Model Selection, Perceptron

CSC 461: Machine Learning

Fall 2022

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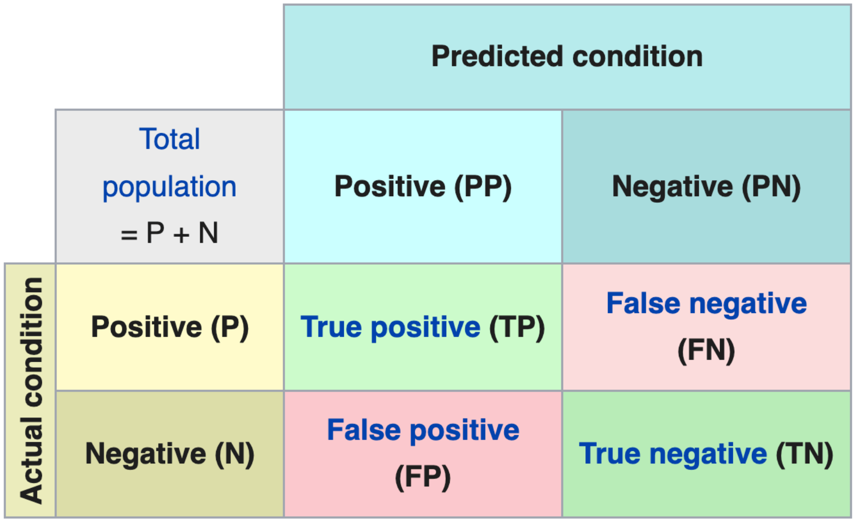
Evaluation (model selection)

Actuals/Predictions (example)

ID	1	2	3	4	5	6	7	8	9	10	11	12
Actual	1	1	1	1	1	1	1	1	0	0	0	0
Predicted	0	0	1	1	1	1	1	1	1	0	0	0
	FN	FN	TP	TP	TP	TP	TP	TP	FP	TN	TN	TN

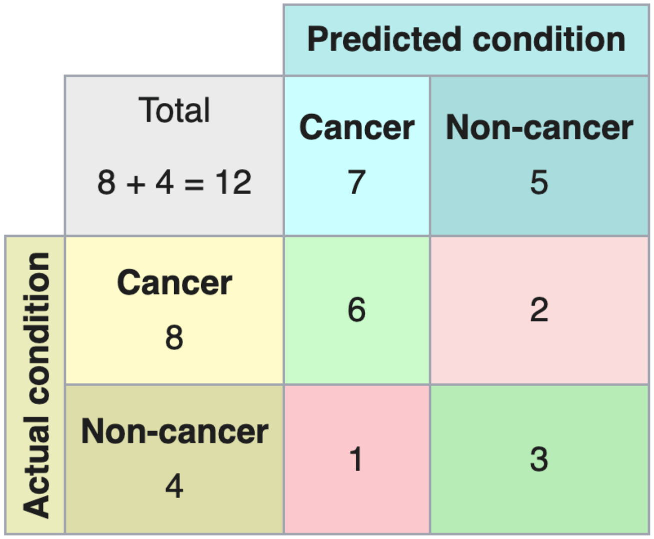
Confusion matrix (2 classes)



		Predicted condition	
	Total population = P + N	Positive (PP)	Negative (PN)
Actual condition	Positive (P)	True positive (TP)	False negative (FN)
	Negative (N)	False positive (FP)	True negative (TN)

https://en.wikipedia.org/wiki/Confusion_matrix

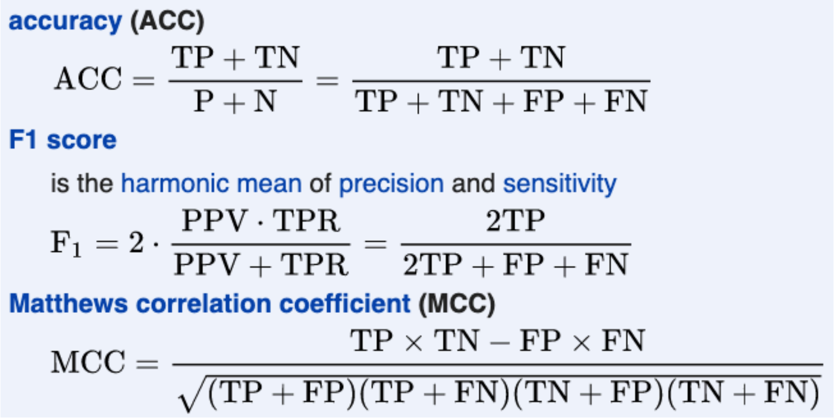
Confusion matrix (example)



