Experimental Setup, Model Selection, Overfitting, Regularization

Explaining concepts with a polynomial fitting example

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Outline

- Learning Goals
- Experimental setup and model selection
- Overfitting and regularization
- Metrics
- Summary

Learning Goals

- Explain how to design your experiment
- Introduce how to select your model
- Introduce the concepts of *over-fitting*, *under-fitting*, and *model generalization*.
- Introduce the concept of *regularization* for reducing model *over-fitting*.

Hands-on Tutorial

- https://github.com/rmsouza01/ENSF617-ENEN-645-W2026

- **Tutorial**: Model selection, overfitting, regularization

- Based on the example presented in chapter 1 of the book: **Christopher M. Bishop. 2006. Pattern Recognition and Machine Learning (Information Science and Statistics). Springer-Verlag New York, Inc., Secaucus, NJ, USA.**

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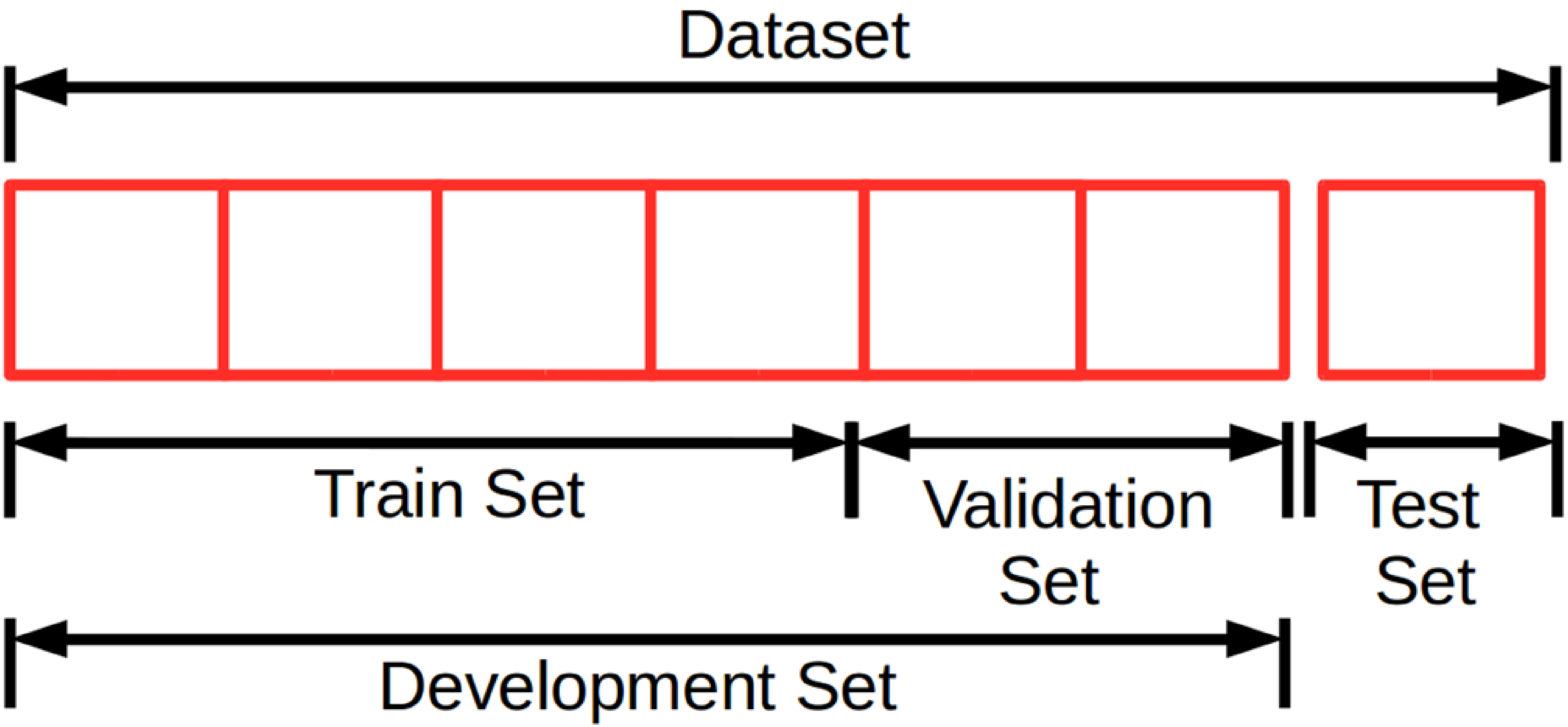
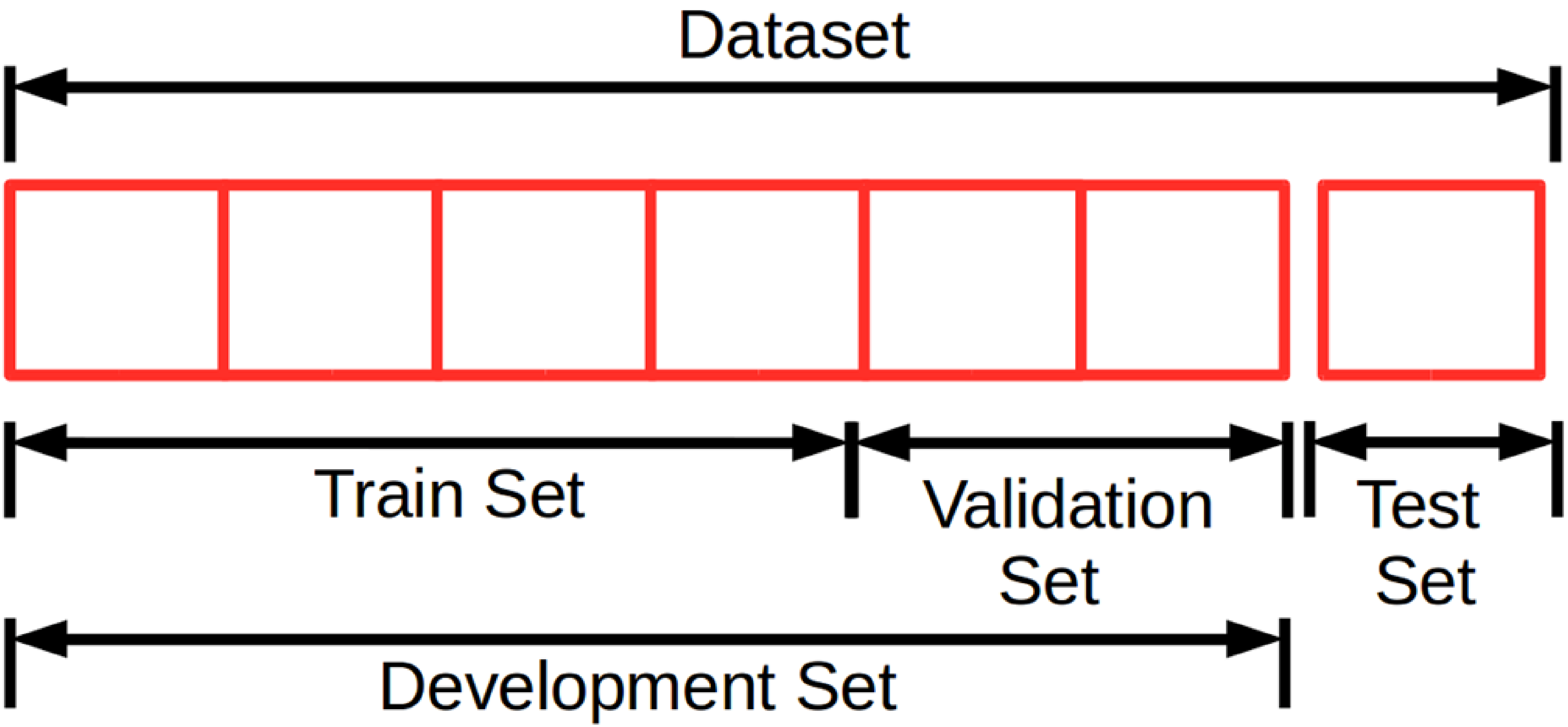
Experiment Design: Train, Validation and Test



