W2. Discrete Classification I - Logistic Regression

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Week 2

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$$\text{Training Error} : \frac{1}{n}\sum_{i=1}^{n} I(f(\boldsymbol{x}_i) \neq y_i)$$

- **Answer**: No, the 0-1 loss function is non-convex and discontinuous, so (sub)gradient methods cannot be applied.

Classification - surrogate loss

- We can replace the 0-1 loss by other loss functions, say surrogate loss

$$\frac{1}{n}\sum_{i=1}^{n} I(f(\boldsymbol{x}_i) \neq y_i) \Rightarrow \frac{1}{n}\sum_{i=1}^{n} L(f(\boldsymbol{x}_i), y_i) = \frac{1}{n}\sum_{i=1}^{n} \phi(f(\boldsymbol{x}_i)y_i)$$

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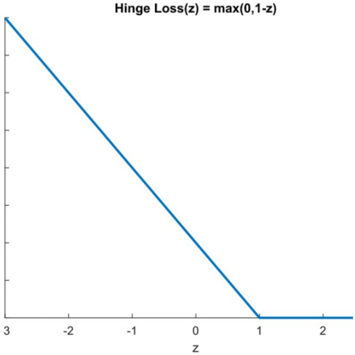
  - Hinge loss: $\phi(x) = \max\{0, 1 - x\}$
  - Logistic loss $\phi(x) = \log(1 + \exp(-x))$

One surrogate loss - Hinge Loss

- Definition of Hinge loss:

$$L_{hinge}(f(\boldsymbol{x}_i), y_i) = \begin{cases} 1 - f(\boldsymbol{x}_i)y_i & \text{if } f(\boldsymbol{x}_i)y_i \leq 1 \\ 0, & \text{if } f(\boldsymbol{x}_i)y_i > 1 \end{cases}$$



Why Hinge Loss?

- Let $\eta(\boldsymbol{x}) = \mathbb{P}(Y = 1 | \boldsymbol{X} = \boldsymbol{x})$. The expected hinge loss: hinge risk.

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R_{hinge}(f) =& \mathbb{E}_{\boldsymbol{X},Y}\left[L_{hinge}(f(\boldsymbol{X}), Y)\right] \\
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Why Hinge Loss?

- The optimal classifier (i.e., Bayes classifier) of Binary loss is defined as

$$f^*(\boldsymbol{x}) = \mathrm{sign}(\eta(\boldsymbol{x}) - 1/2) = \begin{cases} 1 & \text{if } \mathbb{P}(Y = 1|\boldsymbol{X} = \boldsymbol{x}) > 1/2 \\ 0 & \text{if } \mathbb{P}(Y = 1|\boldsymbol{X} = \boldsymbol{x}) < 1/2 \end{cases}$$

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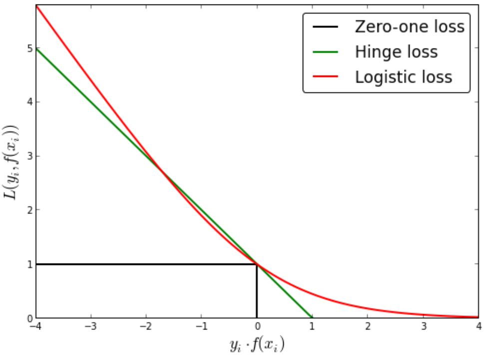
- **Observation**:
  (i) f^*_{hinge} is exactly the Bayes classifier defined above;
  (ii) The hinge loss is a convex function, which makes it possible to minimize the training error in practice.

Another surrogate loss - Logistic Loss

- Definition of Logistic loss:

$$L_{log}(f(\boldsymbol{x}_i), y_i) = \log\left(1 + \exp(-f(\boldsymbol{x}_i)y_i)\right)$$



Why Logistic Loss?

