Lecture 4: Logistic Regression

Machine Learning, Summer Term 2019

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Lecture Overview

1. Motivation
2. The Model
3. How to Derive the Parameters...
4. Wrapup: Summary, Related Topics, Preview

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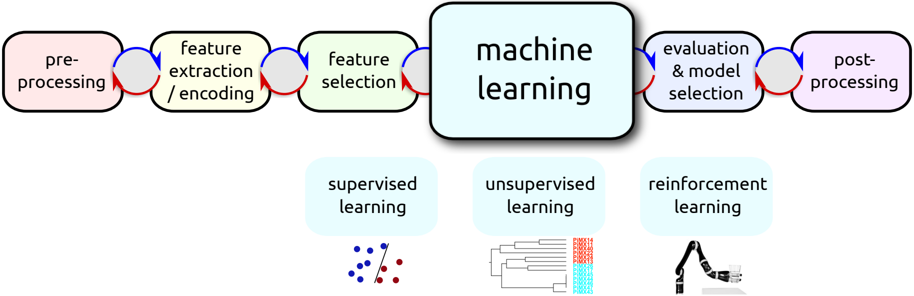
ML Design Cycle



Today's topic is classification:

- Use past experience to predict the future

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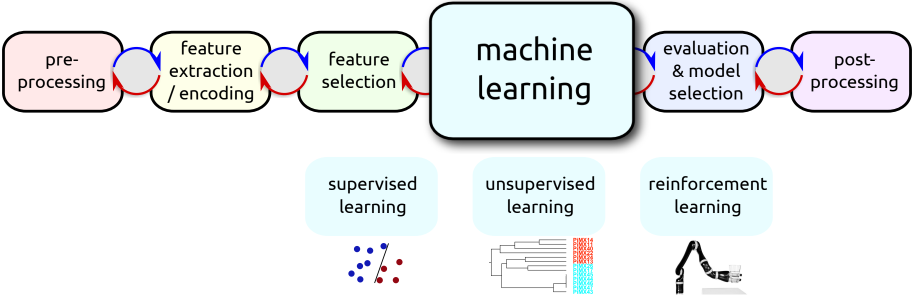

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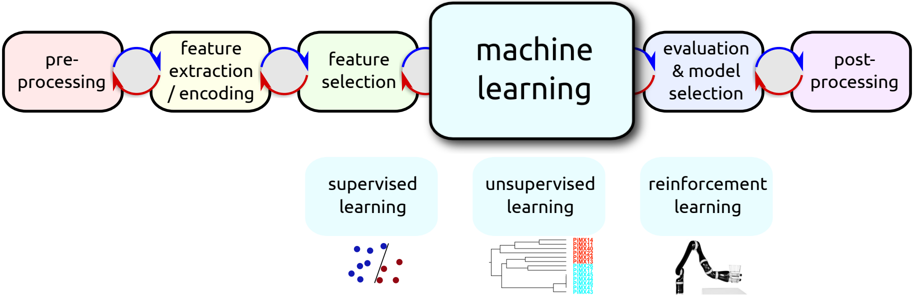

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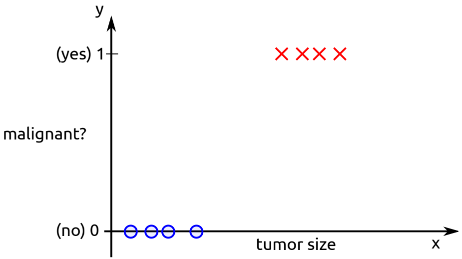
- Use past experience to predict the future
- Use labelled data points $\langle(\mathbf{x}_i, y_i)\rangle_{i=1}^{N}$
- Train a **model** which can predict the label y_{N+1} of a new data point $\mathbf{x}_{N+1}$

Simple Example: Tumor Classification

Is the tumor benign or malignant?

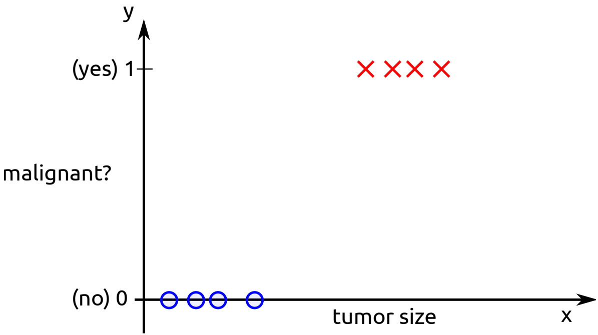
Labels $y \in \{0, 1\}$, with

- $y = 0$: "Negative class" (e.g. benign, not malignant)
- $y = 1$: "Positive class" (e.g. malignant)



Try fitting a (augmented) model $h_{\mathbf{w}}(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$ as in linear regression...