		Predicted condition	
	Total 8 + 4 = 12	**Cancer** 7	**Non-cancer** 5
Actual condition	**Cancer** 8	6	2
	Non-cancer 4	1	3

https://en.wikipedia.org/wiki/Confusion_matrix

Evaluation metrics (2 classes)



accuracy (ACC)

$$\mathrm{ACC} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{P} + \mathrm{N}} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{TN} + \mathrm{FP} + \mathrm{FN}}$$

F1 score

is the harmonic mean of precision and sensitivity

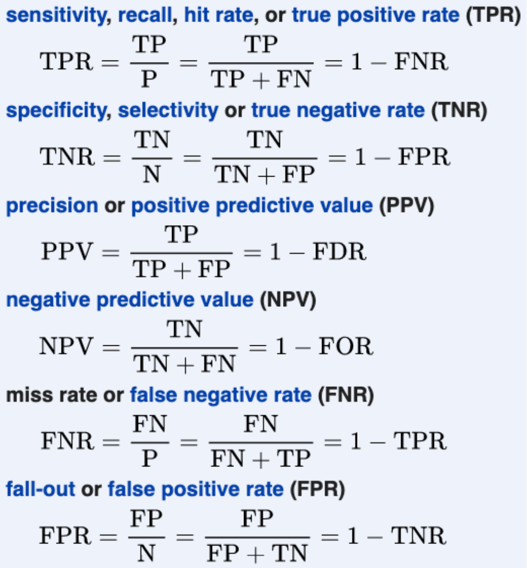
$$\mathrm{F}_1 = 2 \cdot \frac{\mathrm{PPV} \cdot \mathrm{TPR}}{\mathrm{PPV} + \mathrm{TPR}} = \frac{2\mathrm{TP}}{2\mathrm{TP} + \mathrm{FP} + \mathrm{FN}}$$

Matthews correlation coefficient (MCC)

$$\mathrm{MCC} = \frac{\mathrm{TP} \times \mathrm{TN} - \mathrm{FP} \times \mathrm{FN}}{\sqrt{(\mathrm{TP} + \mathrm{FP})(\mathrm{TP} + \mathrm{FN})(\mathrm{TN} + \mathrm{FP})(\mathrm{TN} + \mathrm{FN})}}$$

https://en.wikipedia.org/wiki/Confusion_matrix

Evaluation metrics (2 classes)



sensitivity, recall, hit rate, or true positive rate (TPR)

$$\mathrm{TPR} = \frac{\mathrm{TP}}{\mathrm{P}} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}} = 1 - \mathrm{FNR}$$

specificity, selectivity or true negative rate (TNR)

$$\mathrm{TNR} = \frac{\mathrm{TN}}{\mathrm{N}} = \frac{\mathrm{TN}}{\mathrm{TN} + \mathrm{FP}} = 1 - \mathrm{FPR}$$

precision or positive predictive value (PPV)

$$\mathrm{PPV} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}} = 1 - \mathrm{FDR}$$

negative predictive value (NPV)

$$\mathrm{NPV} = \frac{\mathrm{TN}}{\mathrm{TN} + \mathrm{FN}} = 1 - \mathrm{FOR}$$

miss rate or false negative rate (FNR)

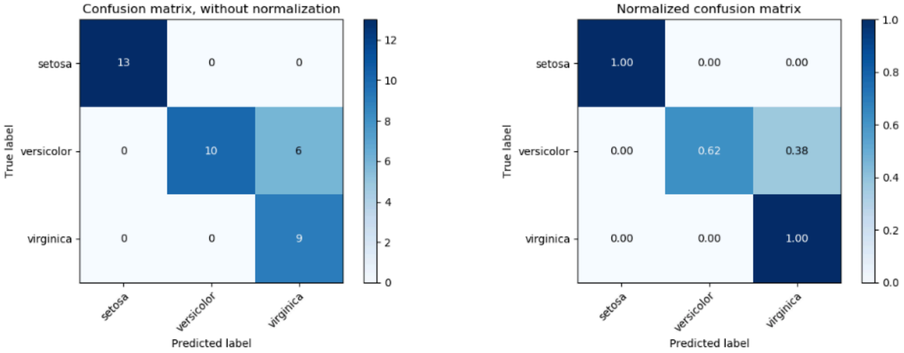
$$\mathrm{FNR} = \frac{\mathrm{FN}}{\mathrm{P}} = \frac{\mathrm{FN}}{\mathrm{FN} + \mathrm{TP}} = 1 - \mathrm{TPR}$$