- The logistic risk:

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- Take the derivative with respect to f, pls verify the following in class

$$-\eta(\boldsymbol{X})\frac{\exp(-f(\boldsymbol{X}))}{1+\exp(-f(\boldsymbol{X}))} + (1-\eta(\boldsymbol{X}))\frac{\exp(f(\boldsymbol{X}))}{1+\exp(f(\boldsymbol{X}))}$$
$$= -\eta(\boldsymbol{X})\frac{1}{1+\exp(f(\boldsymbol{X}))} + (1-\eta(\boldsymbol{X}))\frac{\exp(f(\boldsymbol{X}))}{1+\exp(f(\boldsymbol{X}))}$$
$$= \frac{\exp(f(\boldsymbol{X}))}{1+\exp(f(\boldsymbol{X}))} - \eta(\boldsymbol{X}) = 0 \longleftrightarrow f^*_{log}(\boldsymbol{X}) = \log\frac{\eta(\boldsymbol{X})}{1-\eta(\boldsymbol{X})}$$

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- The optimal classifier of Logistic risk $f^*_{log}(\boldsymbol{x}) = \log \frac{\eta(\boldsymbol{X})}{1-\eta(\boldsymbol{X})}$
- **Question**: what is the connection between these optimal classifiers?
- **Answer**: They are consistent in sign in the sense that signs of $f^*, f^*_{hinge}, f^*_{log}$ are always the same, e.g., always positive as long as $\eta(\boldsymbol{x}) > 1/2$.

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$$\eta(\boldsymbol{x}) = \frac{\exp(\beta_0 + \boldsymbol{\beta}^T\boldsymbol{x})}{1 + \exp(\beta_0 + \boldsymbol{\beta}^T\boldsymbol{x})}, \tag{1}$$

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  - $\boldsymbol{\beta}^T \boldsymbol{x} = \sum_{l=1}^{p} \beta_i x_i$

Rational behind logistic loss: log odds ratio

- By reformulating (1), we have obtained

$$\exp(\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x}) = \frac{\mathbb{P}\Big(Y = 1 \Big| \boldsymbol{X} = \boldsymbol{x}\Big)}{1 - \mathbb{P}\Big(Y = 1 \Big| \boldsymbol{X} = \boldsymbol{x}\Big)} = \frac{\mathbb{P}\Big(Y = 1 \Big| \boldsymbol{X} = \boldsymbol{x}\Big)}{\mathbb{P}\Big(Y = 0 \Big| \boldsymbol{X} = \boldsymbol{x}\Big)},$$

where the last term above is the ratio between the conditional probability of $Y = 1$ and that of $Y = 0$ on $\boldsymbol{X} = \boldsymbol{x}$, i.e., "odds ratio."

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  where the last term above is the ratio between the conditional probability of $Y = 1$ and that of $Y = 0$ on $\boldsymbol{X} = \boldsymbol{x}$, i.e., "odds ratio."
- In other words, we can claim that the log-odds is assumed to be linear with respect to $\boldsymbol{\beta}$:

$$\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x} = \log\left(\frac{\mathbb{P}\Big(Y = 1 \Big| \boldsymbol{X} = \boldsymbol{x}\Big)}{\mathbb{P}\Big(Y = 0 \Big| \boldsymbol{X} = \boldsymbol{x}\Big)}\right)$$

  Interpretability: β_i can then be interpreted as the average change in the log-odds ratio given by a one-unit increase in x_i

Maximum likelihood estimation

- Likelihood function $L(\beta_0, \boldsymbol{\beta})$:

$$L(\beta_0, \boldsymbol{\beta}) = \prod_{i=1}^{n} \Big(\mathbb{P}(Y = 1 \big| \boldsymbol{X} = \boldsymbol{x})\Big)^{y_i} \Big(\mathbb{P}(Y = 0 \big| \boldsymbol{X} = \boldsymbol{x})\Big)^{1-y_i}$$

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- Logarithm of $L(\beta_0, \boldsymbol{\beta})$ (pls verify in class):

$$\begin{aligned} \log L(\beta_0, \boldsymbol{\beta}) &= \sum_{i=1}^{n} \left[y_i \log\left(\mathbb{P}\left(Y = 1 \middle| \boldsymbol{X} = \boldsymbol{x}\right)\right) + (1 - y_i) \log\left(\mathbb{P}\left(Y = 0 \middle| \boldsymbol{X} = \boldsymbol{x}\right)\right)\right] \\ &= \sum_{i=1}^{n} \left[y_i \left(\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x}\right) - \log\left(1 + \exp(\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x})\right)\right] \end{aligned}$$