WHY?

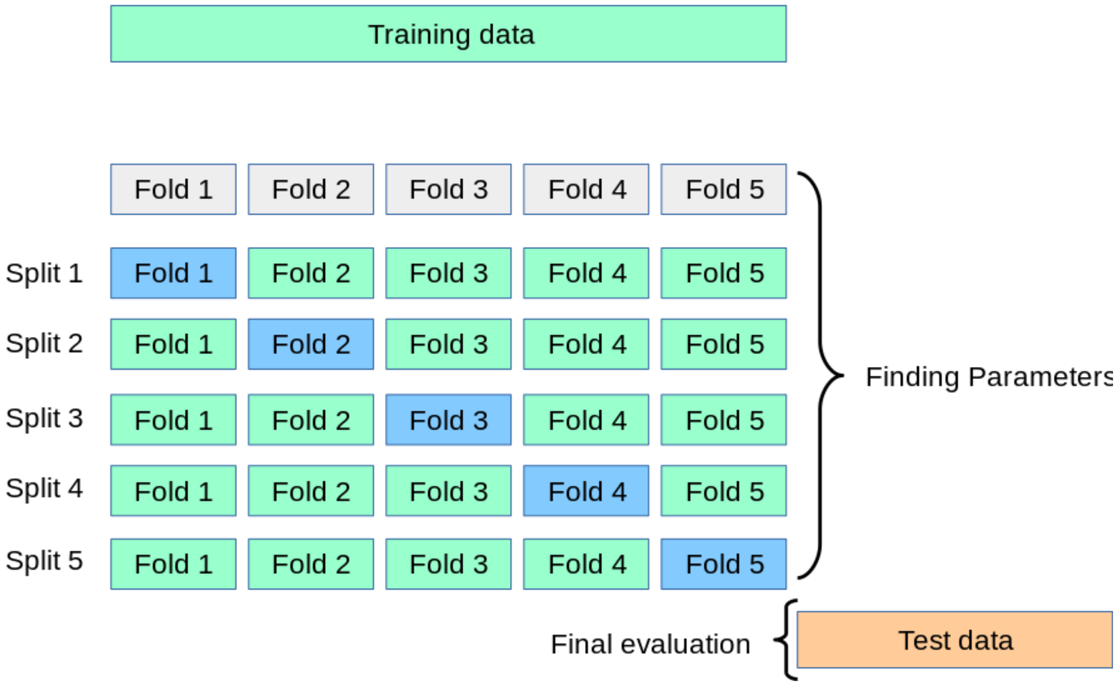
Experiment Design: Train, Validation and Test



- **Train set**: learn parameters of your models
- **Validation set**: model selection
- **Test set**: verify generalizability to unseen data

Experiment Design: k-fold cross validation

- Performs k iterations on the data
- Stratified k-fold: maintain the proportions of each class into folds (unbalance data)

