Classification problem

Logistic regression, decision boundary, overfitting and regularization

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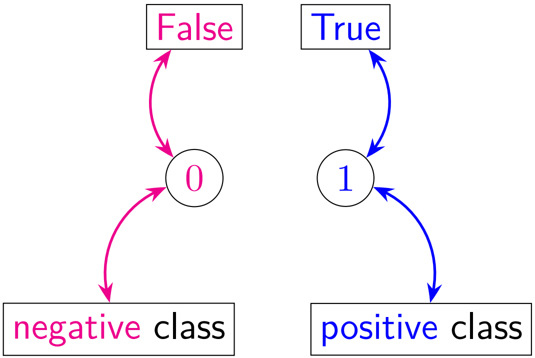
Classification

Question	Answer
Is this email spam?	no yes
Is the transaction fraudulent?	no yes
Is the tumor malignant?	no yes

- y can only be one of two values
  false true
- "binary classification"
- class = category

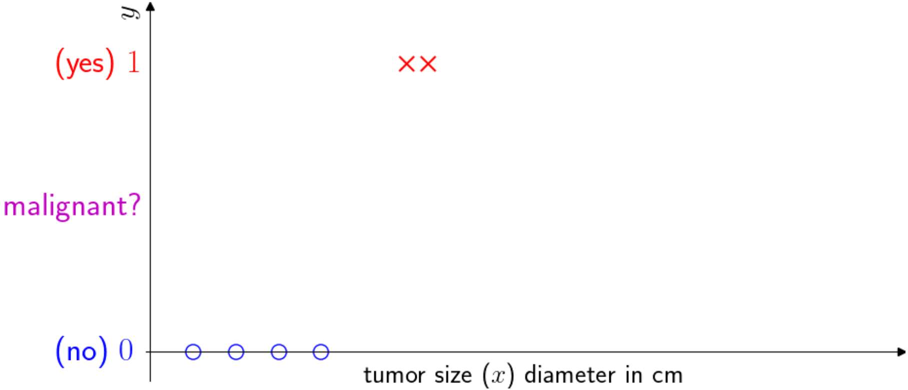


negative $\neq$ bad, positive $\neq$ good.

negative $\longleftrightarrow$ absence of a property

positive $\longleftrightarrow$ presence of a property

Decision boundary



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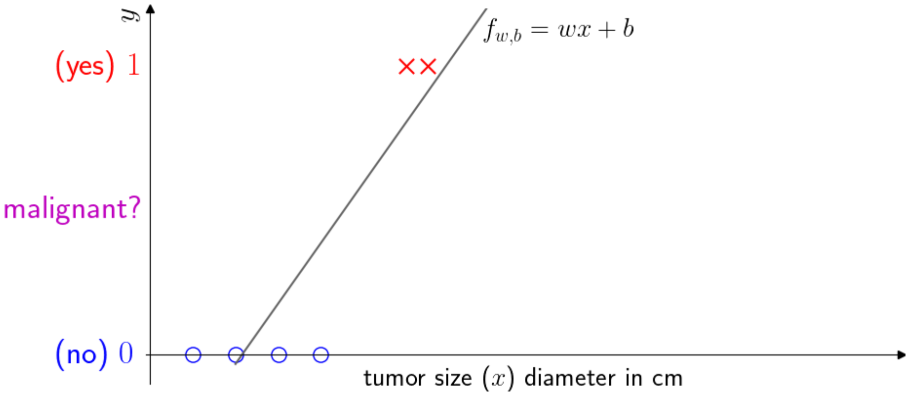

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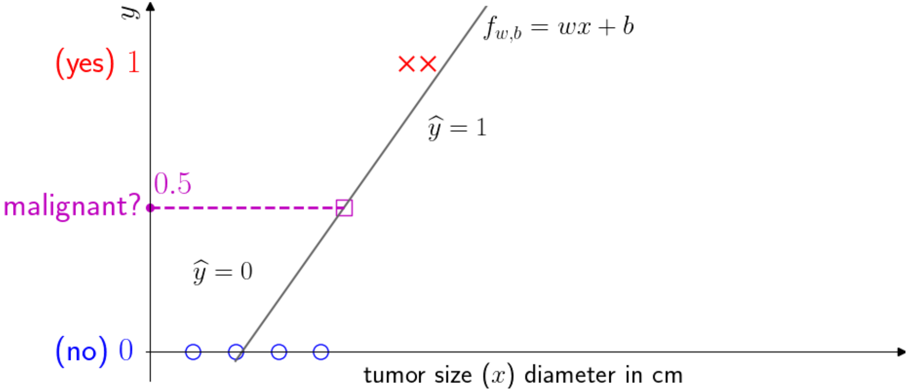
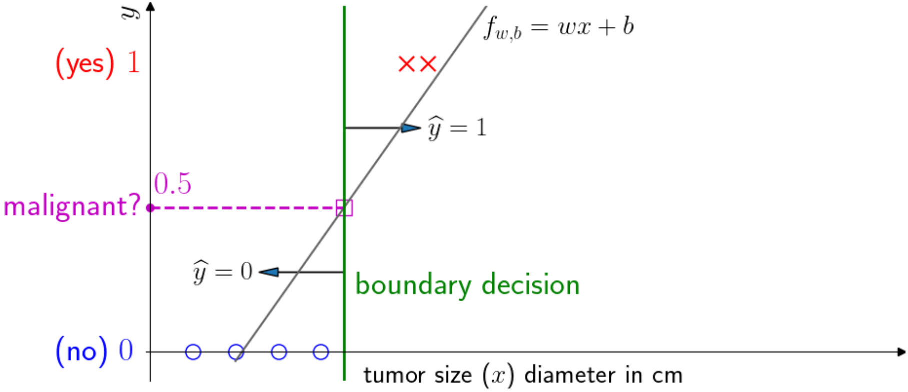