Gradient descent/ascent in the computation

Estimate β_0 and $\boldsymbol{\beta}$ (Gradient Ascent):

$$\beta_0^{(t+1)} \leftarrow \beta_0^{(t)} + \lambda \sum_{i=1}^{n} \left[y_i - \frac{\exp(\beta_0^{(t)} + \boldsymbol{\beta}^{(t)T}\boldsymbol{x})}{1 + \exp(\beta_0^{(t)} + \boldsymbol{\beta}^{(t)}\boldsymbol{x})} \right]$$

$$\boldsymbol{\beta}^{(t+1)} \leftarrow \boldsymbol{\beta}^{(t)} + \lambda \sum_{i=1}^{n} \left[y_i - \frac{\exp(\beta_0^{(t)} + \boldsymbol{\beta}^{(t)T}\boldsymbol{x})}{1 + \exp(\beta_0^{(t)} + \boldsymbol{\beta}^{(t)T}\boldsymbol{x})} \right] \boldsymbol{x}_i$$

Now, we are ready to do classification

We have obtained the estimate for β_0 and $\boldsymbol{\beta}$, denoted as $\widehat{\beta}_0$ and $\widehat{\boldsymbol{\beta}}$, based on which we can estimate $P(Y = 1|\boldsymbol{X})$ as follows:

$$\widehat{\eta}(\boldsymbol{x}) = \frac{\exp(\widehat{\beta}_0 + \widehat{\boldsymbol{\beta}}^T \boldsymbol{x})}{1 + \exp(\widehat{\beta}_0 + \widehat{\boldsymbol{\beta}}^T \boldsymbol{x})}$$

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Then we make predictions by (recall that $\eta(\boldsymbol{x}) = P(Y = 1|\boldsymbol{X})$)

$$\widehat{f}(\boldsymbol{x}) = \begin{cases} 1, & \text{if } \widehat{\eta}(\boldsymbol{x}) > 1/2 \\ 0, & \text{if } \widehat{\eta}(\boldsymbol{x}) < 1/2 \end{cases}$$

If $\widehat{\eta}(\boldsymbol{x}) = 1/2$, then just randomly assign a label to it.

Example

Dataset $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{5000}$, where $\boldsymbol{x}_i = (x_{i1}, x_{i2}, x_{i3}, x_{i4})$.

- Features are generated from uniform distribution $x_{il} \sim Unif(0, 2), l = 1, 2, 3, 4.$

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- Features are generated from uniform distribution $x_{il} \sim Unif(0, 2), l = 1, 2, 3, 4$.
- $\beta_0 = 0.5$ and $\boldsymbol{\beta} = (\beta_1, \beta_2, \beta_3, \beta_4)$ with $\beta_i \sim Unif(-1, 1)$

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- Features are generated from uniform distribution $x_{il} \sim Unif(0, 2), l = 1, 2, 3, 4$.
- $\beta_0 = 0.5$ and $\boldsymbol{\beta} = (\beta_1, \beta_2, \beta_3, \beta_4)$ with $\beta_i \sim Unif(-1, 1)$
- Model:

$$Y_i \sim Bernoulli(\frac{\exp(\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x})}{1 + \exp(\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x})}),$$

  which means

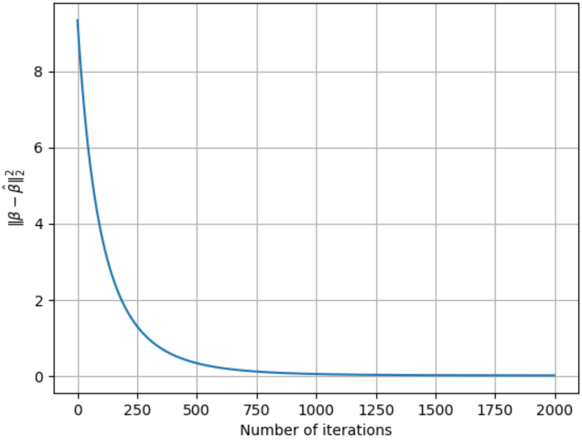
$$P(Y_i = 1|\boldsymbol{X}) = \frac{\exp(\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x})}{1 + \exp(\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x})}$$

