Lecture 6. Linear classification (part 1): Logistic Regression

COMP 551 Applied machine learning

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Outline

Objectives

Linear classifier

Learning logistic regression by gradient descent

Probabilistic view of logistic regression

Application: Titanic surviver prediction

Summary

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Learning objectives

Understanding the following concepts

- linear classifiers
- logistic regression
    - model
    - loss function
- maximum likelihood view multi-class classification

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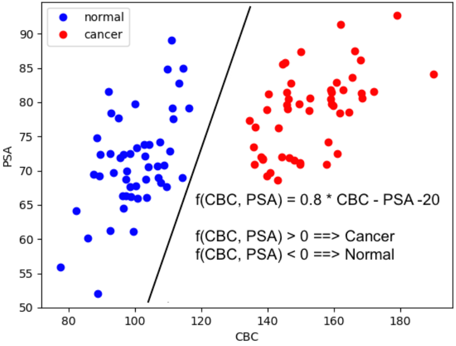
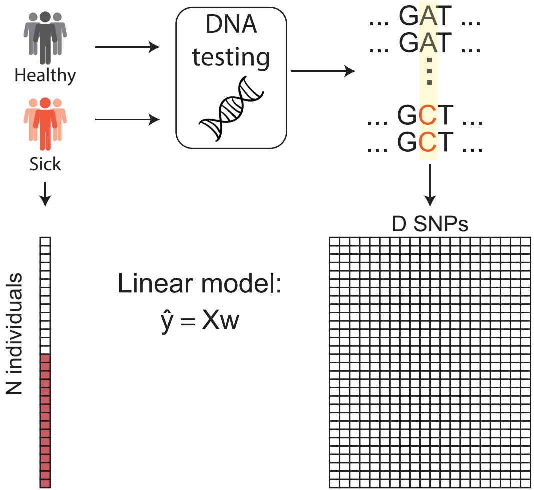
Linear function for binary classification

With one or two-dimensional input, it is not hard to think of a linear function $w_1 x_2 + w_2 x_2$ that separates positive and negative examples.



With high-dimensional input ($D >> 2$), however, it becomes impossible to do.

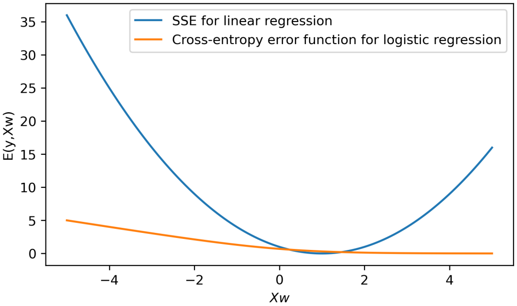


Linear regression for continuous response is not suitable for classification

For a binary classification problem, the target variable $y \in \{0, 1\}$.
Recall from Lecture 5, the cost function for linear regression is sum of squared error (SSE):

$$J(\mathbf{w}) = \sum_{n=1}^{N} (y^{(n)} - \hat{y}^{(n)})^2$$

where $\hat{y}^{(n)} = \sum_d w_d x_d^{(n)}$. However, $\hat{y}^{(n)} \in \mathbb{R}$, which means our prediction is unbounded.



Given that the true label $y = 1$, the SSE is 0 if and only if $\hat{y}^{(n)} = 1$. SEE increases even if $\hat{y}^{(n)}$ is highly positive (indicating that the model is confident about the true positive label). In contrast, another error function called **cross-entropy** decreases $\hat{y}^{(n)}$ becomes more positive and converges to 0 as $\hat{y}^{(n)} \to \infty$.

Logistic function

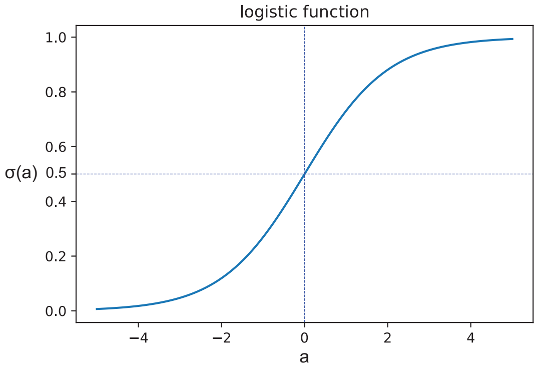
Logistic function transforms the real-value $\mathbf{a} = \mathbf{Xw} \in \mathbb{R}$ into $\hat{y} \in [0, 1]$, which can be interpreted as the *probability* being class 1.

$$\hat{y} = \sigma(a) = \frac{1}{1 + \exp(-a)} \tag{1}$$

The inverse of the logistic function is called **logit function**:

$$\log \frac{\hat{y}}{1 - \hat{y}} = a \tag{2}$$

which is the log-odd ratio of the probability being positive case over the probability being negative class.