$$\text{if } f_{w,b}(x) \leq 0.5 \quad \rightarrow \quad \hat{y} = 0$$

$$\text{if } f_{w,b}(x) < 0.5 \quad \rightarrow \quad \hat{y} = 1$$

Decision boundary



$$\text{if } f_{w,b}(x) \leq 0.5 \quad \rightarrow \quad \hat{y} = 0$$
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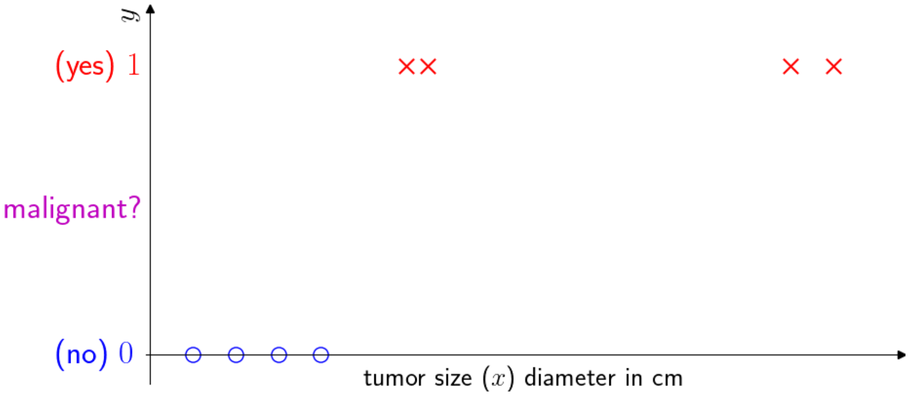

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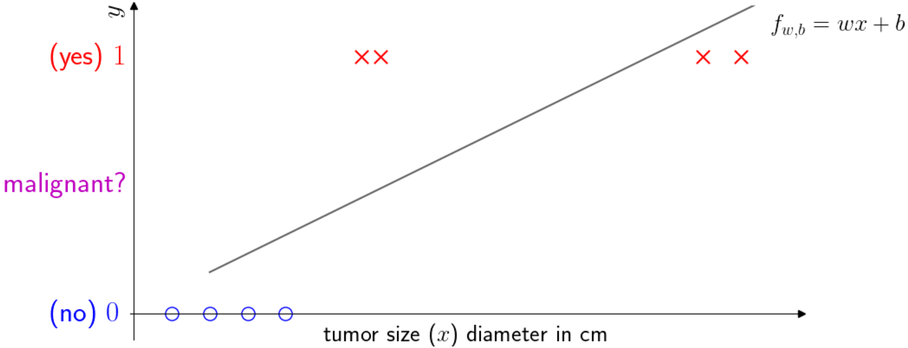

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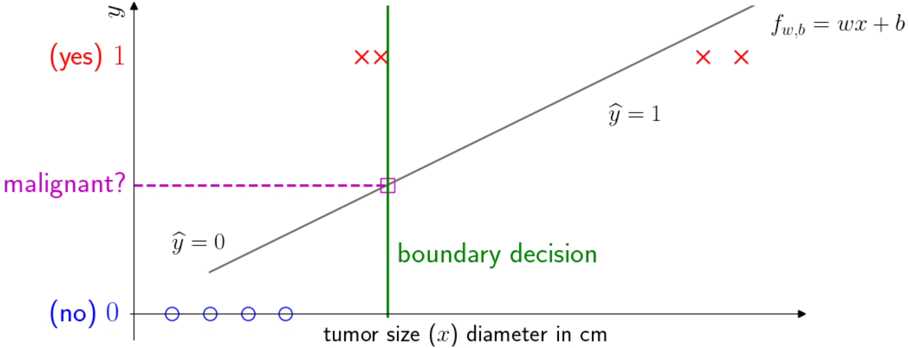

if $f_{w,b}(x) \leq 0.5 \quad \rightarrow \quad \hat{y} = 0$

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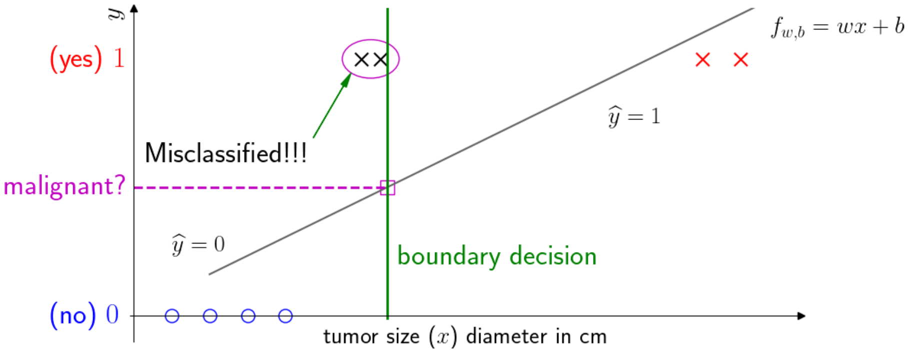

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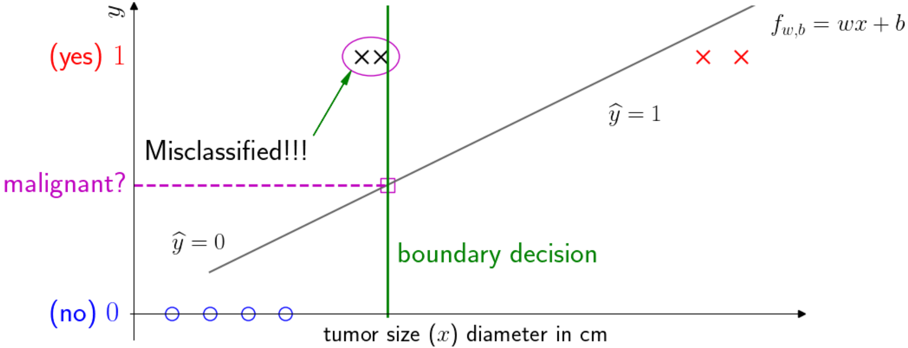