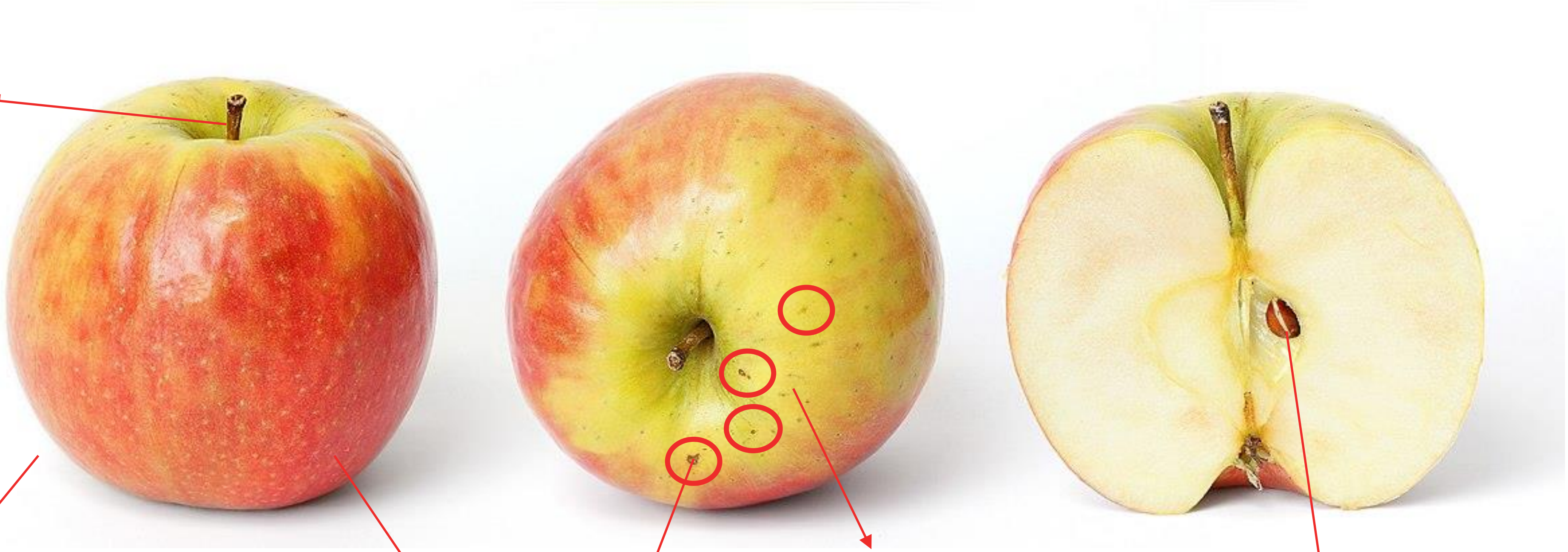


Source: https://scikit-learn.org/stable/modules/cross_validation.html

Under- and Over-fitting

Under- and Over-fitting

Short
stem



Round

Bright red

Yellow-green blush

Seed

Some brown spots: 6

Complex model

Under- and Over-fitting

- What is an apple?

  1 - Short stem
  2 – Round
  3 – Bright and red
  4 – Yellow-green blush
  5 – Seed
  6 – Some brown spots

Under- and Over-fitting

- What is an apple?

  1 - Short stem
  2 – Round
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Under- and Over-fitting

- What is an apple?

~~1 - Short stem~~
~~2 – Round~~
3 – Bright and red or green or yellow
4 – Yellow-green blush
~~5 – Seed~~
~~6 – Some brown spots~~

Simple model

Under- and Over-fitting

- What is an apple?

  ~~1 - Short stem~~
  ~~2 – Round~~
  3 – Bright and red or green or yellow
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  ~~5 – Seed~~
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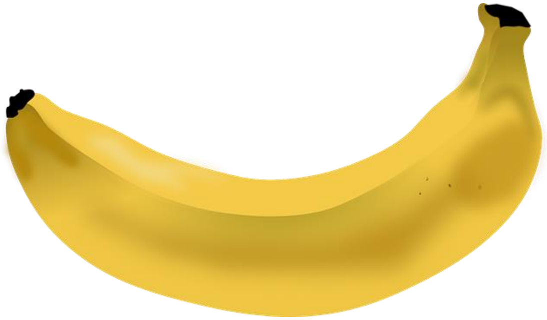
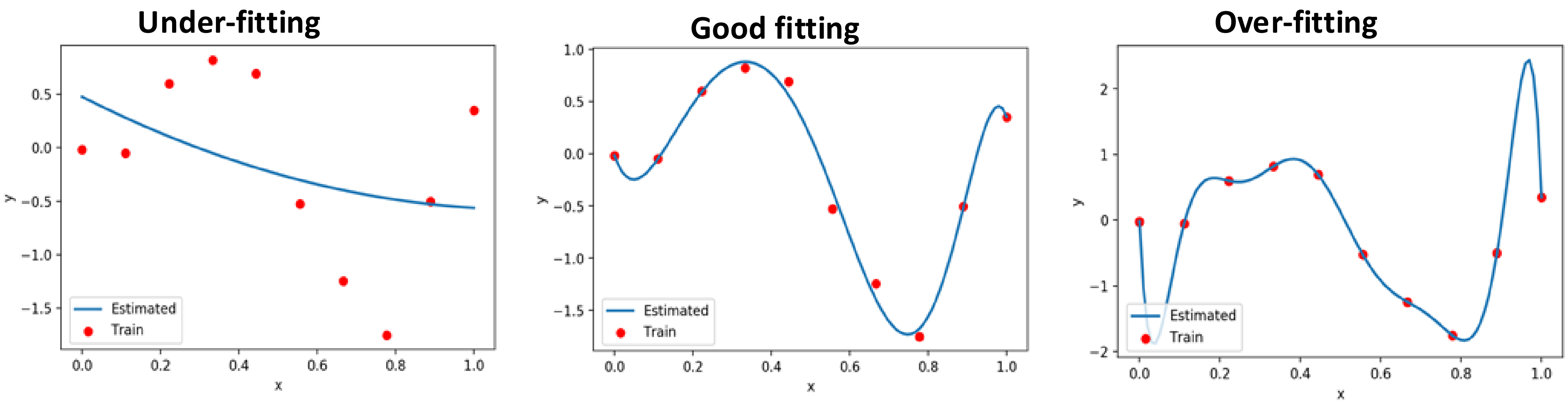


Under- and Over-fitting

- Under-fitting: too inflexible; captures no pattern
  - fitting a linear model to non-linear data
- Over-fitting: too flexible; fits to noise in the data
  - model is excessively complex (#features>>#samples or #parameters too high)
  - decision boundary does not generalize-> poor results for new samples