Python Codes – data generation

```
import numpy as np
np.random.seed(2)
n,p = 5000,4  # Set training datasize and dimension of features
X = np.random.uniform(-1,1,[n,p]) # Generation of features
beta = np.random.uniform(0,2,4) # Generation of parameters
beta_0 = 0.5 # Set the intercept term to 0.5
logOdd = (X * beta).sum(axis=1)+beta_0 # Log-odds
Prob = np.exp(logOdd)/(1+np.exp(logOdd)) # Probability
Y = np.array(Prob - np.random.uniform(0,1,n)>0,dtype=int) # Generate labels
```

```python
Beta_0_hat = 0. # Initialization of intercept term
Beta_hat = np.zeros(p) # Initialization of beta
lamb = 0.1 # Learning rate
Error = [] # Error set
for i in range(2000):# Iterations of gradient ascent
    logOdd_hat = (X * Beta_hat).sum(axis=1)+Beta_0_hat
    Beta_0_hat = Beta_0_hat + lamb * np.mean(Y - np.exp(logOdd_hat)/(1+np.exp(logOdd_hat)))
    Beta_hat = Beta_hat + lamb * ((Y - np.exp(logOdd_hat)/(1+np.exp(logOdd_hat))) * X.T).mean(axis=1)
    Error.append(np.linalg.norm(Beta_hat-beta)**2)
import matplotlib.pyplot as plt
plt.plot(np.arange(0,2000),Error)
plt.xlabel('Number of iterations')
plt.ylabel('$\Vert \\beta - \hat{\\beta}\Vert_2^2$')
plt.grid()
```

Example: gradient ascent for logistic regression



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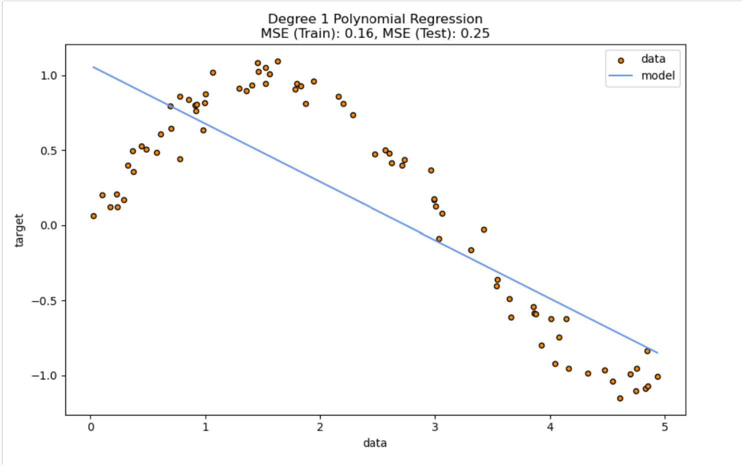
- Let's use a simple example with polynomial regression and visualize the above with the out-of-sample (OOS) metrics.

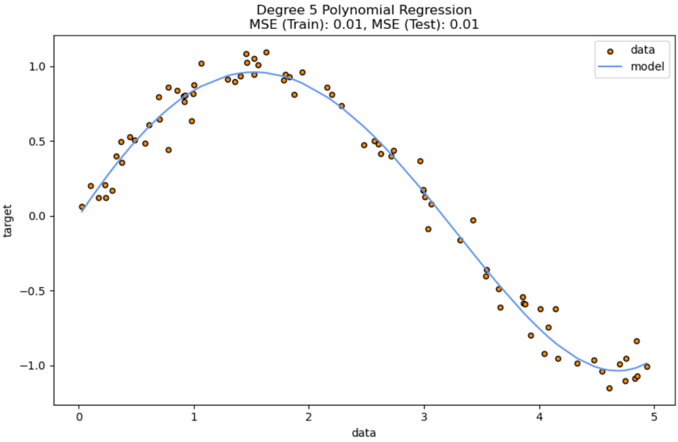
An example - underfitting

Degree 1: Underfitting (Too simple) - The model is not able to capture the underlying pattern in the data.



