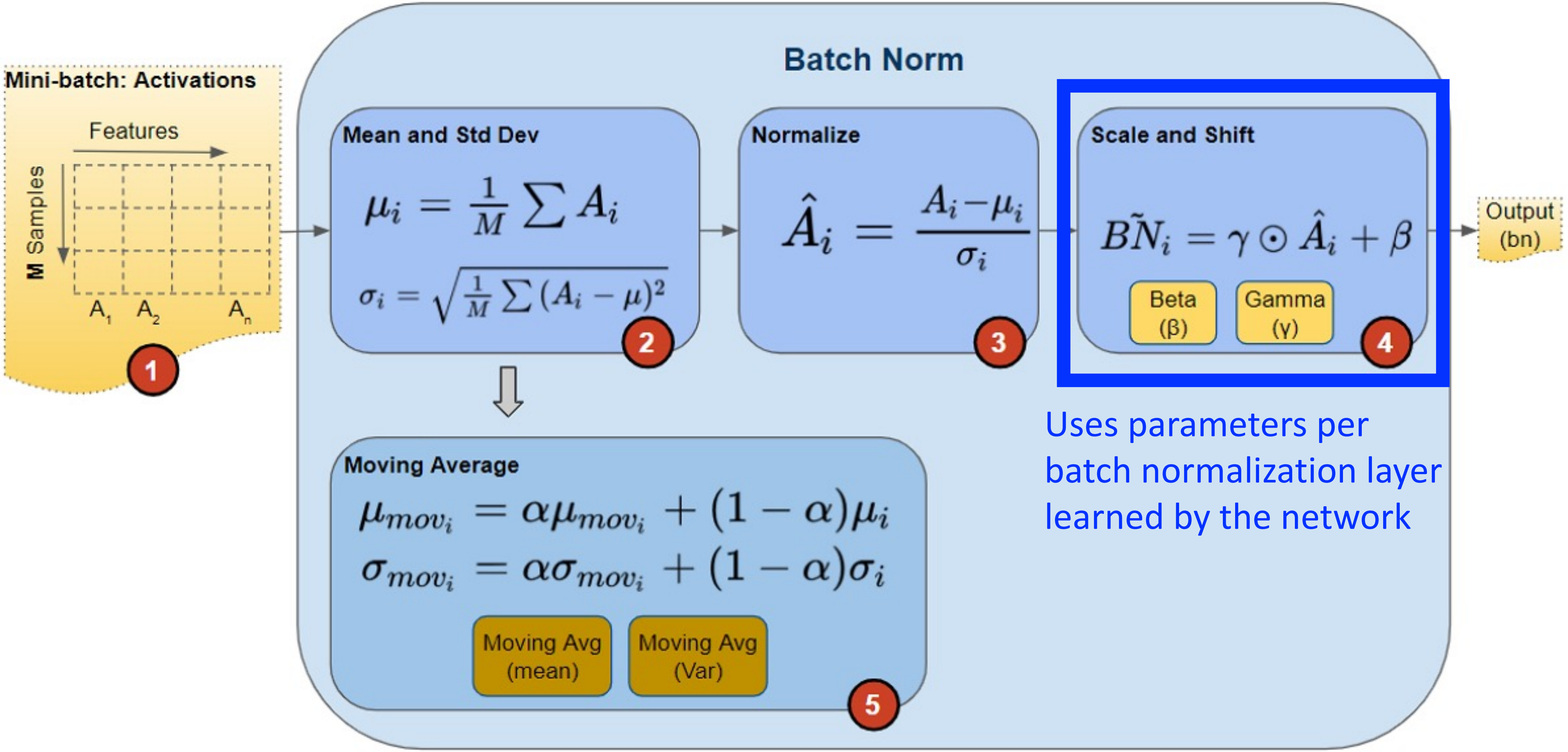
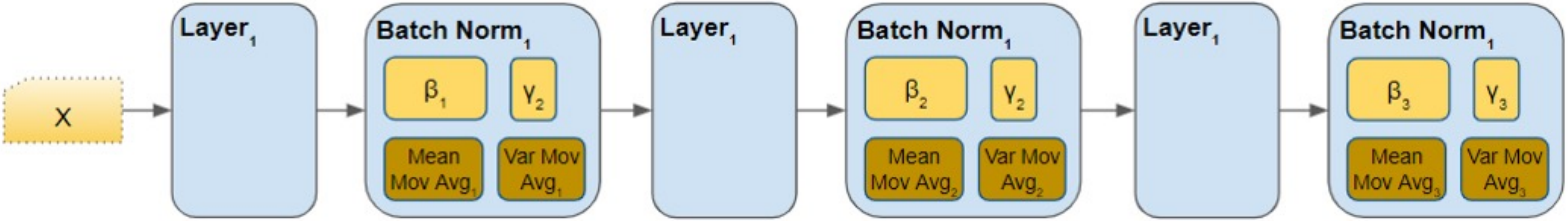
Batch Normalization Layer: Training Operation



https://towardsdatascience.com/batch-norm-explained-visually-how-it-works-and-why-neural-networks-need-it-b18919692739