$\sigma(a) = 0.5$ if $a = 0$, which indicates "neural" (i.e., either positive or negative). Therefore, $a = 0$ is the decision boundary.

Cross entropy loss functions

Given that $\hat{y} = 1/(1 + \exp(-\mathbf{xw}))$, we consider three candidate loss functions.

Direct loss is not differentiable so we cannot use gradient descent (Section 3):

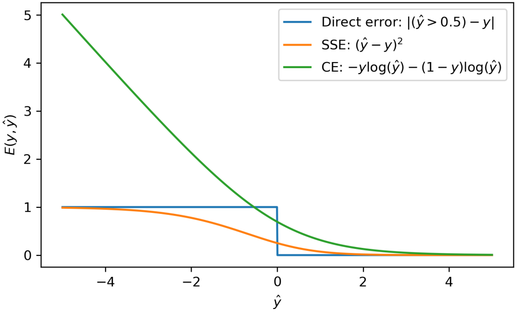
$$\mathcal{L}(\hat{y}, y) = |\mathbb{I}(\hat{y} > 0.5) - y|$$

The SSE loss is non-convex to optimize:

$$\mathcal{L}(\hat{y}, y) = (\hat{y} - y)^2$$

cross-entropy (CE) is convex in **w** and has probabilistic interpretation (Section 4)

$$CE(\hat{y}, y) = -y \log(\hat{y}) - (1 - y) \log(1 - \hat{y})$$



Numerically accurate implementation of the CE loss using `np.log1p`

```
a = np.dot(x, w)
J = np.sum(y * np.log1p(np.exp(-a)) + (1-y) * np.log1p(np.exp(a)))
```

$$
\begin{aligned}
J(w) &= -\sum_n y^{(n)} \log\left(\frac{1}{1+\exp(-a)}\right) - (1-y^{(n)}) \log\left(1 - \frac{1}{1+\exp(-a)}\right) \\
&= \sum_n y^{(n)} \log(1+\exp(-a)) - (1-y^{(n)}) \log\left(\frac{\exp(-a)}{1+\exp(-a)}\right) \\
&= \sum_n y^{(n)} \log(1+\exp(-a)) - (1-y^{(n)}) \log\left(\frac{1}{\exp(a)+1}\right) \\
&= \sum_n y^{(n)} \log(1+\exp(-a)) + (1-y^{(n)}) \log(1+\exp(a))
\end{aligned}
$$

`np.log1p(x)` computes $\log(1+x)$ for accurate floating point. Try this:

```
np.log(1+1e-100) # 0
np.log1p(1e-100) # 1e-100
```

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Gradient calculation

Let's start with one training example $\{\mathbf{x}, y\}$ to not clutter the notation. Let $\hat{y} = 1/(1 + \exp(a))$, where $a = \mathbf{x}\mathbf{w}$. Our goal is to minimize CE w.r.t. $\mathbf{w}$:

$$J(\mathbf{w}) = -y \log(\hat{y}) - (1 - y) \log(1 - \hat{y})$$

We break down the partial derivative of $J(w)$ w.r.t. w_d for feature d by chain rule:

$$\frac{\partial J(\mathbf{w})}{\partial w_d} = \frac{\partial J(\mathbf{w})}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a} \frac{\partial a}{\partial w_d}$$

Let's solve these three gradients one by one:

$$\begin{aligned}
\frac{\partial J(\mathbf{w})}{\partial \hat{y}} &= \frac{\partial}{\partial \hat{y}} - y \log(\hat{y}) - (1 - y) \log(1 - \hat{y}) \\
&= -y \frac{\partial}{\partial \hat{y}} \log \hat{y} - (1 - y) \frac{\partial \log(1 - \hat{y})}{\partial(1 - \hat{y})} \frac{\partial(1 - \hat{y})}{\partial y} \\
&= -\frac{y}{\hat{y}} - \frac{1 - y}{1 - \hat{y}}(-1) = -\frac{y}{\hat{y}} + \frac{1 - y}{1 - \hat{y}}
\end{aligned} \tag{3}$$