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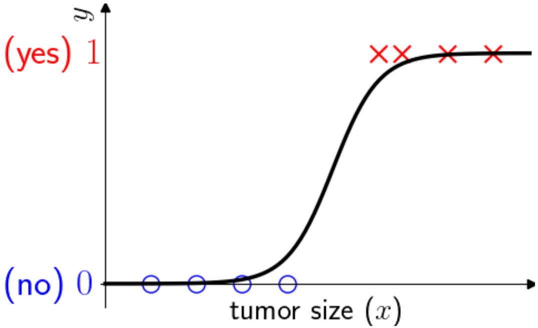
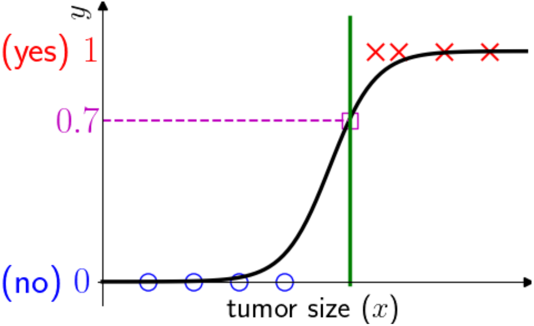
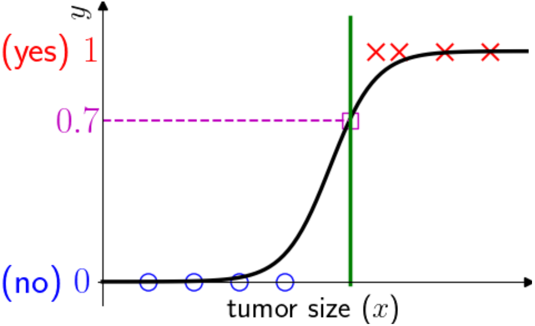
What to do: **logistic regression!!!**

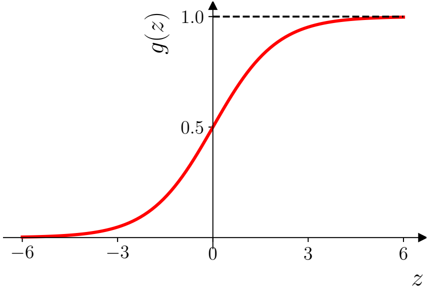
Logistic regression



Logistic regression





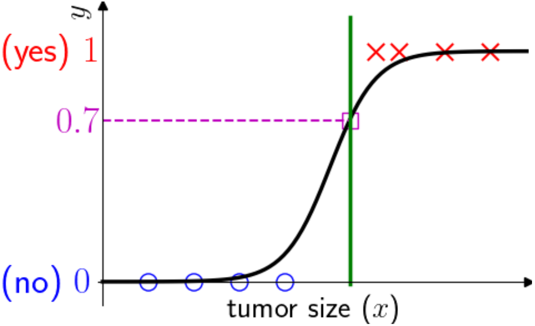


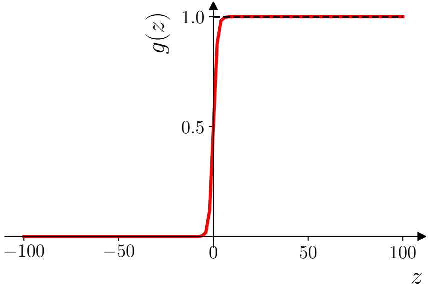
sigmoid function – logistic function

outputs between 0 and 1

$$g(z) = \frac{1}{1 + \mathrm{e}^{-z}} = \frac{1}{1 + \exp(-z)}, \quad 0 < g(z) < 1$$

Logistic regression





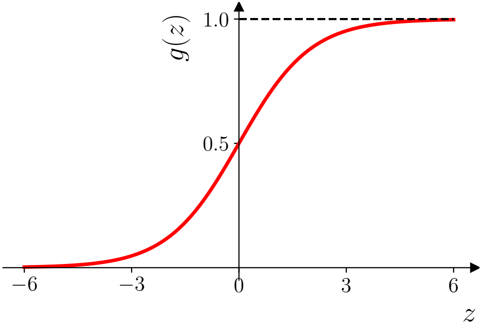
sigmoid function – logistic function

outputs between 0 and 1

$$g(100) \approx \frac{1}{1} = 1, \quad g(-100) \approx \frac{1}{\infty} = 0$$

$$g(\infty) = \frac{1}{1} = 1, \quad g(-\infty) = \frac{1}{+\infty} = 0.$$

Logistic regression



sigmoid function – logistic function
outputs between 0 and 1

$$g(z) = \frac{1}{1+\mathrm{e}^{-z}}, \quad 0 < g(z) < 1$$

$$\boxed{z = \vec{w} \cdot \vec{x} + b}$$

$$\downarrow$$

$$z$$

$$\downarrow$$

$$\boxed{g(z) = \frac{1}{1+\exp(-z)}}$$

$$f_{\vec{w},b}(\vec{x}) = g(\underbrace{\vec{w} \cdot \vec{x} + b}_{z}) = \frac{1}{1+\mathrm{e}^{-(\vec{w}\cdot\vec{x}+b)}}$$

$$= \frac{1}{1+\exp(-(\vec{w} \cdot \vec{x} + b))}$$

logistic regression!