Simple Example: Tumor Classification



Threshold the classifier output $h_{\mathbf{w}}(\mathbf{x})$ at 0.5:

- If $h_{\mathbf{w}}(\mathbf{x}) > 0.5$, predict $y = 1$: (malignant)
- If $h_{\mathbf{w}}(\mathbf{x}) \leq 0.5$, predict $y = 0$: (not malignant)

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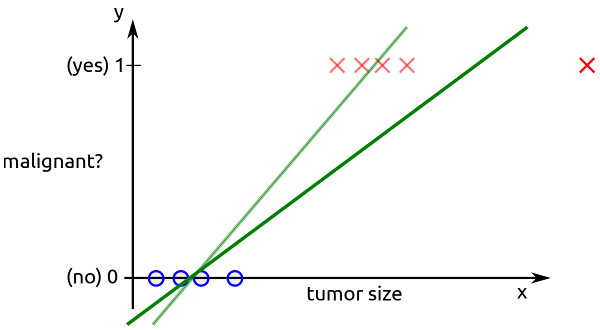

Outliers? Houston, we have a problem...

- For classification case we should only accept $y = 0$ or $y = 1$.
- However, linear regression model $h_{\mathbf{w}}(\mathbf{x})$ can generate $y > 1$ or $y < 0$.

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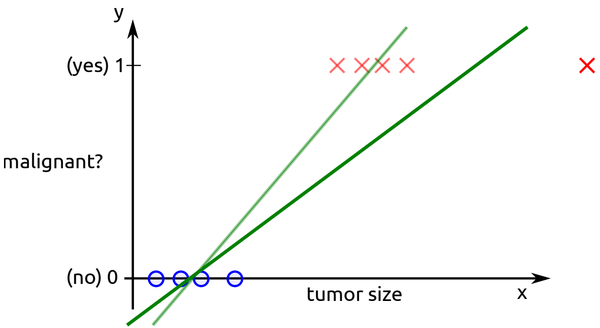

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- However, linear regression model $h_{\mathbf{w}}(\mathbf{x})$ can generate $y > 1$ or $y < 0$.

Solution: logistic regression, which bounds the output to $0 \leq h_{\mathbf{w}}(\mathbf{x}) \leq 1$

Lecture Overview

Logistic Regression Model

We want: $0 \leq h_{\mathbf{w}}(\mathbf{x}) \leq 1$

Standard linear regression
(using the inner product) delivers:
$h_{\mathbf{w}}(\mathbf{x}) = \quad \mathbf{w}^T\mathbf{x}$

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$h_{\mathbf{w}}(\mathbf{x}) = g(\mathbf{w}^T\mathbf{x})$ with $g(z) = \frac{1}{1+e^{-z}}$

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$g(z)$ is called sigmoid function
or logistic function

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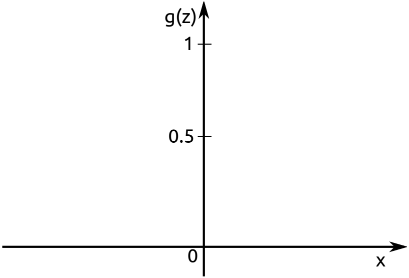
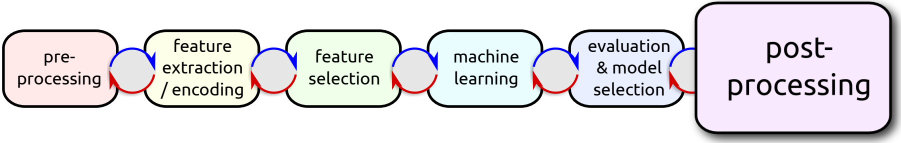


Role of Non-linear Function g



Please observe:

- The use of function $g(\mathbf{x})$ has similarity to a post-processing of a linear method

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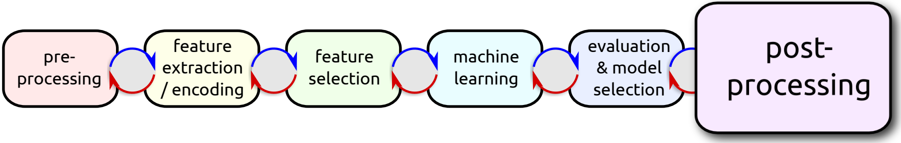

Please observe:

- The use of function $g(\mathbf{x})$ has similarity to a post-processing of a linear method
- You can actually apply a post processing to linear classifier outputs by
  - $\rightarrow$ logistic calibration (making distribution assumptions)
  - $\rightarrow$ isotonic calibration (no assumptions)

Interpretation of Model Output

$h_{\mathbf{w}}(\mathbf{x}) =$ estimated probability, that $y = 1$ on input $\mathbf{x}$

Example with tumor size:

$$x = \begin{bmatrix} \mathbf{x}_0 \\ \mathbf{x}_1 \end{bmatrix} = \begin{bmatrix} 1 \\ tumorSize \end{bmatrix}$$

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How can we interpret the model output $h_{\mathbf{w}}(\mathbf{x}) = 0.7$?