$$
\begin{aligned}
\frac{\partial \hat{y}}{\partial a} &= \frac{\partial}{\partial a}(1+\exp(-a))^{-1} \\
&= \frac{\partial (1+\exp(-a))^{-1}}{\partial 1+\exp(-a)} \frac{\partial 1+\exp(-a)}{\partial -a} \frac{\partial -a}{a} \\
&= -(1+\exp(-a))^{-2}\exp(-a)(-1) \\
&= (1+\exp(-a))^{-2}\exp(-a) \\
&= \frac{1}{1+\exp(-a)} \frac{\exp(-a)}{1+\exp(-a)} \\
&= \frac{1}{1+\exp(-a)} \left(1 - \frac{1}{1+\exp(-a)}\right) \\
&= \hat{y}(1-\hat{y}) \\
\frac{\partial a}{\partial w_d} &= \frac{\partial}{\partial w_d} \sum_d x_d w_d = x_d
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial J(\mathbf{w})}{\partial w_d} &= \frac{\partial J(\mathbf{w})}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a} \frac{\partial a}{\partial w_d} \\
&= (-\frac{y}{\hat{y}} + \frac{1-y}{1-\hat{y}})(\hat{y}(1-\hat{y}))x_d \\
&= -y(1-\hat{y})x_d + (1-y)\hat{y}x_d \\
&= -yx_d + y\hat{y}x_d + \hat{y}x_d - y\hat{y}x_d \\
&= (\hat{y}-y)x_d
\end{aligned}
$$

The gradient suggests that to update weight w_d, we use the prediction error weighted by the corresponding feature x_d. We can represent the gradients over all features $d \in \{1 \ldots, D\}$ in matrix form:

$$
\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}} = (\hat{y}-y)\mathbf{x}
$$

Logistic regression training algorithm by gradient descent

For N individuals, we can adding the gradients together for each feature:

$$\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}} = \sum_{n=1}^{N} (\hat{y}^{(n)} - y^{(n)}) \mathbf{x}^{(n)} = \mathbf{X}^\intercal (\hat{\mathbf{y}} - \mathbf{y})$$

Unlike in the linear regression case, where we have closed-form solution for **w** (i.e., $\mathbf{w} = (\mathbf{X}^\intercal \mathbf{X})^{-1} \mathbf{X}^\intercal \mathbf{y}$), to train a logistic regression, we cannot solve $\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}} = 0$ for **w**. To update the logistic regression model, we perform **gradient descent** by *subtracting* the gradients from the existing weight *iteratively*:

$$\mathbf{w}^t \leftarrow \mathbf{w}^{t-1} - \alpha \frac{\partial J(\mathbf{w})}{\partial \mathbf{w}}$$

- We do subtracting because we want to minimize the error function.
- We multiple the gradient by a learning rate $\alpha \in [0, 1]$ to avoid overshoot the optimal value

Logistic regression training algorithm by gradient descent

Algorithm 1 LogisticRegression.fit($\mathbf{X}$, $\mathbf{y}$, $\alpha = 0.005$, $\epsilon = 10^{-5}$, max_iter$=10^5$)

Randomly initialize regression coefficients $w_d \sim \mathcal{N}(0,1)\,\forall d$

for niter $= 1 \ldots$ max_iter **do**

  $\mathbf{w}^{(t)} \leftarrow \mathbf{w}^{(t-1)} - \alpha \frac{\partial J(\mathbf{w}^{(t-1)})}{\partial \mathbf{w}^{(t-1)}}$

  $\hat{\mathbf{y}} = 1/(1 + \exp(-\mathbf{X}\mathbf{w}^{(t)}))$

  $J(\mathbf{w}^{(t)}) = \sum_n -y^{(n)} \log(\hat{y}^{(n)}) - (1 - y^{(n)}) \log(1 - \hat{y}^{(n)})$