fall-out or false positive rate (FPR)

$$\mathrm{FPR} = \frac{\mathrm{FP}}{\mathrm{N}} = \frac{\mathrm{FP}}{\mathrm{FP} + \mathrm{TN}} = 1 - \mathrm{TNR}$$

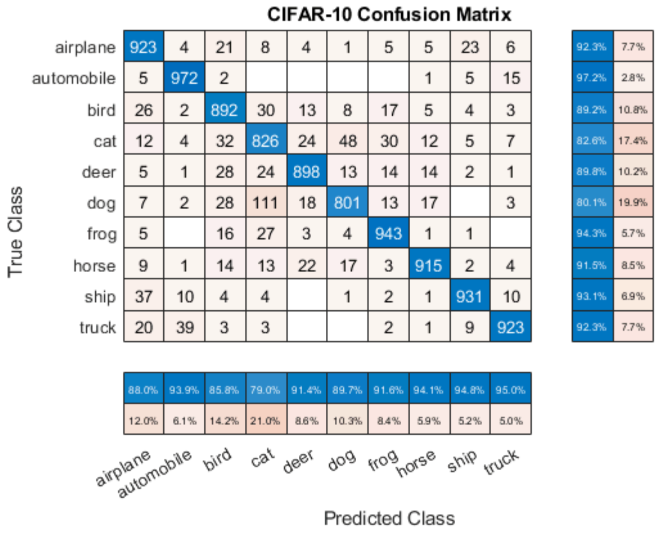
https://en.wikipedia.org/wiki/Confusion_matrix

Confusion matrix (>2 classes)



https://scikit-learn.org/stable/auto_examples/model_selection/plot_confusion_matrix.html

Confusion matrix (>2 classes)



CIFAR-10 Confusion Matrix

True Class	airplane	automobile	bird	cat	deer	dog	frog	horse	ship	truck		
airplane	923	4	21	8	4	1	5	5	23	6	92.3%	7.7%
automobile	5	972	2					1	5	15	97.2%	2.8%
bird	26	2	892	30	13	8	17	5	4	3	89.2%	10.8%
cat	12	4	32	826	24	48	30	12	5	7	82.6%	17.4%
deer	5	1	28	24	898	13	14	14	2	1	89.8%	10.2%
dog	7	2	28	111	18	801	13	17		3	80.1%	19.9%
frog	5		16	27	3	4	943	1	1		94.3%	5.7%
horse	9	1	14	13	22	17	3	915	2	4	91.5%	8.5%
ship	37	10	4	4		1	2	1	931	10	93.1%	6.9%
truck	20	39	3	3			2	1	9	923	92.3%	7.7%
	88.0%	93.9%	85.8%	79.0%	91.4%	89.7%	91.6%	94.1%	94.8%	95.0%		
	12.0%	6.1%	14.2%	21.0%	8.6%	10.3%	8.4%	5.9%	5.2%	5.0%		