Interpretation of logistic regression input

$$f_{w,b}(\vec{x}) = \frac{1}{1 + \mathrm{e}^{-(\vec{w}\cdot\vec{x}+b)}}$$

$$f_{\vec{w},b}(\vec{x}) = P(y = 1|\vec{x}; \vec{w}, b)$$

Interpretation: probability that class of $\vec{x}$ is 1

Probability that y is 1,

given input $\vec{x}$, parameters $\vec{w}, b$

Example:

- x is "tumor size"
- y is 0 (not malignant) or 1 (malignant)

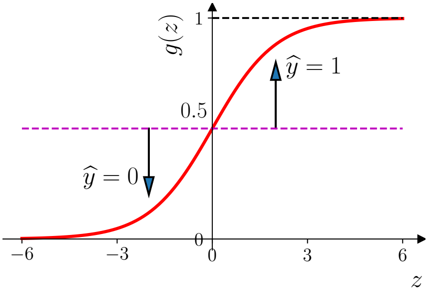
$$P(y = 0) + P(y = 1) = 1$$

$f_{\vec{w},b}(\vec{x}) = 0.7$ implies 70%

chance that y given $\vec{x}$ is 1.

$$\Rightarrow P(y = 0) = 1 - P(y = 1)$$

Decision boundary



$$f_{\vec{w},b}(\vec{x}) = g(\underbrace{\vec{w} \cdot \vec{x} + b}_{z}) = \frac{1}{1 + \mathrm{e}^{-(\vec{w} \cdot \vec{x} + b)}}$$
$$= P(y = 1 | x; \vec{w}, b)$$

0 or 1?: Is $f_{\vec{w},b}(\vec{x}) \geq 0.5$, $\quad 0.5 \rightarrow$ threshold

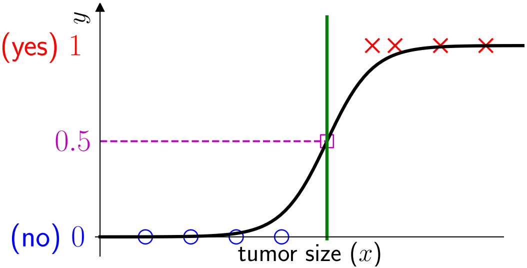
Yes: $\hat{y} = 1$ $\qquad$ No: $\hat{y} = 0$

When is $f_{\vec{w},b}(\vec{x}) \geq 0.5$?	$f_{\vec{w},b}(\vec{x}) \leq 0.5$?
$g(z) \geq 0.5$	$\cdots$
$z \geq 0$	$\cdots$
$\vec{w} \cdot \vec{x} + b \geq 0$	$\vec{w} \cdot \vec{x} + b \leq 0$
$\hat{y} = 1$	$\hat{y} = 0$

Decision boundary: 1D problem

- For single variable input, the decision boundary is

$$wx + b = 0 \quad \Leftrightarrow \quad x = -b/w$$



Question: What happen if we change the threshold from 0.5 to 0.7?

Decision boundary: 1D problem

- Denote the threshold τ with $0 < \tau < 1$:

$$
\begin{aligned}
& \frac{1}{1+\exp(-(\vec{w}\cdot\vec{x}+b))} = \tau \\
\Leftrightarrow \quad & \tau + \tau\exp(-(\vec{w}\cdot\vec{x}+b)) = 1 \\
\Leftrightarrow \quad & \tau\exp(-(\vec{w}\cdot\vec{x}+b)) = 1-\tau \\
\Leftrightarrow \quad & \exp(-(\vec{w}\cdot\vec{x}+b)) = \frac{1}{\tau} - 1 \\
\Leftrightarrow \quad & -\vec{w}\cdot\vec{x}+b = \log(\kappa), \quad \kappa = \frac{1}{\tau} - 1
\end{aligned}
$$

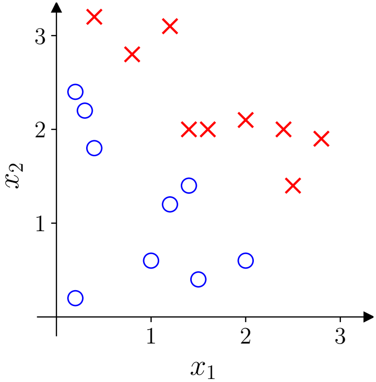
- For 1D problem:

$$
wx + b = \log(\kappa) \quad \Leftrightarrow \quad x = \frac{\log(\kappa) - b}{w}
$$

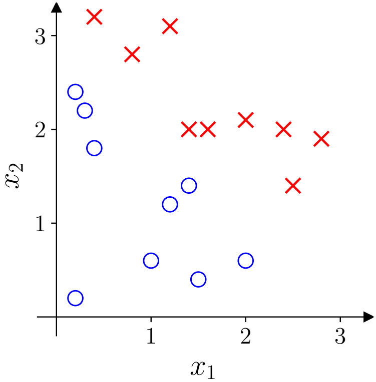
$\rightarrow$ a vertical straight line different from

$x = -b/w$ corresponding to the threshold $\tau = 0.5 \leftrightarrow \kappa = 1, \log(\kappa) = 0$

Decision boundary: 2D problem



Decision boundary: 2D problem



$$f_{\vec{w},b}(\vec{x}) = g(z) = g(w_1x_1 + w_2x_2 + b)$$

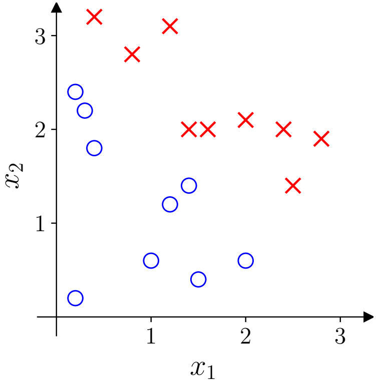
Decision boundary:

Assume the threshold $y_{\text{threshold}} = 0.5$

$$z = \vec{w} \cdot \vec{x} + b = 0 \quad \Leftrightarrow \quad w_1x_1 + w_2x_2 + b = 0$$

Clearly, this is just a line in 2D plane

Decision boundary: 2D problem



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Clearly, this is just a line in 2D plane

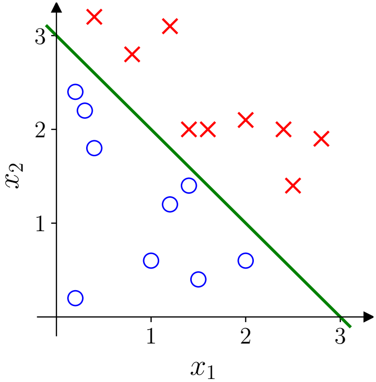
Assume after 'training': $w_1 = w_2 = 1, b = -3$
$\rightarrow$

$$w_1x_1 + w_2x_2 + b = 0$$

$$x_1 + x_2 - 3 = 0$$

$$x_1 + x_2 = 3$$

Decision boundary: 2D problem



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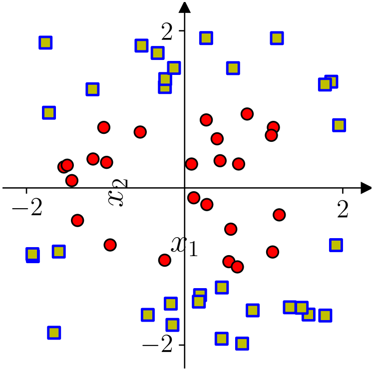
$$w_1x_1 + w_2x_2 + b = 0$$

$$x_1 + x_2 - 3 = 0$$

$$x_1 + x_2 = 3$$

Nonlinear decision boundary



$$f_{\vec{w},b}(\vec{x}) = g(z) = g(w_1 x_1^2 + w_2 x_2^2 + b)$$

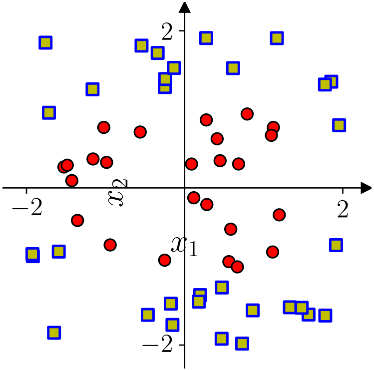
Decision boundary:

Assume the threshold $= 0.5$

$$z = w_1 x_1^2 + w_2 x^2 - 1 = 0$$

Ellipse in 2D plane

Nonlinear decision boundary



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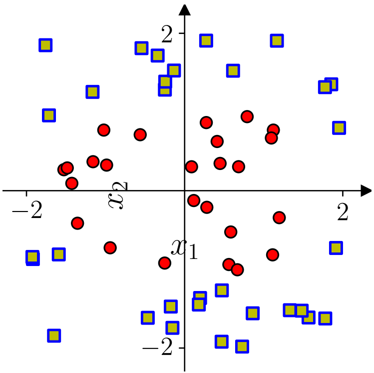
Ellipse in 2D plane

Nonlinear decision boundary



$$f_{\vec{w},b}(\vec{x}) = g(z) = g(w_1 x_1^2 + w_2 x_2^2 + b)$$

Decision boundary:

Assume the threshold $= 0.5$

$$z = w_1 x_1^2 + w_2 x^2 - 1 = 0$$

Ellipse in 2D plane

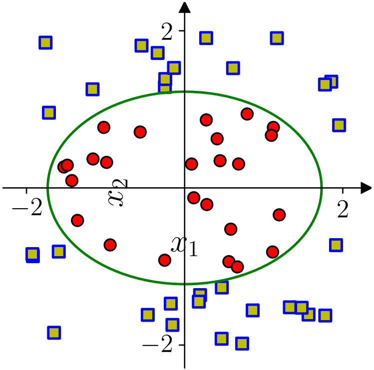
Assume after 'training':
$w_1 = 1, w_2 = 2, b = -3$

$$w_1 x_1 + w_2 x_2 + b = 0$$

$$x_1^2 + 2x_2^2 - 3 = 0$$

$$x_1^2 + 2x_2^2 = 3$$

Nonlinear decision boundary



$$f_{\vec{w},b}(\vec{x}) = g(z) = g(w_1 x_1^2 + w_2 x_2^2 + b)$$

Decision boundary:

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$$z = w_1 x_1^2 + w_2 x^2 - 1 = 0$$

Ellipse in 2D plane

Assume after 'training':
$w_1 = 1, w_2 = 2, b = -3$

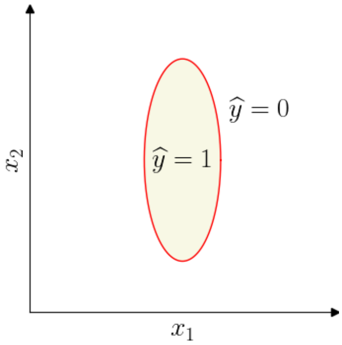
$$w_1 x_1 + w_2 x_2 + b = 0$$

$$x_1^2 + 2x_2^2 - 3 = 0$$

$$x_1^2 + 2x_2^2 = 3$$

Nonlinear decision boundary

The decision boundary can be as wiggly and complex as we may want.