  if $||J(\mathbf{w}^{(t)}) - J(\mathbf{w}^{(t-1)})||_2) < \epsilon$ **then**

    break // *Converged so we quite before completing all iterations*

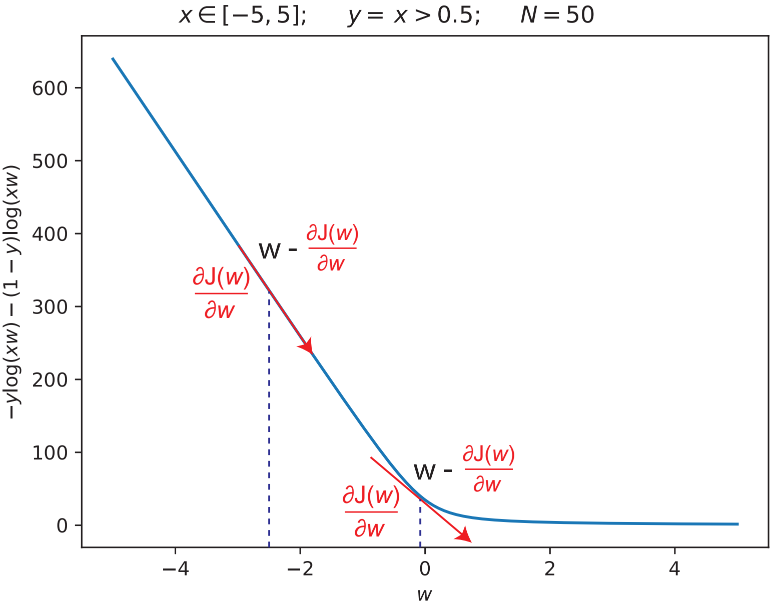
  end if

end for

Toy data

```
N=50
x = np.linspace(-5,5, N)
y = (x > 0.5).astype(int)

lr = 0.001
niter = 10000
w = np.random.randn(1)
w0 = w
ce_all = np.zeros(niter)
for i in range(niter):
    y_hat = 1 / (1 + np.exp(-w * x))
    ce_all[i] = np.sum(-y * np.log(y_hat) - (1-y) * np.log(1-y_hat))
    dw = np.sum((y_hat - y) * x)
    w = w - lr * dw
```

Cross-entropy as a function of w



Verifying gradient calculation 1: small perturbation

Gradient calculation by hand as shown above can be error-prone. We can verify the gradient as follow:

1. $\epsilon \sim \mathit{Uniform}([0, 1])$
2. $w_d^{(+)} = w_d + \epsilon$
3. $w_d^{(-)} = w_d - \epsilon$
4. $\nabla w_d = \frac{J(w_d^{(+)}) - J(w_d^{(-)})}{2\epsilon}$ (numerically estimated gradient)
5. $\frac{(\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}} - \nabla w_d)^2}{(\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}} + \nabla w_d)^2}$ must be small (e.g., 10^{-8}) otherwise your gradient calculation and/or your loss function is incorrect

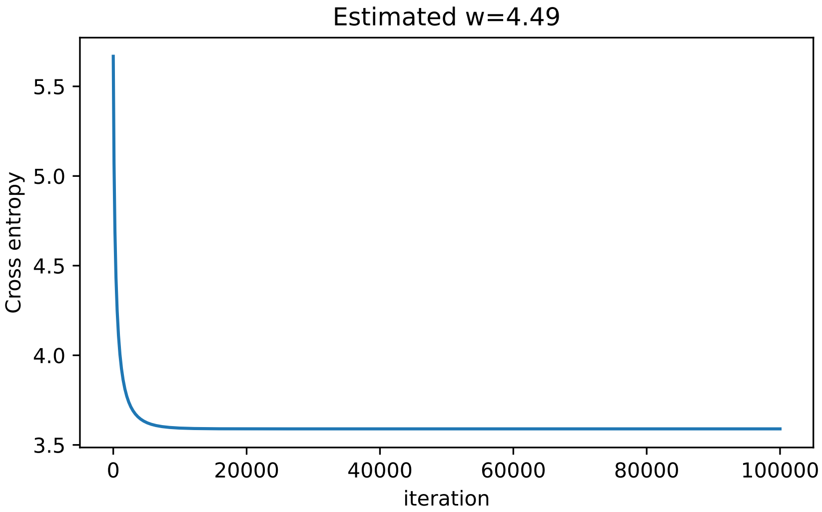
Python code for small perturbation test on a toy data

```
N=50
x = np.linspace(-5,5, N)
y = (x > 0.5).astype(int)

# small perturbation
w = np.random.randn(1)
w0 = w
epsilon = np.random.randn(1)[0] * 1e-5
w1 = w0 + epsilon
w2 = w0 - epsilon
a1 = w1*x
a2 = w2*x
ce1 = np.sum(y * np.log1p(np.exp(-a1)) + (1-y) * np.log1p(np.exp(a1)))
ce2 = np.sum(y * np.log1p(np.exp(-a2)) + (1-y) * np.log1p(np.exp(a2)))
dw_num = (ce1 - ce2)/(2*epsilon) # approximated gradient

yh = 1/(1+np.exp(-x * w))
dw_cal = np.sum((yh - y) * x) # hand calculated gradient

print(dw_cal)
print(dw_num)
print((dw_cal - dw_num)**2/(dw_cal + dw_num)**2)
```