Predicted Class

https://www.mathworks.com/help/deeplearning/ref/confusionchart.html

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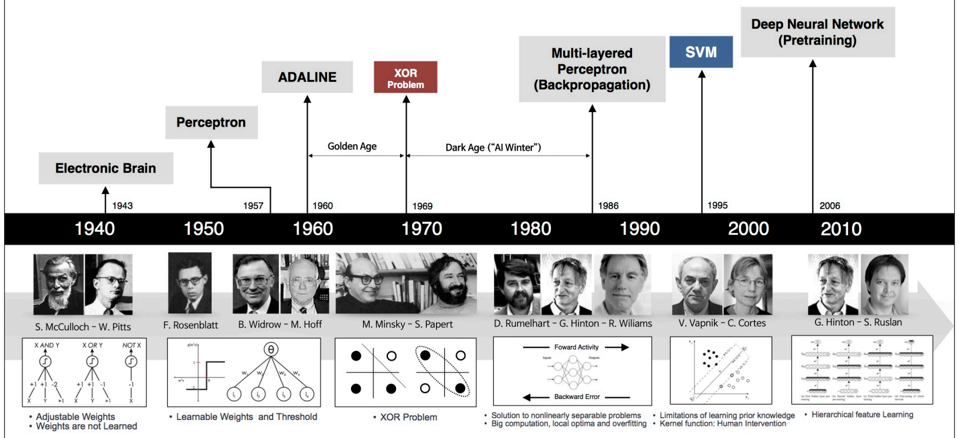
The Perceptron

Neural Networks



http://beamandrew.github.io/deeplearning/2017/02/23/deep_learning_101_part1.html

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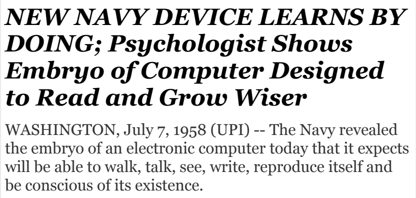
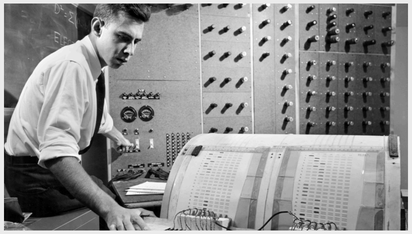
Rosenblatt (1958)

- Perceptron introduced by Frank Rosenblatt (psychologist, logician)
  - ✓ based on work from McCulloch-Pitts and Hebb
  - ✓ very powerful **learning** algorithm with high expectations

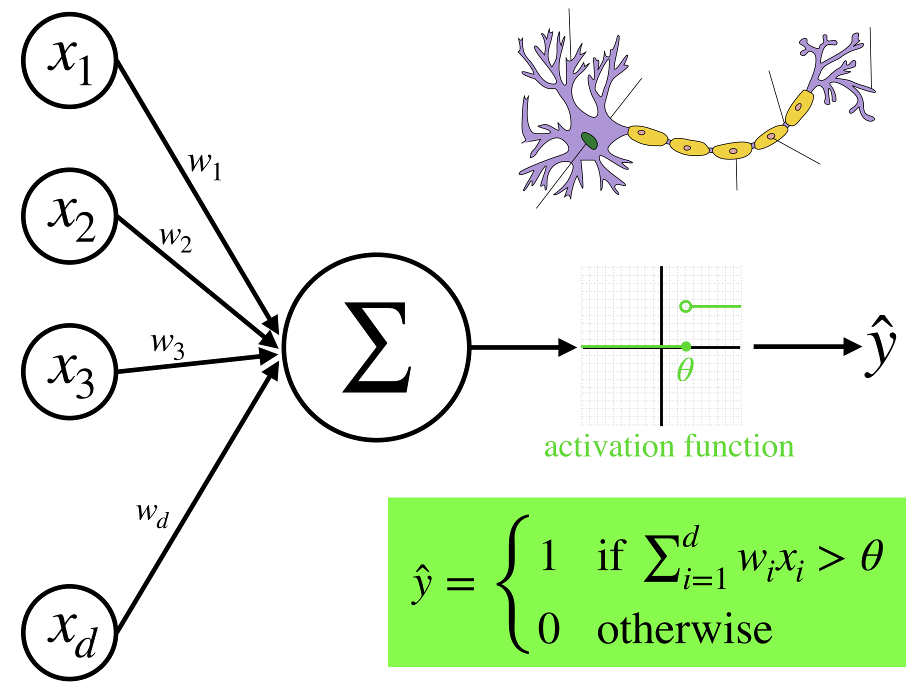


NEW NAVY DEVICE LEARNS BY DOING; Psychologist Shows Embryo of Computer Designed to Read and Grow Wiser

WASHINGTON, July 7, 1958 (UPI) -- The Navy revealed the embryo of an electronic computer today that it expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence.



https://news.cornell.edu/stories/2019/09/professors-perceptron-paved-way-ai-60-years-too-soon



$$\hat{y} = \begin{cases} 1 & \text{if } \sum_{i=1}^{d} w_i x_i > \theta \\ 0 & \text{otherwise} \end{cases}$$