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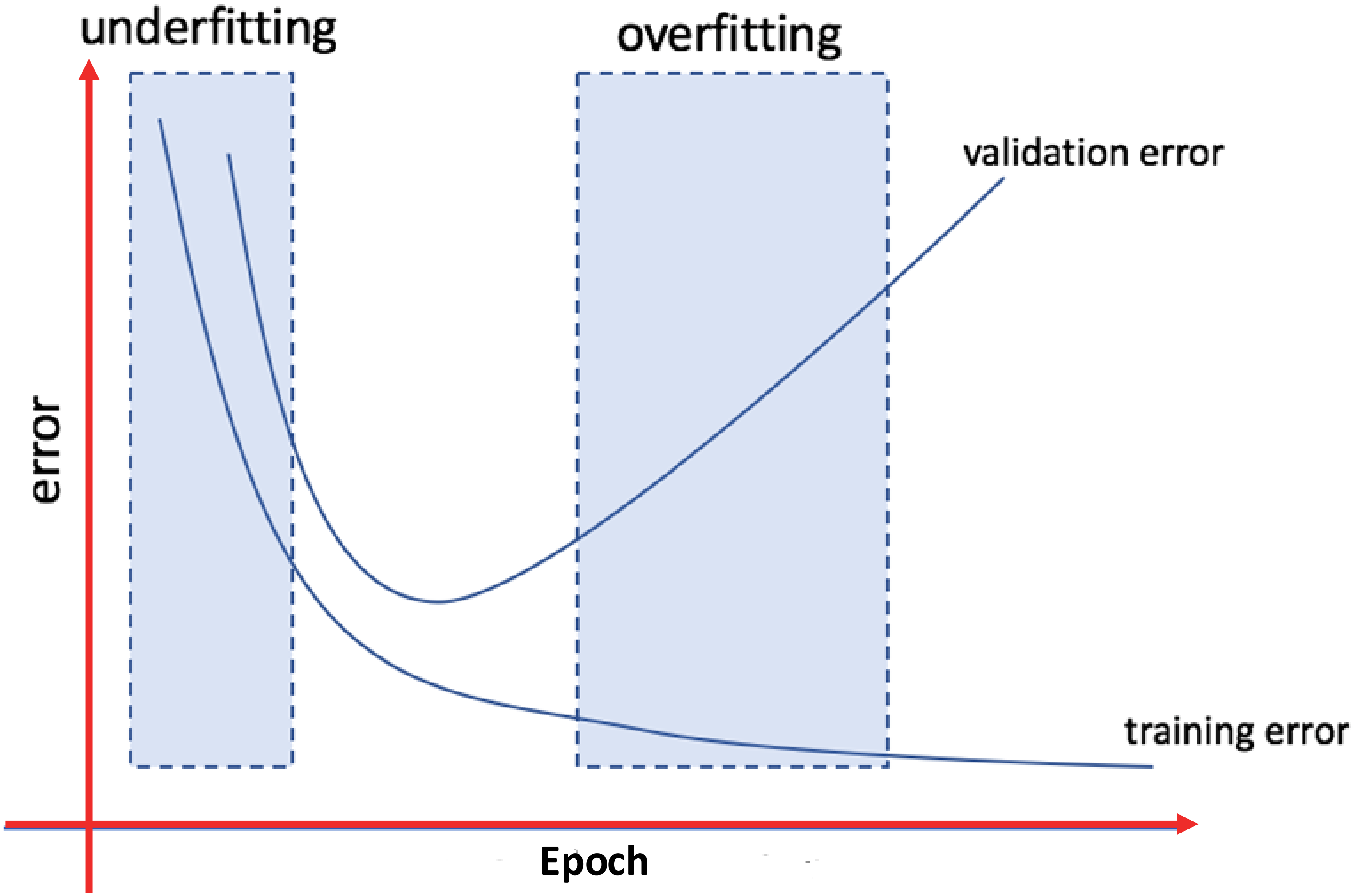
Under- and Over-fitting