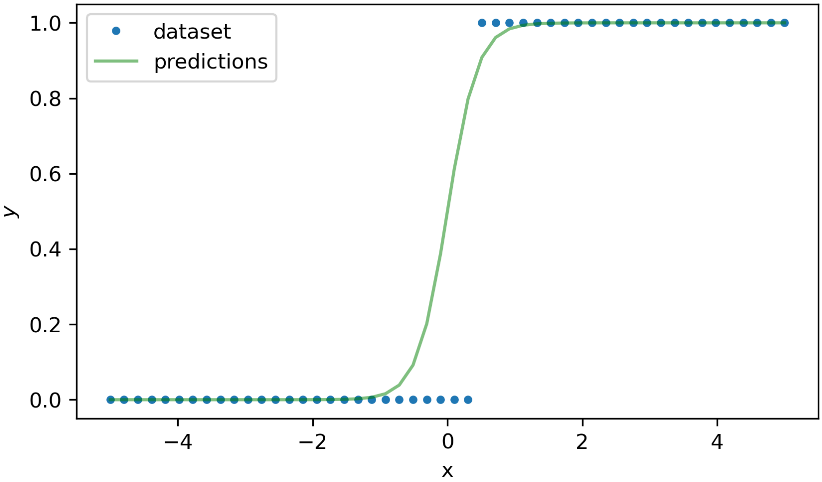
Verifying gradient calculation 2: Monitor error decreases at each iteration

```
N=50
x = np.linspace(-5,5, N)
y = (x > 0.5).astype(int)

lr = 0.001
niter = 10000
w = np.random.randn(1)
w0 = w
ce_all = np.zeros(niter)
for i in range(niter):
    a = w * x
    ce_all[i] = np.sum(y * np.log1p(np.exp(-a)) \
        + (1-y) * np.log1p(np.exp(a)))
    dw = np.sum((y_hat - y) * x)
    w = w - lr * dw
```

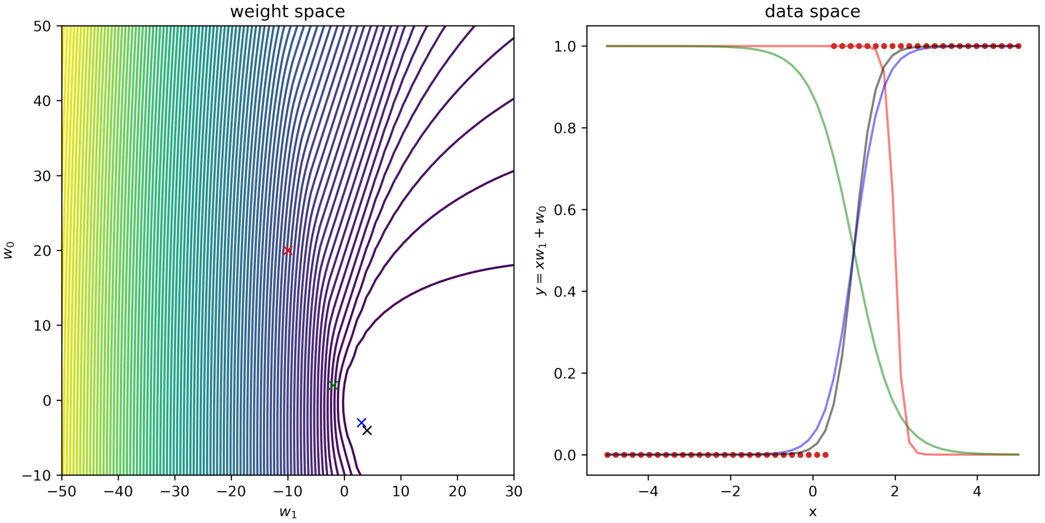
Verifying gradient calculation 2: Monitor error decreases at each iteration



Visualizing predictions on 1D data



Visualizing weights contour and their predictions



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Bernoulli distribution

A Bernoulli distribution has the following probability distribution function (PDF):

$$p(y|\pi) = \pi^y (1-\pi)^{1-y} \tag{4}$$

where π is the rate of $y = 1$. A common example used is coin toss. If the coin lands on its head $y = 1$; otherwise $y = 0$. A fair coin will have $\pi = 0.5$.

We can toss N times to get a dataset of $\mathcal{D} = \{y^{(n)}\}^N$, where $y^{(n)} \in \{0, 1\}$. Assuming the coin tosses are i.i.d., we can express the joint distribution of N tosses as the product of PDF or the *likelihood*:

$$p(\mathbf{y}|\pi) = \prod_{n=1}^{N} \pi^{y^{(n)}} (1-\pi)^{1-y^{(n)}} \tag{5}$$

It is more convent to work with logarithmic form of the likelihood or log likelihood because **the log of the products equal to the sum of the log**:

$$\mathcal{L}(\pi) = \log p(\mathbf{y}|\pi) = \log \prod_{n=1}^{N} \pi^{y^{(n)}} (1-\pi)^{1-y^{(n)}} = \sum_{n=1}^{N} y^{(n)} \log \pi + (1 - y^{(n)}) \log(1-\pi) \tag{6}$$