Absorbing the threshold/bias

$$\hat{y} = \begin{cases} 1 & \text{if } \sum_{i=1}^{d} w_i x_i > \theta \\ 0 & \text{otherwise} \end{cases}$$

$$\hat{y} = \begin{cases} 1 & \text{if } \sum_{i=1}^{d} w_i x_i - \theta > 0 \\ 0 & \text{otherwise} \end{cases}$$

$$\hat{y} = \begin{cases} 1 & \text{if } \sum_{i=0}^{d} w_i x_i > 0 \\ 0 & \text{otherwise} \end{cases}$$

$$x_0 = +1, \quad w_0 = -\theta$$

Another look

For convenience we will use +1 and -1 instead of 1 and 0

$$h_{\mathbf{w}}(\mathbf{x}) = \sigma\left(\sum_{i=0}^{d} w_i x_i\right) = \sigma(\mathbf{w}^T\mathbf{x})$$

$$\sigma(z) = \begin{cases} 1 & \text{if } z > 0 \\ -1 & \text{if } z \leq 0 \end{cases}$$

$$\mathscr{H} = \{h_w : \mathbf{w} \in \mathbb{R}^{d+1}\}$$

Perceptron Algorithm

- Start with a null vector **w**
- Repeat for T epochs
  - ✓ shuffle the data instances
  - ✓ for all examples in training data
    - ✓ if misclassified
      - update the weight vector by adding **x** to **w** if the actual label is positive and subtracting **x** from **w** otherwise
- Return **w**

Write the pseudocode

https://colab.research.google.com/drive/1p7LjENLd6whkoVY2yRGg-Nm5v4XNjdDt

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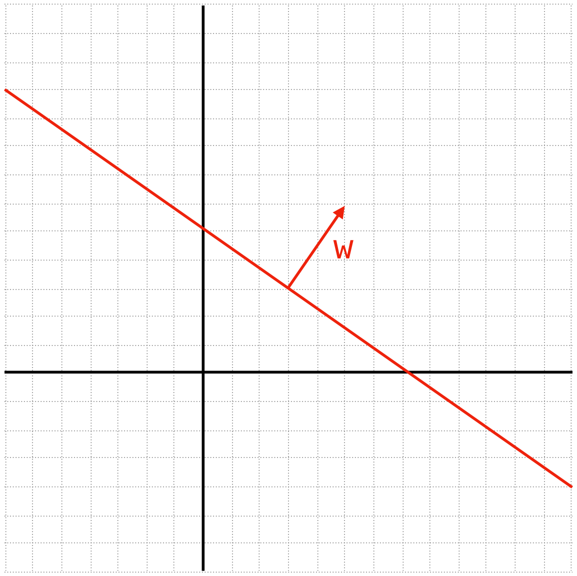
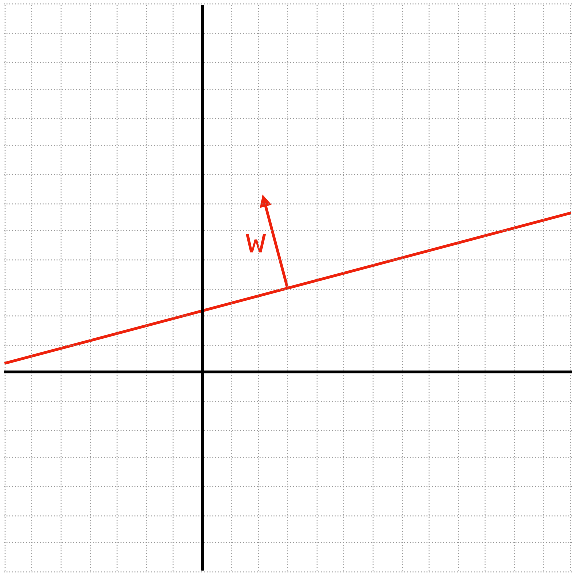
Mistake on a positive (update)



Mistake on a negative (update)



Intuition

- Suppose a mistake on the positive side:

$$y = +1 \qquad \mathbf{w}^T x \leq 0$$

- After 1 update the new weight vector will be:

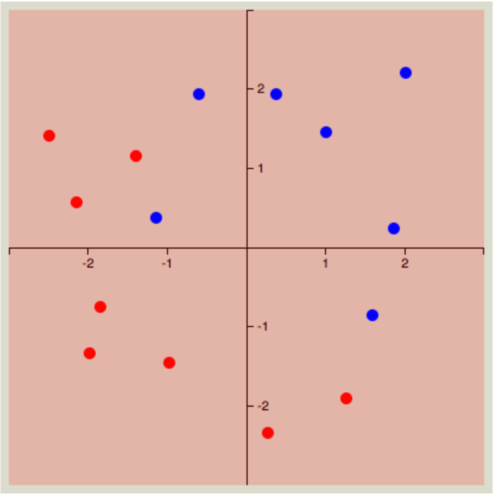
$$\mathbf{w}_{t+1} = \mathbf{w}_t + \mathbf{x}$$

- Classifying the datapoint with the new weight vector:

$$\mathbf{w}_{t+1}{}^T\mathbf{x} = (\mathbf{w}_t + \mathbf{x})^T\mathbf{x} = \mathbf{w}_t^T\mathbf{x} + \mathbf{x}^T\mathbf{x} \geq \mathbf{w}_t^T\mathbf{x}$$

use same idea for mistakes on the negative side

Demo



https://planspace.org/20150907-interactive_perceptron_training_toy/

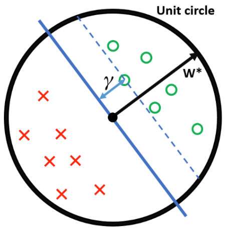
Perceptron convergence theorem

The argument goes as follows: Suppose $\exists \mathbf{w}^*$ such that $y_i(\mathbf{x}^\top \mathbf{w}^*) > 0 \; \forall (\mathbf{x}_i, y_i) \in D$.

Now, suppose that we rescale each data point and the $\mathbf{w}^*$ such that

$$||\mathbf{w}^*|| = 1 \qquad \text{and} \qquad ||\mathbf{x}_i|| \le 1 \;\; \forall \mathbf{x}_i \in D$$

Let us define the Margin γ of the hyperplane $\mathbf{w}^*$ as $\gamma = \min_{(\mathbf{x}_i, y_i) \in D} |\mathbf{x}_i^\top \mathbf{w}^*|$.



To summarize our setup:

- All inputs $\mathbf{x}_i$ live within the unit sphere
- There exists a separating hyperplane defined by $\mathbf{w}^*$, with $\|\mathbf{w}\|^* = 1$ (i.e. $\mathbf{w}^*$ lies exactly on the unit sphere).
- γ is the distance from this hyperplane (blue) to the closest data point.

Theorem: If all of the above holds, then the Perceptron algorithm makes at most $1/\gamma^2$ mistakes.

http://www.cs.cornell.edu/courses/cs4780/2018fa/lectures/lecturenote03.html

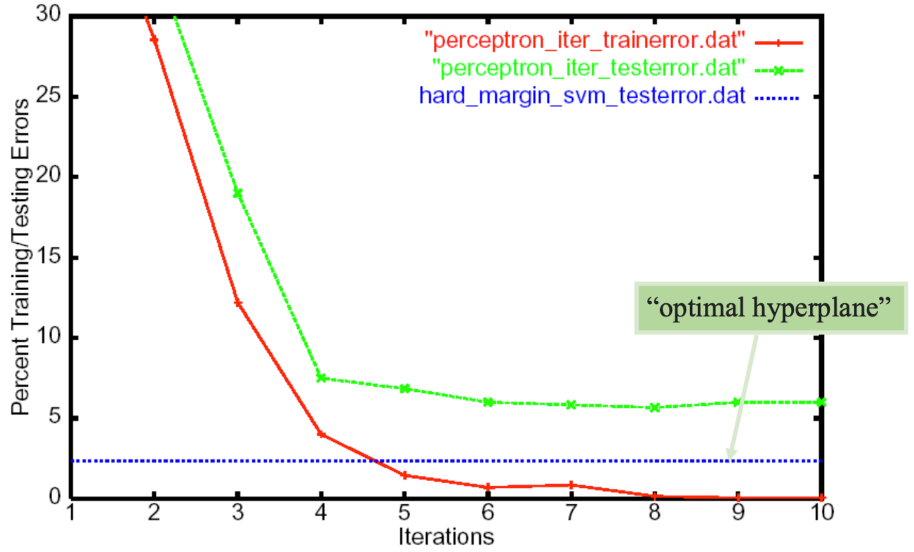
Perceptron (remarks)