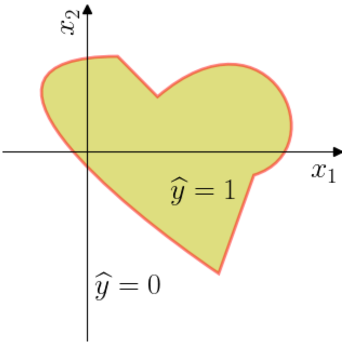


Table of Contents

Training set

tumor size (cm) x_1	$\cdots$	age x_n	malignant? y
10		52	1
2		73	0
5		55	0
12		49	1
$\vdots$		$\vdots$	$\vdots$

Training set

tumor size (cm) x_1	$\cdots$	age x_n	malignant? y
10		52	1
2		73	0
5		55	0
12		49	1
$\vdots$		$\vdots$	$\vdots$

$i = 1, \dots, m \quad \longleftarrow$ training examples

$j = 1, \dots, n \quad \longleftarrow$ features

target y is 0 or 1

Model function

$$f_{\vec{w},b}(\vec{x}) = \frac{1}{1 + \mathrm{e}^{-(\vec{w}\cdot\vec{x}+b)}}$$

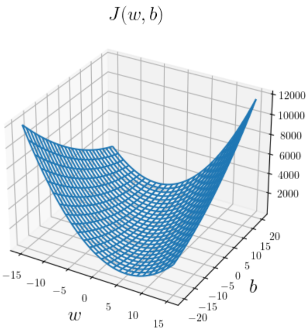
Squared error cost

$$J(\vec{w}, b) = \frac{1}{m}\sum_{i=1}\frac{1}{2}(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)})^2 = \frac{1}{m}\sum_{i=1}^{m}\underbrace{L\big[f_{\vec{w},b}(\vec{x}^{(i)}), y^{(i)}\big]}_{\text{loss (the example } (i))}$$

Squared error cost

$$J(\vec{w}, b) = \frac{1}{m} \sum_{i=1} \frac{1}{2}(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)})^2 = \frac{1}{m} \sum_{i=1}^{m} \underbrace{L\left[f_{\vec{w},b}(\vec{x}^{(i)}), y^{(i)}\right]}_{\text{loss (the example } (i))}$$

$$f_{\vec{w},b}(\vec{x}) = \vec{w} \cdot \vec{x} + b$$

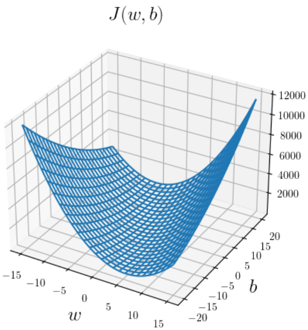


Convex cost function

Squared error cost

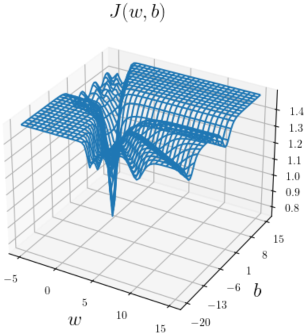
$$J(\vec{w},b) = \frac{1}{m}\sum_{i=1} \frac{1}{2}(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)})^2 = \frac{1}{m}\sum_{i=1}^{m} \underbrace{L\left[f_{\vec{w},b}(\vec{x}^{(i)}), y^{(i)}\right]}_{\text{loss (the example } (i))}$$

$$f_{\vec{w},b}(\vec{x}) = \vec{w}\cdot\vec{x} + b$$



Convex cost function

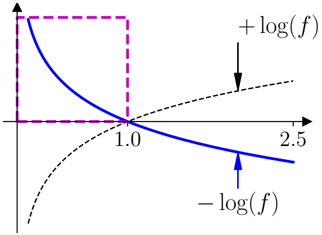
$$f_{\vec{w},b}(\vec{x}) = \frac{1}{1+\mathrm{e}^{-(\vec{w}\cdot\vec{x}+b)}}$$



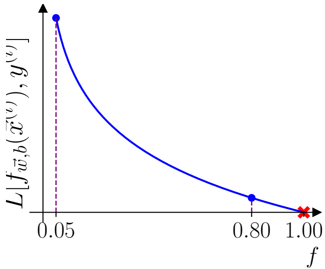
Non-convex cost function

Logistic loss function

$$L\left[f_{\vec{w},b}(\vec{x}^{(i)}), y^{(i)}\right] = \begin{cases} -\log\left(f_{\vec{w},b}(\vec{x}^{(i)})\right) & \text{if } y^{(i)} = 1 \\ -\log\left(1 - f_{\vec{w},b}(\vec{x}^{(i)})\right) & \text{if } y^{(i)} = 0 \end{cases}$$



Loss is lowest when $f_{\vec{w},b}(x^{(i)}))$ predicts close to true label $y^{(i)}$ and highest when f predicts far from true label.

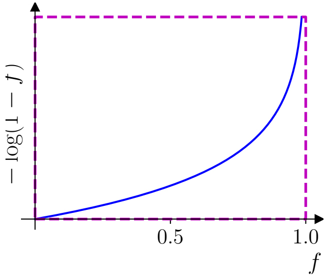


As $f_{\vec{w},b}(x^{(i)}) \to 0$, then loss $\to \infty$ ☹☹☹

As $f_{\vec{w},b}(x^{(i)}) \to 1$, then loss $\to 0$ ☺☺☺

Logistic loss function

$$L\left[f_{\vec{w},b}(\vec{x}^{(i)}), y^{(i)}\right] = \begin{cases} -\log\left(f_{\vec{w},b}(\vec{x}^{(i)})\right) & \text{if } y^{(i)} = 1 \\ -\log\left(1 - f_{\vec{w},b}(\vec{x}^{(i)})\right) & \text{if } y^{(i)} = 0 \end{cases}$$