Maximum likelihood estimation w.r.t. the Bernoulli rate π

Suppose we are interested in knowing the Bernoulli rate π. We can directly maximize the log likelihood w.r.t. π. We do this by trying to solve for π by setting $\frac{\partial \mathcal{L}}{\partial \pi} = 0$:

$$\frac{\partial \mathcal{L}}{\partial \pi} = \frac{\partial}{\partial \pi} \sum_{n=1}^{N} y^{(n)} \log \pi + (1 - y^{(n)}) \log(1 - \pi) = \sum_{n=1}^{N} y^{(n)} \frac{\partial \log \pi}{\partial \pi} + (1 - y^{(n)}) \frac{\partial \log(1 - \pi)}{\partial \pi}$$

$$= \sum_{n=1}^{N} \frac{y^{(n)}}{\pi} - \frac{1 - y^{(n)}}{1 - \pi} = \frac{\sum_{n=1}^{N} y^{(n)}}{\pi} - \frac{\sum_{n=1}^{N} 1 - y^{(n)}}{1 - \pi} = \frac{N_1}{\pi} - \frac{N - N_1}{1 - \pi}$$

where $N_1 = \sum_n y^{(n)}$. Solving $\frac{N_1}{\pi} - \frac{N - N_1}{1 - \pi} = 0$ for π:

$$\frac{N_1}{\pi} - \frac{N - N_1}{1 - \pi} = 0 \implies N_1 - N_1 \pi = \pi N - \pi N_1 \implies \pi = \frac{N_1}{N}$$

Therefore, the maximum likelihood estimate of π is simply the proportion of the positive values.

Maximum likelihood estimation w.r.t. the logistic regression coefficients

Replacing the Bernoulli rate π with predicted probability $\hat{y}^{(n)} = \sigma(\mathbf{x}^{(n)}\mathbf{w} + w_0)$ by the logistic regression for each example:

$$\mathcal{L}(\mathbf{w}) = \log p(\mathbf{y}|\hat{\mathbf{y}}) = \sum_{n=1}^{N} y^{(n)} \log \hat{y}^{(n)} + (1 - y^{(n)}) \log(1 - \hat{y}^{(n)}) \tag{7}$$

We can solve $\frac{\partial \mathcal{L}}{\partial \hat{y}^{(n)}} = 0$ in Eq (3) for $\hat{y}^{(n)}$ and realize that the solution is trivial: $\hat{y}^{(n)} = y$.

Recall the inverse of the logistic function is the logit function:

$$\log \frac{\hat{y}^{(n)}}{1 - \hat{y}^{(n)}} = \mathbf{x}^{(n)}\mathbf{w} + w_0 \tag{8}$$

If $\mathbf{x}^{(n)}\mathbf{w} = 0 \, \forall n$, we have $\hat{y}^{(n)} = \sigma(b) \equiv \pi \, \forall n$ and

$$\log \frac{\hat{y}^{(n)}}{1 - \hat{y}^{(n)}} = \log \frac{\pi}{1 - \pi} = w_0 \quad \forall n \tag{9}$$

So the intercept b here captures the log odds of the prior probability.

Maximum likelihood estimation w.r.t. the logistic regression coefficients

However, our main interest is in $\mathbf{w}$. It is easy to see that maximizing this likelihood w.r.t. $\mathbf{w}$ is equivalent to minimizing the cross entropy (CE) since $CE = -\mathcal{L}(\mathbf{w})$:

$$\begin{aligned} -\mathcal{L}(\mathbf{w}) &= -\log p(\mathbf{y}|\hat{\mathbf{y}}) \\ &= -\left(\sum_{n=1}^{N} y^{(n)} \log \hat{y}^{(n)} + (1 - y^{(n)}) \log(1 - \hat{y}^{(n)})\right) \\ &= \sum_{n=1}^{N} -y^{(n)} \log \hat{y}^{(n)} - (1 - y^{(n)}) \log(1 - \hat{y}^{(n)}) \\ &= J(\mathbf{w}) \end{aligned}$$

That is,

$$\mathbf{w}^* = \arg\max_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = \arg\min_{\mathbf{w}} J(\mathbf{w}) \tag{10}$$