- Assumes data is linearly separable
  - ✓ **does not converge** if classes are not linearly separable
- Different correct solutions can be found
  - ✓ most are not optimal in terms of generalization
- Averaged Perceptron
  - ✓ returns a weighted average of earlier hypotheses

Parameters vs Hyperparameters

- Parameters
  - ✓ weights and bias
- **Hyperparameters**
  - ✓ number of epochs (one epoch is one pass over the training data)

Example: Reuters Text Classification



"optimal hyperplane"

Credit: http://www.cs.cornell.edu/courses/cs4780/2019fa/lectures/06-perceptron.pdf

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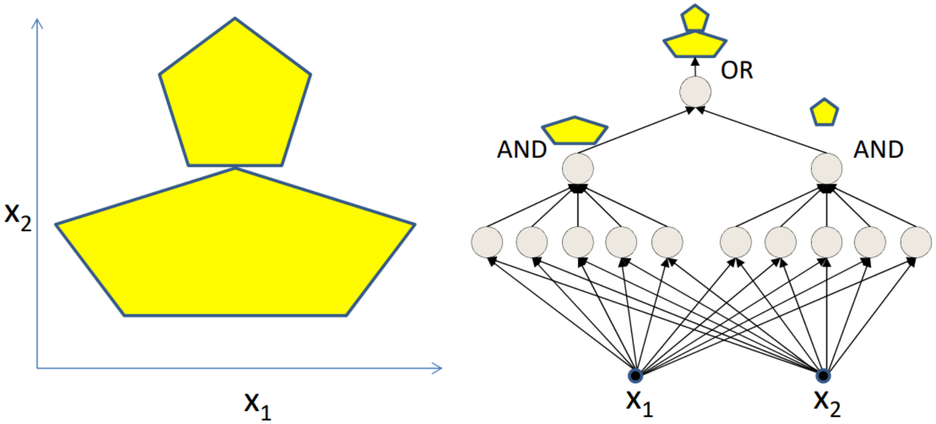
Spoiler alert (neural nets)



http://deeplearning.cs.cmu.edu/document/lecture/lecture-1.pdf

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Data, Loss, and a Linear Model

X0	X1	X2	Y
1	0	0	-1
1	1	0	+1
1	1	1	+1
1	0	1	+1

$$\sigma(z) = \begin{cases} +1 & \text{if } z > 0 \\ -1 & \text{if } z \le 0 \end{cases}$$

$$h_w(\mathbf{x}) = \sigma\left(\sum_{i=0}^{d} w_i x_i\right) = \sigma(\mathbf{w}^T\mathbf{x})$$

$$L_{0/1}(h, \mathscr{D}) = \frac{1}{n} \sum_{(x_i, y_i) \in \mathscr{D}} I(h(x_i) \neq y_i)$$

$$\mathbf{w}_a = [0,0,0]^T$$
$$\mathbf{w}_b = [0,1,0]^T$$
$$\mathbf{w}_c = [-1,2,2]^T$$

$$L_{0/1}(h_{w_a}, \mathscr{D}) = ?$$
$$L_{0/1}(h_{w_b}, \mathscr{D}) = ?$$
$$L_{0/1}(h_{w_c}, \mathscr{D}) = ?$$

Applying SGD to the Perceptron

Back to the perceptron …

$$L(\mathbf{w}) = \sum_{i=1}^{n} -y^{(i)}\mathbf{w}^T\mathbf{x}^{(i)}$$

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} L(\mathbf{w})$$

Note this loss function has a problem, it is not bounded below

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Gradient

With respect to a single w_j

$$\frac{\partial}{\partial w_j}L(\mathbf{w}) = \frac{\partial}{\partial w_j}\left[-\sum_{i=1}^{m} y^{(i)}\mathbf{w}^T\mathbf{x}^{(i)}\right]$$

$$= -\sum_{i=1}^{m} y^{(i)}x_j^{(i)}$$

The training algorithm can focus on batches of misclassified instances, then the batch loss cannot be negative

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Pseudocode