$\rightarrow$ We would infer that with a probability of 70% the patient's tumor is malignant.

Interpretation of Model Output

$h_{\mathbf{w}}(\mathbf{x}) \approx$ estimated probability, that $y = 1$

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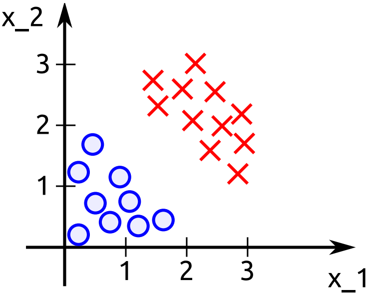
The actual labels are still discrete ($y = 0$ or $y = 1$), but the probabilities need to add to one:

$$P(y = 0|\mathbf{x}; \mathbf{w}) + P(y = 1|\mathbf{x}; \mathbf{w}) = 1$$

$$P(y = 0|\mathbf{x}; \mathbf{w}) = 1 - P(y = 1|\mathbf{x}; \mathbf{w})$$

Example in $\mathbb{R}^2$

Where is the decision boundary?



$$h_{\mathbf{w}}(\mathbf{x}) = g(\mathbf{w}_0 + \mathbf{w}_1\mathbf{x}_1 + \mathbf{w}_2\mathbf{x}_2)$$

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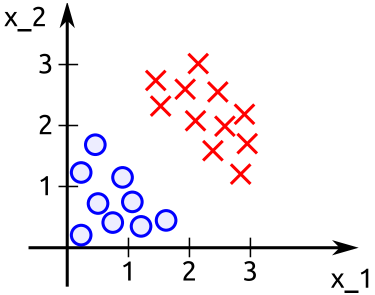

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$$\mathbf{w} = \begin{bmatrix} -3 \\ 1 \\ 1 \end{bmatrix}$$

Predict "$y = 1$" if $\quad -3 + \mathbf{x}_1 + \mathbf{x}_2 \geq 0$

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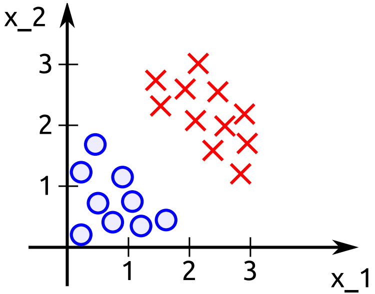

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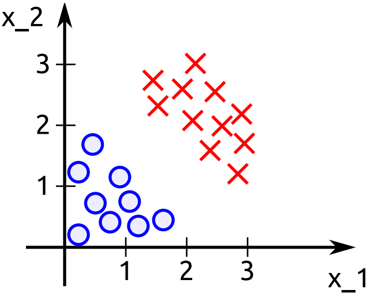

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Remark: as in linear models, the use of additional dimensions and basis functions allows for non-linear decision boundaries!

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- If we use the augmented notation – what is the dimensionality of the data? 
- Answer: $\mathbf{x} \in \mathbb{R}^{D+1}$ with first dimension $x_0 = 1$

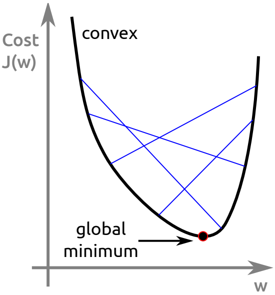
Our model is:

$$h_{\mathbf{w}}(\mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x}}}$$

How can we choose the parameters $\mathbf{w}$?

Reminder: Loss Function Punishes Wrong Predictions

- To tune the weight vector $\mathbf{w}$, we should check the costs / losses generated by data points, which have not been fitted perfectly (and thus show non-zero residuals).



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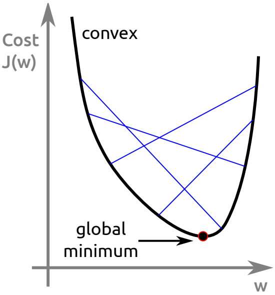

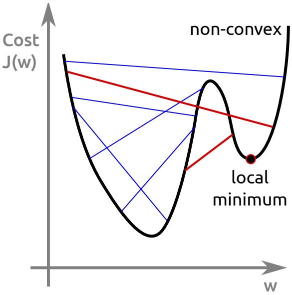

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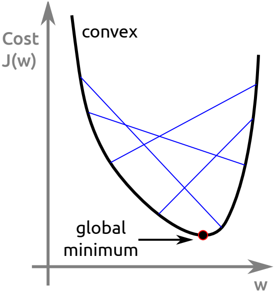
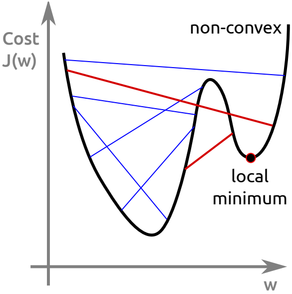
- Loss for data point $(\mathbf{x}, y)$ depends on the choice of $\mathbf{w}$: $Cost(h_{\mathbf{w}}, y)$.
- Parameters w_i can be optimized easier, if the loss function is convex and (continuously) differentiable.