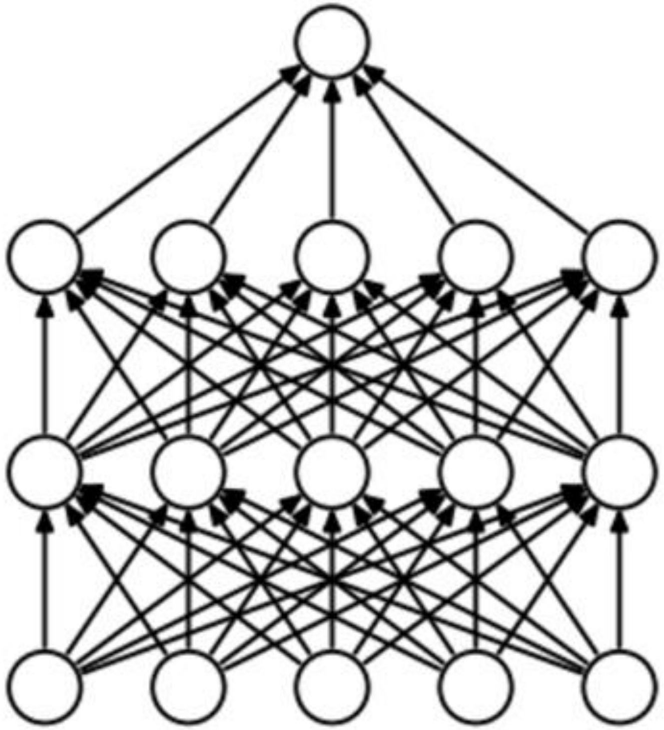


Techniques to Avoid Over-fitting

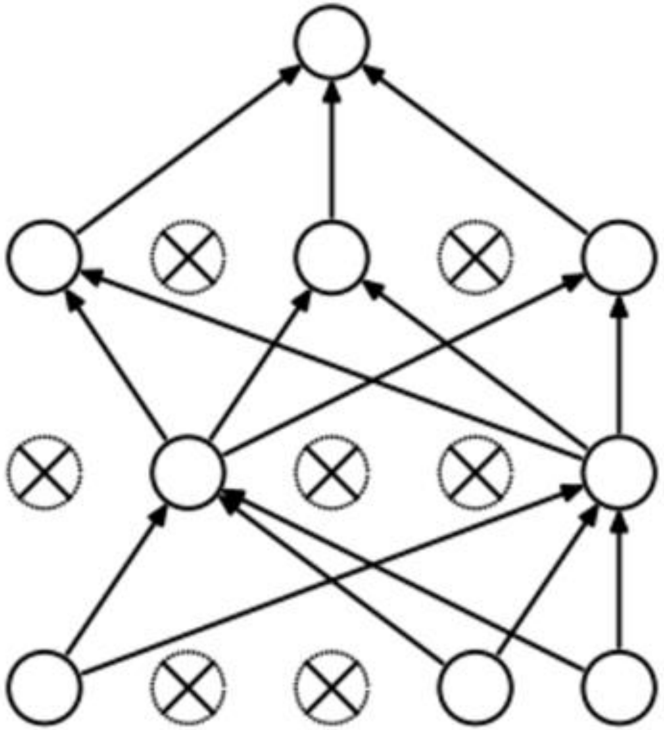
- More data
- Reduce model complexity (*i.e.*, number of trainable parameters)
- Regularization
  - Dropout
  - L1 & L2 regularization
- Data augmentation

Dropout

- Learn redundant paths -> gain robustness



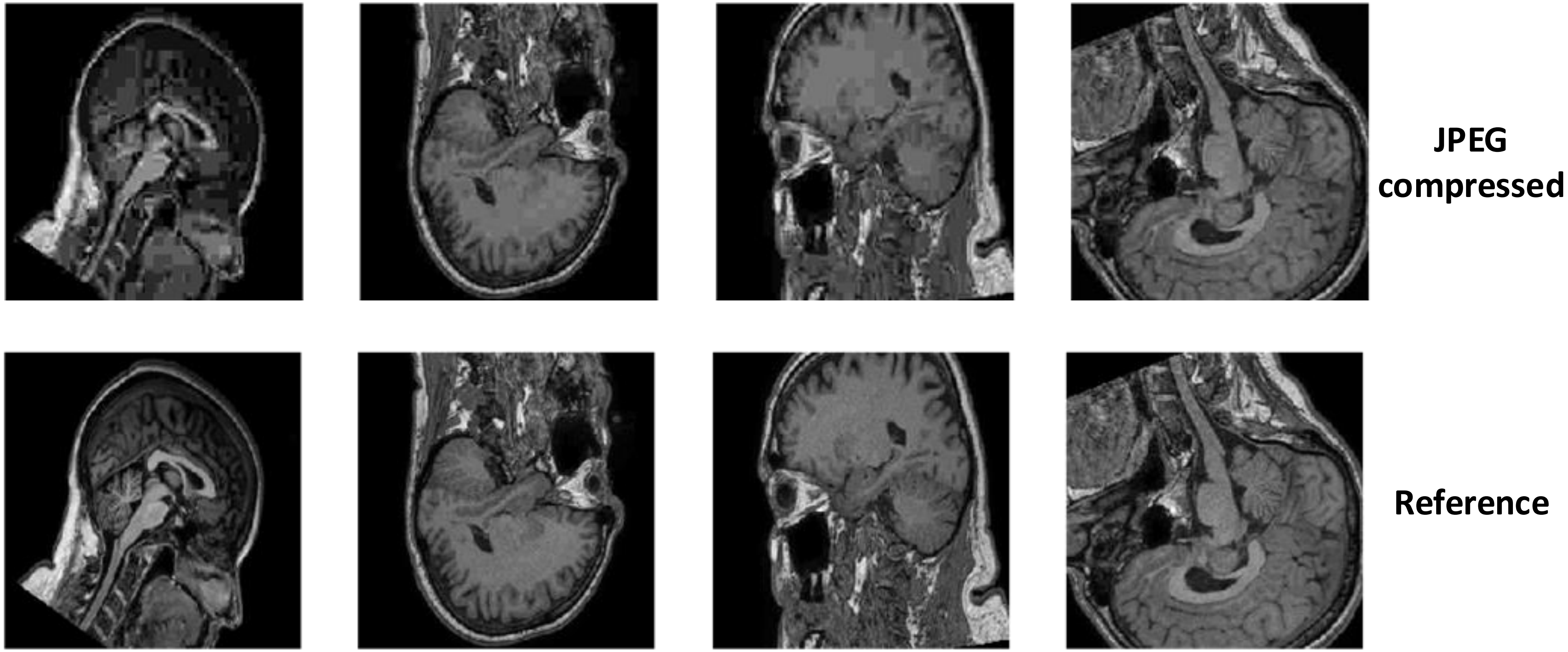
(a) Standard Neural Net



(b) After applying dropout.