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Titanic dataset

1. ‘pclass’ - passenger class (1 = first; 2 = second; 3 = third)
2. ‘survived’ - yes (1) or no (0)
3. ‘sex’ - sex of passenger (binary) (‘male’=0 and ‘female’ = 1)
4. ‘age’ - age of passenger in years (float)
5. ‘sibsp’ - number of siblings/spouses aboard (integer)
6. ‘parch’ - number of parents/children aboard (integer)
7. ‘fare’ - fare paid for ticket (float)

	pclass	survived	sex	age	sibsp	parch	fare
0	1.0	1.0	1	29.0000	0.0	0.0	211.3375
1	1.0	1.0	0	0.9167	1.0	2.0	151.5500
2	1.0	0.0	1	2.0000	1.0	2.0	151.5500
3	1.0	0.0	0	30.0000	1.0	2.0	151.5500
4	1.0	0.0	1	25.0000	1.0	2.0	151.5500
...	...	...	...	...	...	...	...
1040	3.0	0.0	0	45.5000	0.0	0.0	7.2250
1041	3.0	0.0	1	14.5000	1.0	0.0	14.4542
1042	3.0	0.0	0	26.5000	0.0	0.0	7.2250
1043	3.0	0.0	0	27.0000	0.0	0.0	7.2250
1044	3.0	0.0	0	29.0000	0.0	0.0	7.8750

Classifying survivor and non-survivor from Titanic

Goal: For a given passenger, we want to predict whether he or she survive using the rest of the variables.
We split the data into 80% training and 20% testing

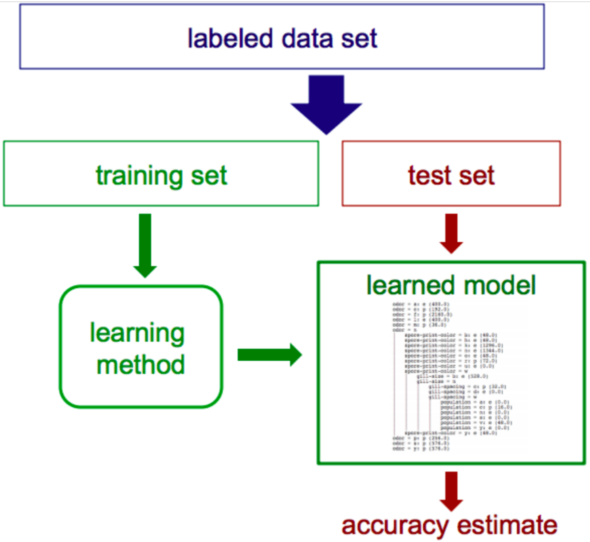
```
from sklearn import model_selection
import pandas as pd
from sklearn.preprocessing import normalize

data = pd.read_csv('data/LogisticRegression/titanic.csv')

X = data.drop(["survived"], axis=1).values
y = data["survived"].values
X_train, X_test, y_train, y_test = model_selection.train_test_split(
    X, y, test_size = 0.2, random_state=1, shuffle=True)

X_train = normalize(X_train)
X_test = normalize(X_test)
```

Recall the typical workflow to evaluate a classification model



Logistic regression classification

```
logitreg = LogisticRegression() # create an object (OOP)
fit = logitreg.fit(X_train, y_train)
effect_size = pd.DataFrame(fit.w[:(len(fit.w)-1)]).transpose() #
↪  linear coeffficents
effect_size.columns = data.drop(["survived"], axis=1).columns
print(effect_size.to_string(index=False))
#    pclass       sex       age     sibsp    parch     fare
# -1.051683  2.326165 -0.037907 -0.348339  0.151557  0.001107
```

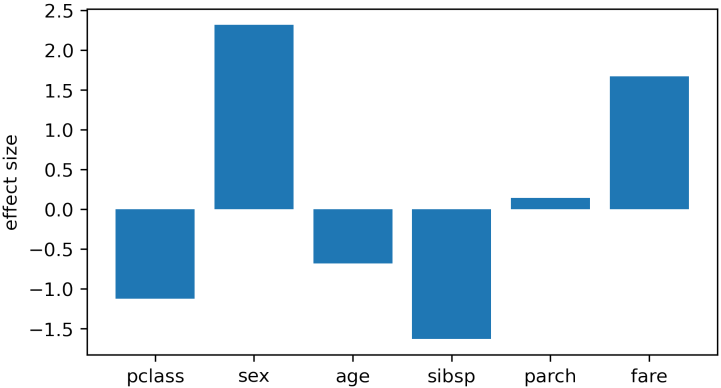
$$a = w_0 + w_{pclass}\mathbf{x}_{pclass} + w_{sex}\mathbf{x}_{sex} + w_{age}\mathbf{x}_{age} + w_{sidsp}\mathbf{x}_{sidsp} + w_{parch}\mathbf{x}_{parch}$$

$$\hat{y} = \frac{1}{1 + \exp(-a)}$$

- We train logistic regression on the training data: `logitreg.fit(X_train, y_train)`
- We can examine which variables are important in predicting survivor based on the linear coefficients b_j: `print(effect_size.to_string(index=False))`

Which variables are important in predicting survior?

```python
import matplotlib.pyplot as plt
plt.bar(list(effect_size.columns.values),
    effect_size.stack().tolist())
plt.ylabel("effect size")
plt.show()
```



Logistic regression prediction

Model training:

```
logitreg = LogisticRegression() # create an object (OOP)
fit = logitreg.fit(X_train, y_train)
```

Model prediction:

```
y_test_pred = fit.predict(X_test)
```

- We then apply the trained model `fit` to predict survivor: `y_train_pred=fit.predict(X_train)`, `y_test_pred=fit.predict(X_test)`
- Our prediction is binary 0 (not survived) or 1 (survived) based on whether the predicted probabilities are greater than 0.5.