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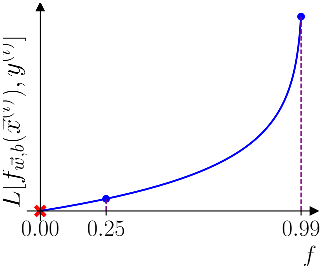


As $f_{\vec{w},b}(x^{(i)}) \to 1$, then loss $\to \infty$ ☹☹☹

As $f_{\vec{w},b}(x^{(i)}) \to 0$, then loss $\to 0$ ☺☺☺

Cost function for logistic regression

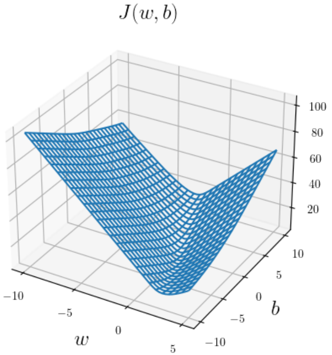
$$J(\overrightarrow{w}, b) = \frac{1}{m}\sum_{i=1}^{m} L[f_{\overrightarrow{w},b}(\vec{x}^{(i)}), y^{i}]$$

$$L[f_{\overrightarrow{w},b}(\vec{x}^{(i)}), y^{(i)}] = \begin{cases} -\log\left(f_{\overrightarrow{w},b}(\vec{x}^{(i)})\right) & \text{if } y^{(i)} = 1 \\ -\log\left(1 - f_{\overrightarrow{w},b}(\vec{x}^{(i)})\right) & \text{if } y^{(i)} = 0 \end{cases}$$

Cost function for logistic regression

$$J(\overrightarrow{w}, b) = \frac{1}{m}\sum_{i=1}^{m} L[f_{\overrightarrow{w},b}(\vec{x}^{(i)}), y^{i}]$$

$$L[f_{\overrightarrow{w},b}(\vec{x}^{(i)}), y^{(i)}] = \begin{cases} -\log\left(f_{\overrightarrow{w},b}(\vec{x}^{(i)})\right) & \text{if } y^{(i)} = 1 \\ -\log\left(1 - f_{\overrightarrow{w},b}(\vec{x}^{(i)})\right) & \text{if } y^{(i)} = 0 \end{cases}$$



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Cost function $J(\overrightarrow{w}, b)$ is convex $\rightarrow$ can reach a global minimum

Find $\overrightarrow{w}, b$: Minimize $J(\overrightarrow{w}, b)$ with respect to $\overrightarrow{w}, b$

$$\boxed{\min_{\overrightarrow{w},b} J(\overrightarrow{w}, b)}$$

Simplified cost function

$$L\left[f_{\overrightarrow{w},b}(\vec{x}^{(i)}), y^{(i)}\right] = \begin{cases} -\log\left(f_{\overrightarrow{w},b}(\vec{x}^{(i)})\right) & \text{if } y^{(i)} = 1 \\ -\log\left(1 - f_{\overrightarrow{w},b}(\vec{x}^{(i)})\right) & \text{if } y^{(i)} = 0 \end{cases}$$

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- If $y^{(i)} = 1$

$$L\left[f_{\vec{w},b}(\vec{x}^{(i)}), y^{(i)}\right] = -1 \times \log(f_{\vec{w},b}(\vec{x}^{(i)})) - (1-1) \times \smiley = -\log(f)$$

Simplified cost function

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- If $y^{(i)} = 0$

$$L\left[f_{\vec{w},b}(\vec{x}^{(i)}), y^{(i)}\right] = -0 \times ☺ - (1-0) \times \log(1 - f_{\vec{w},b}(\vec{x}^{(i)})) = -\log(1 - f)$$

Simplified cost function

➥ For one training example:

$$L\left[f_{\vec{w},b}(\vec{x}^{(i)}), y^{(i)}\right] = -y^{(i)} \log\left(f_{\vec{w},b}(\vec{x}^{(i)})\right) - (1-y^{(i)}) \log\left(1 - f_{\vec{w},b}(\vec{x}^{(i)})\right)$$

➥ Cost function [Note the minus sign in front of summation!]:

$$J(\vec{w}, b) = \frac{1}{m} \sum_{i=1}^{m} L\left[f_{\vec{w},b}(\vec{x}^{(i)}), y^{i}\right]$$

$$= -\frac{1}{m} \sum_{i=1}^{m} \left[y^{(i)} \log\left(f_{\vec{w},b}(\vec{x}^{(i)})\right) + (1-y^{(i)}) \log\left(1 - f_{\vec{w},b}(\vec{x}^{(i)})\right)\right]$$

maximum likelihood

(don't worry about it – it's just a name from statistics ☺☺)

Simplified cost function

- For one training example:

$$L\left[f_{\overrightarrow{w},b}(\vec{x}^{(i)}), y^{(i)}\right] = -y^{(i)} \log\left(f_{\overrightarrow{w},b}(\vec{x}^{(i)})\right) - (1 - y^{(i)}) \log\left(1 - f_{\overrightarrow{w},b}(\vec{x}^{(i)})\right)$$

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maximum likelihood

(don't worry about it – it's just a name from statistics ☺☺)

Find $\overrightarrow{w}, b$: Minminize $J(\overrightarrow{w}, b)$ with respect to $\overrightarrow{w}, b \quad \rightarrow \quad \min_{\overrightarrow{w},b} J(\overrightarrow{w}, b)$

Convex cost function

$$J(\vec{w}, b) = -\frac{1}{m} \sum_{i=1}^{m} \left[y^{(i)} \log\left(f_{\vec{w},b}(\vec{x}^{(i)}) \right) + (1 - y^{(i)}) \log\left(1 - f_{\vec{w},b}(\vec{x}^{(i)}) \right) \right]$$