Data Augmentation

- Supervised Data = Images + labels

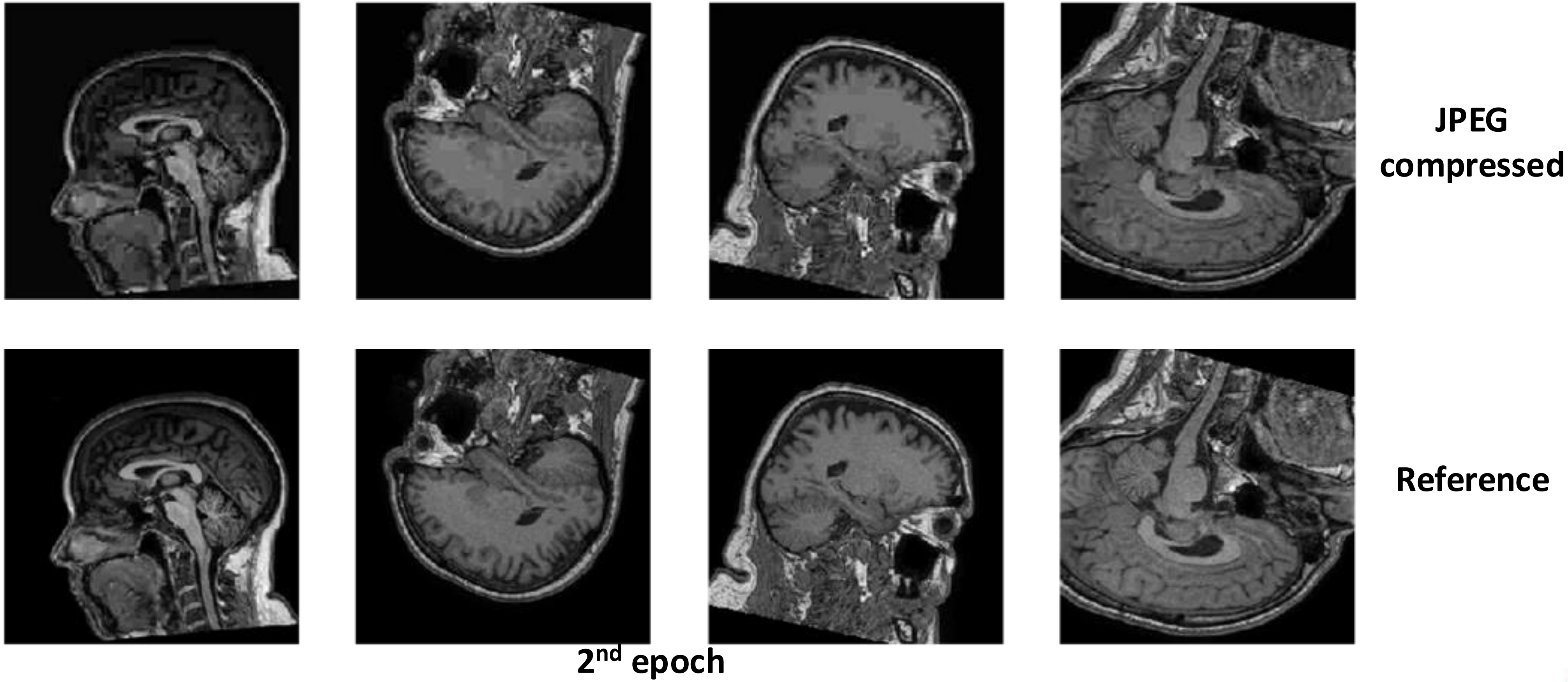


1st epoch

Data augmentation illustration (regression)

Data Augmentation

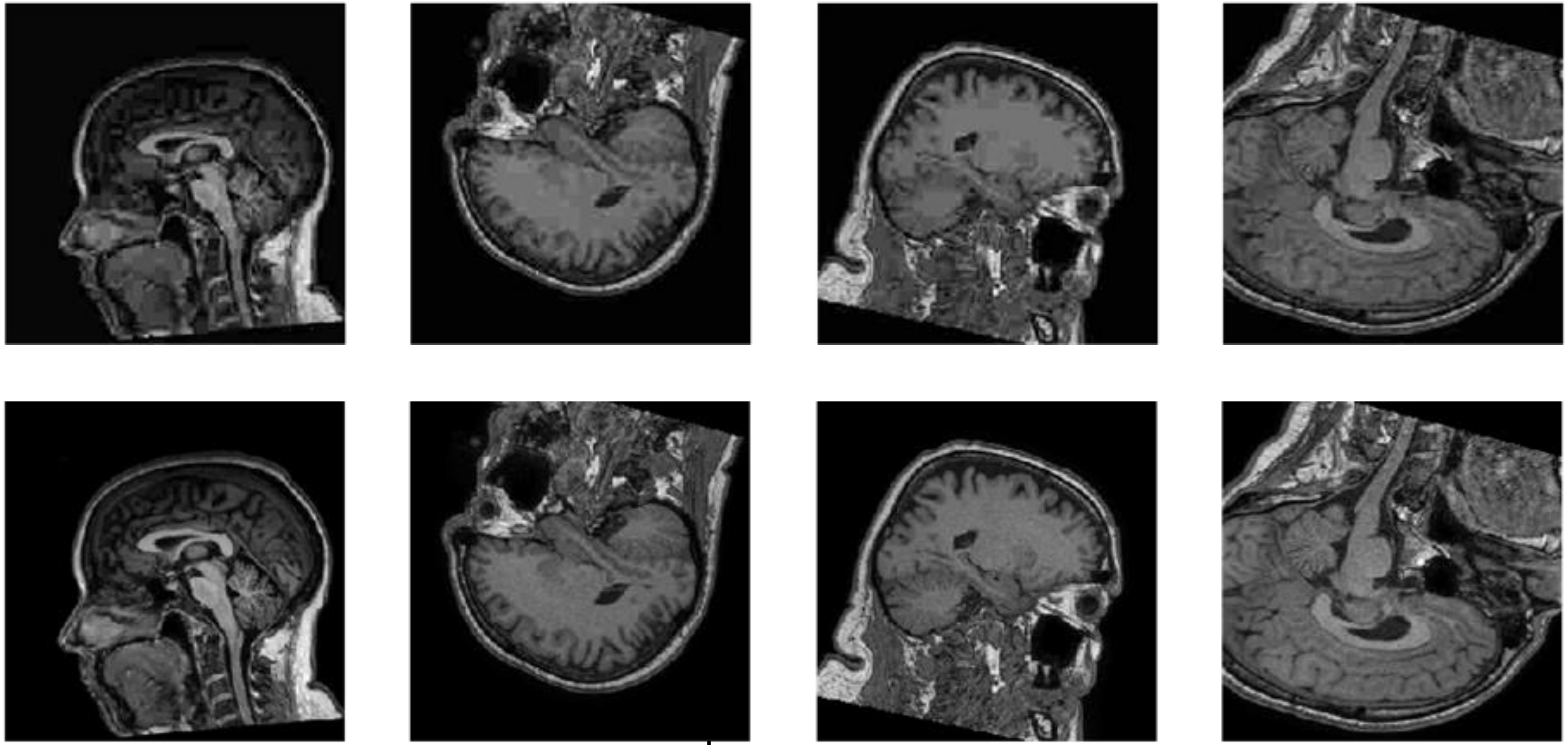
- Supervised Data = Images + labels



Data augmentation illustration (regression)

Data Augmentation

- Supervised Data = Images + labels



JPEG compressed

Reference

3rd epoch

Data augmentation illustration (regression)