Classification Accuracy

```python
# accuracy = correctly classified / total classified
acc_train = sum(y_train_pred==y_train)/len(y_train)
acc_test = sum(y_test_pred==y_test)/len(y_test)
print(f"train accuracy: {acc_train:.3f}; test accuracy:
 ↪  {acc_test:.3f}")
# train accuracy: 0.778; test accuracy: 0.823
```

- We then evaluate the prediction accuracy:

$$Accuracy = \frac{\text{Correctly classified passengers}}{\text{Total number of classified passengers}}$$

- The accuracy for predicting survivors in the training dataset (77.8%) is a bit lower than the accuracy in predicting survivors in the testing dataset (82.3%).
- In practice, the accuracy for the training tends to be higher than the accuracy on the testing
- When the training accuracy is much higher than the testing accuracy, the model is *overfitting* the data

Code to generate ROC curve and calculate AUROC

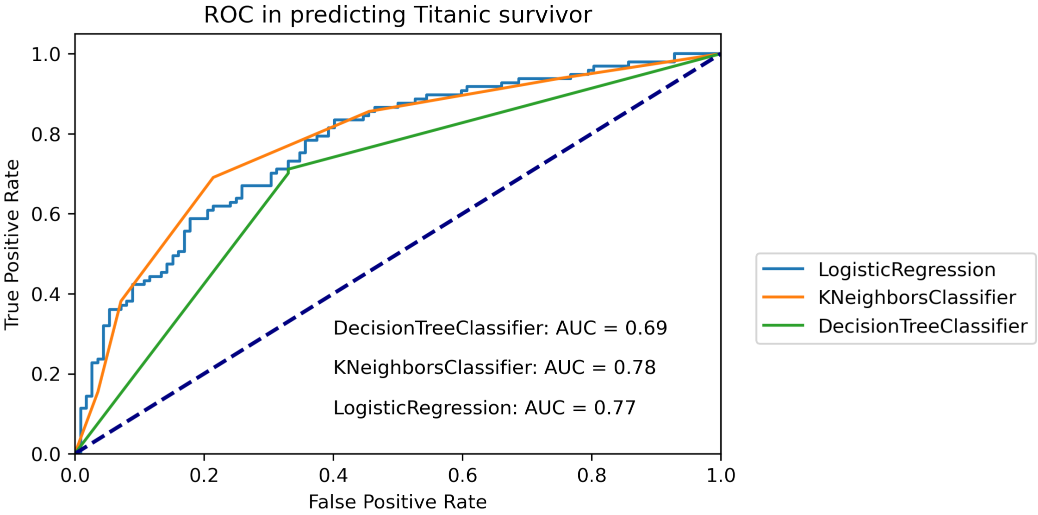
```
from sklearn.metrics import roc_curve, roc_auc_score
from sklearn.linear_model import LogisticRegression
from sklearn.tree import DecisionTreeClassifier
from sklearn.neighbors import KNeighborsClassifier

models = [LogisticRegression(), KNeighborsClassifier(), DecisionTreeClassifier()]

perf = {}
for model in models:
    fit = model.fit(X_train, y_train)
    y_test_prob = fit.predict_proba(X_test)[:,1]
    fpr, tpr, thresholds = roc_curve(y_test, y_test_prob)
    auroc = roc_auc_score(y_test, y_test_prob)
    perf[type(model).__name__] = {'fpr':fpr,'tpr':tpr,'auroc':auroc}

i = 0
for model_name, model_perf in perf.items():
    plt.plot(model_perf['fpr'], model_perf['tpr'],label=model_name)
    plt.text(0.4, i+0.1, model_name + ': AUC = '+ str(round(model_perf['auroc'],2)))
    i += 0.1
```

ROC curve on Titanic survivor prediction



Summary

- logistic regression
  - logistic activation function: sigmoid
  - cross-entropy (CE) loss
  - Gradient descent
- probabilistic interpretation
  - Bernoulli distribution
  - Maximum likelihood estimate of Bernoulli is equivalent to minimizing CE loss
  - Recall in linear regression: MLE of Gaussian is equivalent to minimizing SSE loss
- Application and interpretation of logistic regression linear coefficients