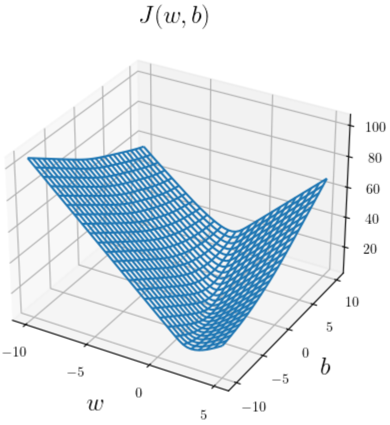

Table of Contents

Training logistic regression: Gradient descent

$$J(\vec{w}, b) = -\frac{1}{m} \sum_{i=1}^{m} \left[y^{(i)} \log\left(f_{\vec{w},b}(\vec{x}^{(i)}) \right) + (1 - y^{(i)}) \log\left(1 - f_{\vec{w},b}(\vec{x}^{(i)}) \right) \right]$$

Training logistic regression: Gradient descent

$$J(\vec{w}, b) = -\frac{1}{m} \sum_{i=1}^{m} \left[y^{(i)} \log\left(f_{\vec{w},b}(\vec{x}^{(i)})\right) + (1 - y^{(i)}) \log\left(1 - f_{\vec{w},b}(\vec{x}^{(i)})\right) \right]$$

Repeat

$$\begin{cases} w_j = w_j - \alpha \dfrac{\partial J}{\partial w_j}(\vec{w}, b) \\ \\ b = b - \alpha \dfrac{\partial J}{\partial b}(\vec{w}, b) \end{cases}$$

simultaneous updates

Training logistic regression: Gradient descent

$$J(\vec{w}, b) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log\left(f_{\vec{w},b}(\vec{x}^{(i)})\right) + (1-y^{(i)})\log\left(1-f_{\vec{w},b}(\vec{x}^{(i)})\right)\right]$$

Repeat

$$\begin{cases} w_j = w_j - \alpha\dfrac{\partial J}{\partial w_j}(\vec{w}, b) \\ \\ b = b - \alpha\dfrac{\partial J}{\partial b}(\vec{w}, b) \end{cases}$$

simultaneous updates

$$\frac{\partial J}{\partial w_j}(\vec{w}, b) = \frac{1}{m}\sum_{i=1}^{m}\left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)}\right)x_j^{(i)}$$

$$\frac{\partial J}{\partial b}(\vec{w}, b) = \frac{1}{m}\sum_{i=1}^{m}\left(f_{\vec{w},b}(x^{(i)}) - y^{(i)}\right)1$$

looks like linear regression!

$\rightarrow$ Not the same though as $f_{\vec{w},b}$ is different

same same but different

Gradient descent for logistic regression

Repeat

$$\begin{cases} w_j = w_j - \alpha\left[\dfrac{1}{m}\displaystyle\sum_{i=1}^{m}\left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)}\right)x_j^{(i)}\right] \\ b = b - \alpha\left[\dfrac{1}{m}\displaystyle\sum_{i=1}^{m}\left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)}\right)\right] \end{cases}$$

simultaneous updates

Linear regression: $f_{\vec{w},b}(\vec{x}) = \vec{w} \cdot \vec{x} + b$

Logistic regression:

$$f_{\vec{w},b}(\vec{x}) = \frac{1}{1 + \mathrm{e}^{-(\vec{w}\cdot\vec{x}+b)}}$$

Same concepts:

- Monitor gradient descent (learning curve)
- Vectorized implementation
- Feature scaling

LogisticRegression from sklearn

```
class sklearn.linear_model.LogisticRegression(penalty='l2', *, dual=False, tol=0.0001,
C=1.0, fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None,
solver='lbfgs', max_iter=100, multi_class='deprecated', verbose=0, warm_start=False,
n_jobs=None, l1_ratio=None)
```
[source]

Logistic Regression (aka logit, MaxEnt) classifier.

In the multiclass case, the training algorithm uses the one-vs-rest (OvR) scheme if the 'multi_class' option is set to 'ovr', and uses the cross-entropy loss if the 'multi_class' option is set to 'multinomial'. (Currently the 'multinomial' option is supported only by the 'lbfgs', 'sag', 'saga' and 'newton-cg' solvers.)

This class implements regularized logistic regression using the 'liblinear' library, 'newton-cg', 'sag', 'saga' and 'lbfgs' solvers. **Note that regularization is applied by default**. It can handle both dense and sparse input. Use C-ordered arrays or CSR matrices containing 64-bit floats for optimal performance; any other input format will be converted (and copied).

The 'newton-cg', 'sag', and 'lbfgs' solvers support only L2 regularization with primal formulation, or no regularization. The 'liblinear' solver supports both L1 and L2 regularization, with a dual formulation only for the L2 penalty. The Elastic-Net regularization is only supported by the 'saga' solver.

Figure: LogisticRegression from sklearn

https://scikit-learn.org/1.5/modules/generated/sklearn.linear_model.LogisticRegression.html

LogisticRegression from sklearn

Examples

```
>>> from sklearn.datasets import load_iris
>>> from sklearn.linear_model import LogisticRegression
>>> X, y = load_iris(return_X_y=True)
>>> clf = LogisticRegression(random_state=0).fit(X, y)
>>> clf.predict(X[:2, :])
array([0, 0])
>>> clf.predict_proba(X[:2, :])
array([[9.8...e-01, 1.8...e-02, 1.4...e-08],
       [9.7...e-01, 2.8...e-02, ...e-08]])
>>> clf.score(X, y)
0.97...
```

Figure: LogisticRegression from sklearn

https://scikit-learn.org/1.5/modules/generated/sklearn.linear_model.LogisticRegression.html