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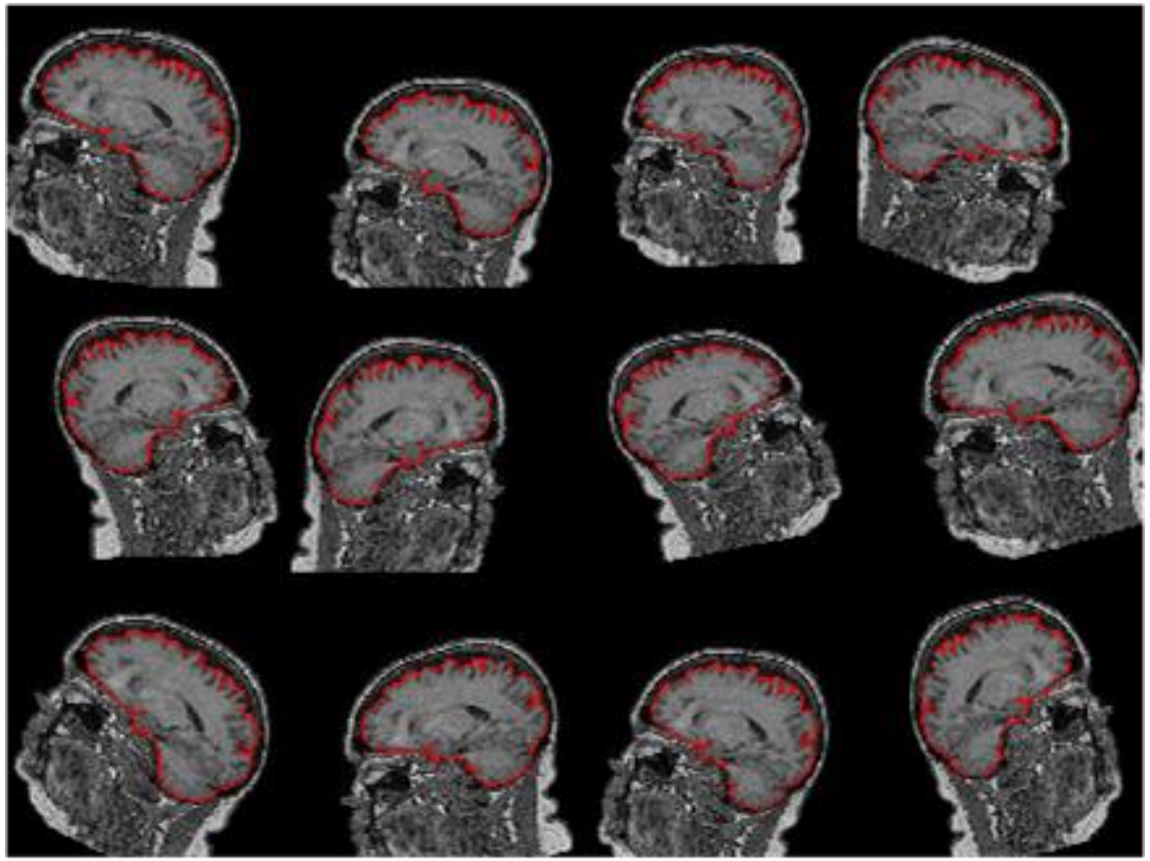
Data Augmentation

- Supervised Data = Images + labels



Data augmentation illustration (segmentation)

L1 & L2 Regularization

- L1 regularization (Lasso)

The idea of the regularization is to penalize your model by decreasing its complexity.

L1 regularization can be seen as a feature selection because by zeroing some of the weights it can tell us what features are not important

L1 Regularization

$$\text{Cost} = \sum_{i=0}^{N}(y_i - \sum_{j=0}^{M} x_{ij}W_j)^2 + \underbrace{\lambda \sum_{j=0}^{M} |W_j|}_{\text{Quickly to zero}}$$

~~1 - Short stem~~

~~2 – Round~~

3 – Bright and red or green or yellow

4 – Yellow-green blush

~~5 – Seed~~

~~6 – Some brown spots~~

L1 & L2 Regularization

- L2 regularization (Weight Decay)

L2 regularization is commonly known as weight decay because it shrinks the weight according to the regularize factor

L2 Regularization

$$\text{Cost} = \sum_{i=0}^{N}(y_i - \sum_{j=0}^{M} x_{ij}W_j)^2 + \underbrace{\lambda \sum_{j=0}^{M} W_j^2}_{\text{Become smaller (Not necessarily zero)}}$$

1 - Short stem x 0.1
2 – Round x 0.9
3 – Bright and red or green or yellow x 0.9
4 – Yellow-green blush x 0.8
5 – Seed x 0.3
6 – Some brown spots x 0.01

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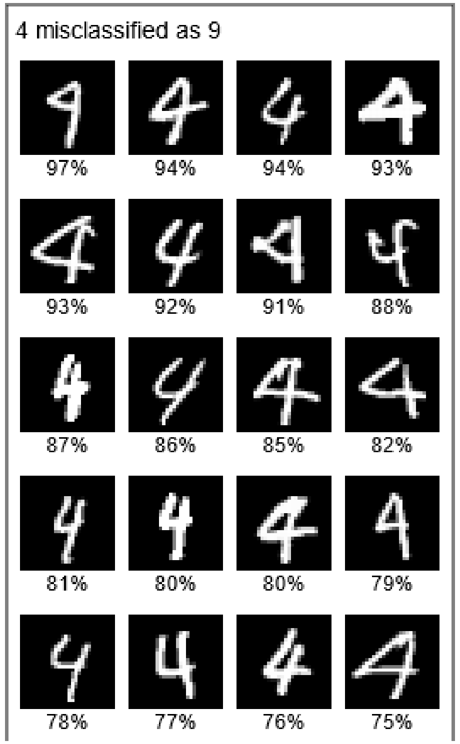
Metrics - Classification

- Confusion matrix

		Prediction outcome: positive	Prediction outcome: negative	
Actual value	positive	TP	FN	$TP+FN$
	negative	FP	TN	$FP+TN$
		$TP+FP$	$FN+TN$	