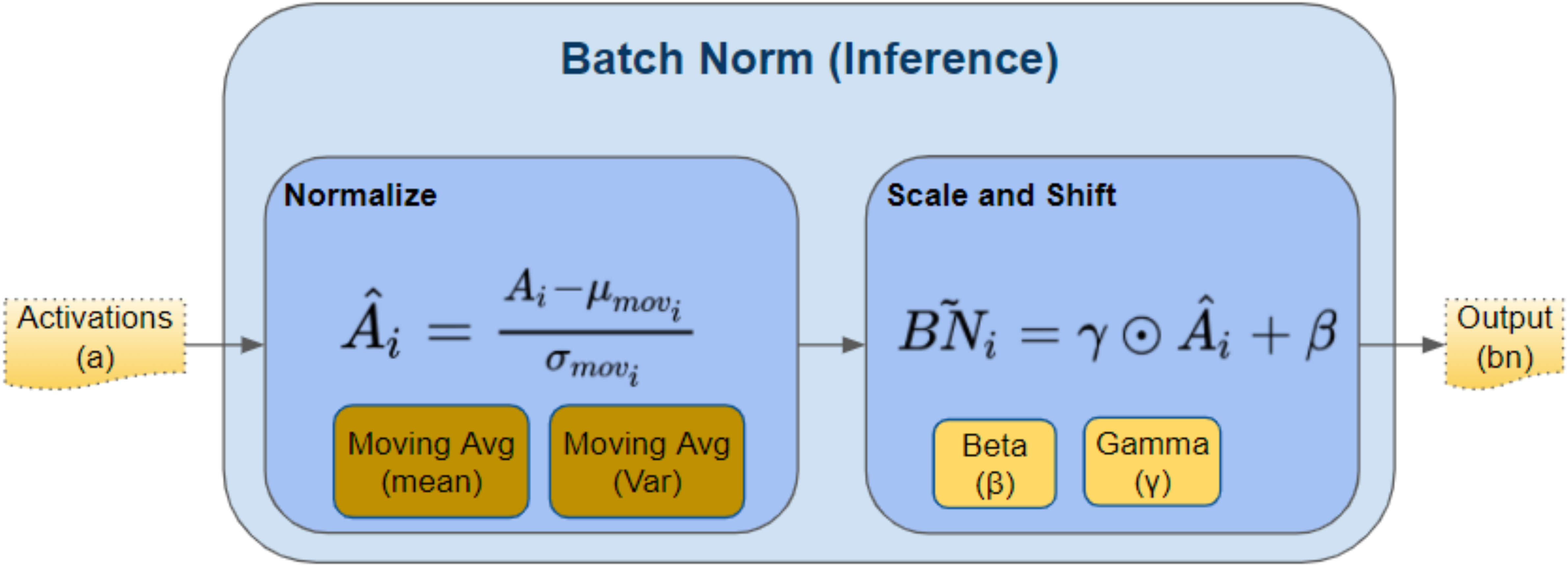
Batch Normalization Layer: Training Operation

How many trainable parameters must be learned during training for this subnetwork?



https://towardsdatascience.com/batch-norm-explained-visually-how-it-works-and-why-neural-networks-need-it-b18919692739

Batch Normalization Layer: Test-Time Operation



Layer brings a regularizing effect by introducing additive and multiplicative “noise”

https://towardsdatascience.com/batch-norm-explained-visually-how-it-works-and-why-neural-networks-need-it-b18919692739

Benefits and Limitations

- Pros - smooths the optimization function leading to:
  - Faster training convergence
  - More stable learning when paired with different hyperparameters and initializations
  - Better generalization performance

- Cons - extra layer(s) introduce more training and testing time

Santurkar et al. How Does Batch Normalization Help Optimization? Neurips 2018.

Today’s Topics

- Regularization
- Parameter norm penalty
- Early stopping
- Dataset augmentation
- Dropout
- Batch normalization
- Programming tutorial

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The End

Layer Normalization

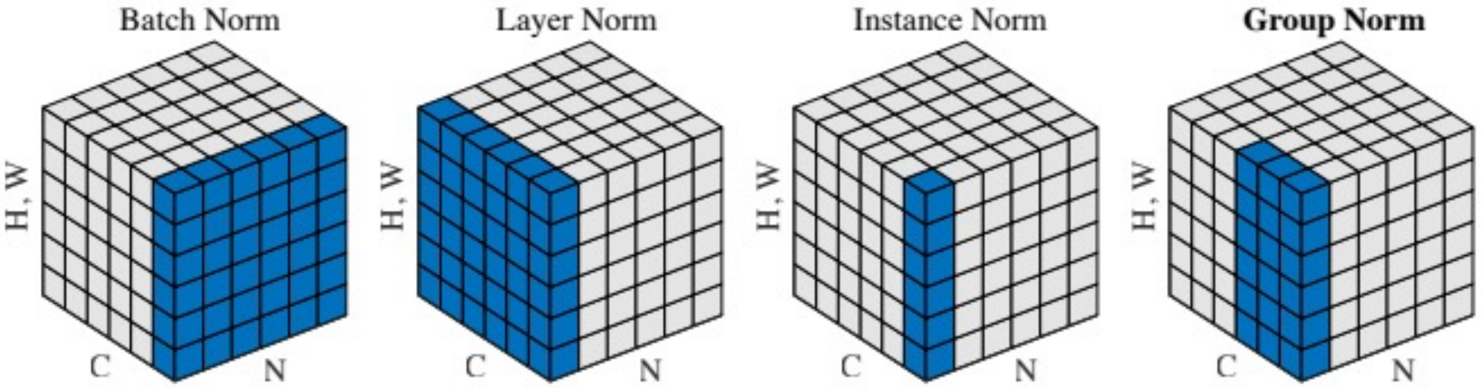

Image source: Wu, Y., & He, K. (2018). Group normalization. ECCV

https://sebastianraschka.com/pdf/lecture-notes/stat453ss21/L19_seq2seq_rnn-transformers__slides.pdf