Quadratic Loss is Unfavorable for Logistic Regression

Unfortunately, a quadratic loss function (as e.g. im LDA)

$$J(\mathbf{w}) = ||h_{\mathbf{w}}(\mathbf{x}), y||^2$$

would lead to a non-convex optimization problem with local minima.

- What may cause this trouble? 

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- How can we derive better loss functions? 

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- What may cause this trouble? 
- Answer: the sigmoid function in $h_{\mathbf{w}}(\mathbf{x})$

- How can we derive better loss functions? 
- Answer: talk to domain experts!

Adapted Loss Function of Logistic Regression (I)

Proposed loss function (specifically adapted to logistic regression):

$$J(h_{\mathbf{w}}(\mathbf{x}), y) = \begin{cases} -\log(h_{\mathbf{w}}(\mathbf{x})) & \text{for} \quad y = 1 \text{ (malignant)} \\ -\log(1 - h_{\mathbf{w}}(\mathbf{x})) & \text{for} \quad y = 0 \end{cases}$$

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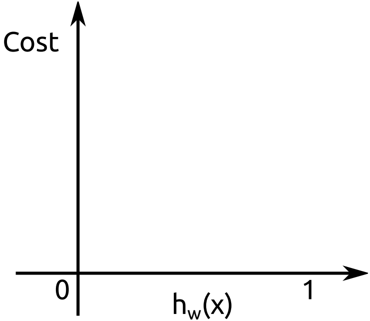
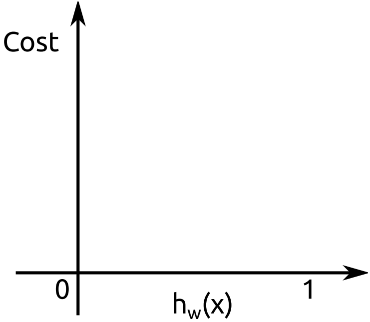


Adapted Loss Function of Logistic Regression (I)

Proposed cost function for the logistic regression model:

$$Cost(h_{\mathbf{w}}(\mathbf{x}), y) = \begin{cases} -\log(h_{\mathbf{w}}(\mathbf{x})) & \text{for} \quad y = 1 \\ -\log(1 - h_{\mathbf{w}}(\mathbf{x})) & \text{for} \quad y = 0 \end{cases}$$

Case: $y = 0$



Adapted Loss Function for Logistic Regression (II)

The case distinction can be avoided using this formulation
(check by setting $y = 0$ and $y = 1$):

$$J(h_{\mathbf{w}}(\mathbf{x}), y) = -y \log(h_{\mathbf{w}}(\mathbf{x})) - ((1 - y) \log(1 - h_{\mathbf{w}}(\mathbf{x})))$$

- Nice property: J is convex.
- Not so nice property: There is no analytic solution (but gradient descent works well).

Literature:

- Big parts of this section are based on the lectures by Andrew Ng (see youtube channel) on logistic regression.
- For a good reading on logistic calibration of linear classifiers, see Section 7.4 (Obtaining probabilities from linear classifiers) in Peter Flach: Machine Learning (Cambridge Univ. Press, 2012)

For Toolbox Use: Check Definition of Labels

For the assignment, you have used / will use the scikit-learn toolbox. Please note, that this toolbox uses labels $y \in \{-1, 1\}$. By reformulation, this leads to the following alternative loss function for logistic regression:

$$J(\mathbf{w}) = \sum_{i=1}^{N} log(exp(-y_i(\mathbf{w}^T \mathbf{x}_1)) + 1)$$

Again, check by setting the labels to fixed values and compare the both formulations:

- Case 1: $y = 0$ (our cost function / Andrew Ng) and $y = -1$ (scikit-learn)
- Case 1: $y = 1$ (our cost function / Andrew Ng) and $y = 1$ (scikit-learn)

Lecture Overview

Summary by learning goals

Having heard this lecture, you can now ...

- explain, why probability outputs instead of class values may be desired
- describe the logistic function
- formulate the logistic regression hypothesis
- formulate the optimization criterion and explain, how parameters are determined
- explain, how the output of logistic regression is interpreted
- (assignments) formulate pros and cons of LDA and logistic regression
- (assignments) compare assumptions and the effects of their violation for the two classification approaches