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN}$$

	predicted 0	predicted 1	predicted 2	predicted 3	predicted 4	predicted 5	predicted 6	predicted 7	predicted 8	predicted 9
actual 0	954	0	0	7	1	10	6	3	7	3
actual 1	0	1031	4	3	1	4	1	2	16	2
actual 2	12	21	852	18	11	8	14	20	29	5
actual 3	2	5	9	899	1	71	0	12	23	7
actual 4	2	8	2	2	861	7	7	1	4	89
actual 5	7	5	9	24	3	833	12	8	12	2
actual 6	11	6	2	0	6	31	902	0	8	1
actual 7	3	10	5	3	7	7	1	1041	0	14
actual 8	2	28	4	29	2	31	1	9	882	21
actual 9	7	3	1	7	10	11	1	44	4	873



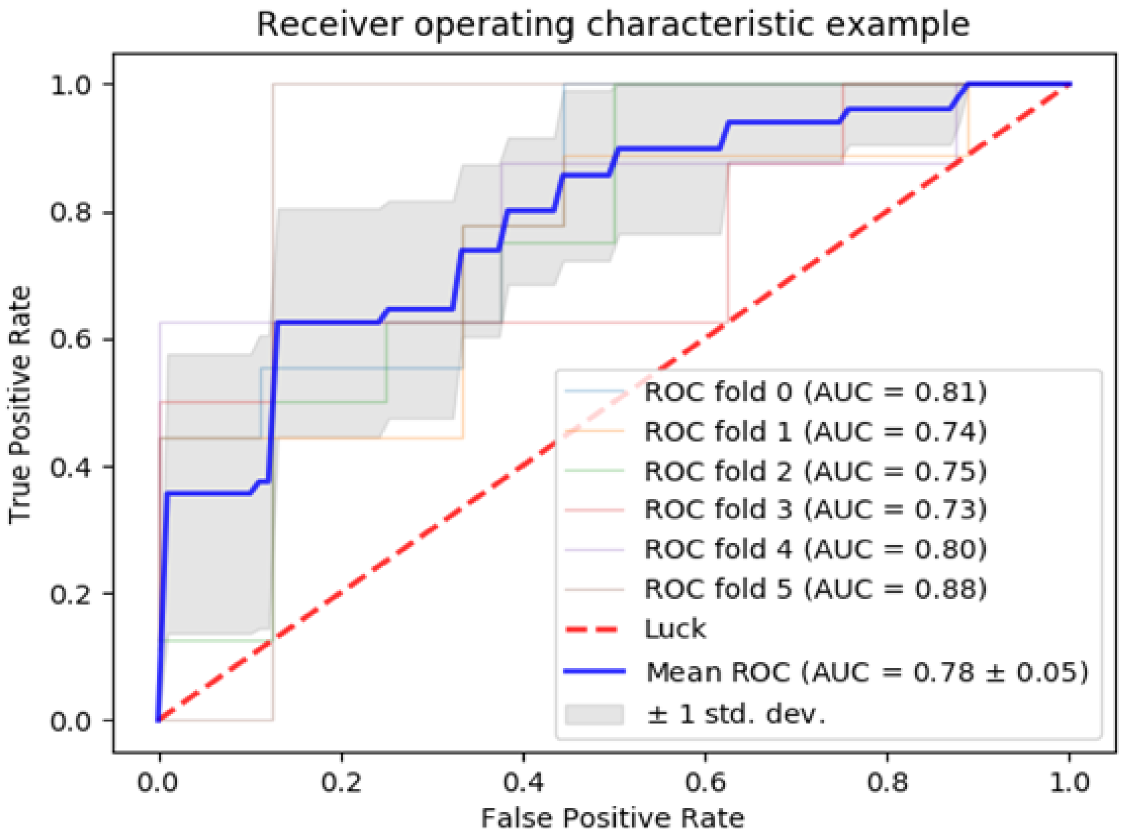
Source: Adapted from https://ml4a.github.io/demos/confusion_mnist/

Metrics - Classification

- Receiver operating characteristic (ROC) curve

$$Sensitivity = TP / P$$

$$Specificity = TN / N$$



Metrics - Regression

- Structural Similarity (SSIM)

$$\mathrm{SSIM}(x,y) = \frac{(2\mu_x\mu_y + c_1)(2\sigma_{xy} + c_2)}{(\mu_x^2 + \mu_y^2 + c_1)(\sigma_x^2 + \sigma_y^2 + c_2)}$$

Luminance, Contrast, and Structure

Source: Understanding SSIM

Metrics - Regression

- Normalized Root Mean Squared Error (NRMSE)

$$\operatorname{RMSD}(\hat{\theta}) = \sqrt{\operatorname{MSE}(\hat{\theta})} = \sqrt{\operatorname{E}((\hat{\theta} - \theta)^2)}.$$

$$\mathrm{NRMSD} = \frac{\mathrm{RMSD}}{y_{\max} - y_{\min}}$$

E = target – prediction
E = 0.5 – 1.0
E = -0.5

$E^2 = 0.25$
E = 0.5

Metrics - Regression

- Peak Signal to Noise Ratio (PSNR)

$$MSE = \frac{1}{m\,n}\sum_{i=0}^{m-1}\sum_{j=0}^{n-1}[I(i,j) - K(i,j)]^2$$

$$\begin{aligned} PSNR &= 10 \cdot \log_{10}\left(\frac{MAX_I^2}{MSE}\right) \\ &= 20 \cdot \log_{10}\left(\frac{MAX_I}{\sqrt{MSE}}\right) \\ &= 20 \cdot \log_{10}(MAX_I) - 10 \cdot \log_{10}(MSE) \end{aligned}$$

E = target – prediction
E = 0.5 – 1.0
E = -0.5

MAX = 255
PSNR = 20 x log10 (255) – 10 x log(0.25)
PSNR = 48.1

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Summary

- For large datasets, a single train/val/test split is often sufficient
- The validation set is used for model selection
- Overfitting makes your model less generalizable to new datasets
- Model overfitting can be mitigated by employing techniques, such as regularization

Thank you!

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