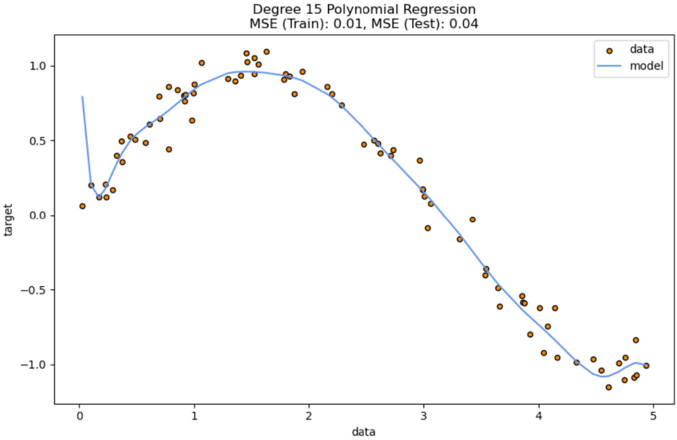
An example - good fit

Degree 5: Good fit - The model captures the underlying pattern well and generalizes to the test data.



An example - overfitting

Degree 15: Overfitting (Too complex) - The model fits the training data too closely, capturing noise and performing poorly on new data.



Confusion matrix – measure the performance of classification

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- A confusion matrix is a matrix that displays the number of accurate and inaccurate classification outcomes for each input instance $\boldsymbol{X}$.

Classification outcomes

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- true positives (TP): occurs when the model accurately predicts a positive data point, i.e., $\widehat{y} = y = 1$.

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An example : dog recognition

Dog: $Y = 1$ & Not Dog: $Y = -1$ (pls verify this table in class!)

index	actual	predicted	Result
1	Dog	Dog	TP
2	Dog	Not Dog	FN
3	Dog	Dog	TP
4	Not Dog	Not Dog	TN
5	Dog	Dog	TP
6	Not Dog	Dog	FP
7	Dog	Dog	TP
8	Dog	Dog	TP
9	Not Dog	Not Dog	TN
10	Not Dog	Not Dog	TN

An example - counts

Pls take a min to count....

- Actual Dog Counts = ?

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- Actual Dog Counts = ?
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- True Positive Counts = ?
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An example - counts

- Actual Dog Counts $= 6$

An example - counts

- Actual Dog Counts $= 6$
- Actual Not Dog Counts $= 4$

An example - counts

- Actual Dog Counts $= 6$
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An example - construct the confusion matrix

- Construct the Confusion Matrix

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Predicted	Dog	True Positive (TP =5)	False Positive (FP=1)
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- How to use the Confusion Matrix for assessing a classification model's performance ?

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- For the above case: Accuracy $= (5+3)/(5+3+1+1) = 8/10 = 0.8$

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- The harmonic mean is often used to calculate the average of the ratios or rates.
- The harmonic mean can be expressed as the reciprocal of the arithmetic mean of the reciprocals of the given set of observations.
- For example, harmonic mean of $1, 4, 4$ is

$$(\frac{1^{-1} + 4^{-1} + 4^{-1}}{3})^{-1} = 2$$

Classification metrics based on confusion matrix: F-1 Score

- Pls verify this in class: F1-score $= \frac{2 \cdot \text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$

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- For the above case: F1-Score=?
- For the above case: F1-Score $= (2 * 0.8333 * 0.8333)/(0.8333 + 0.8333) = 0.8333$

Exercise: Confusion Matrix and Classification Metrics Calculation

Problem statement

- You have a binary classification model used to predict whether an email is spam (positive class) or not spam (negative class). After testing the model on a dataset of 100 emails, you get the following results:

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Solution

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- Recall $= \frac{40}{40+20} = \frac{2}{3}$
- F-1 Score $= 2 \times \frac{0.8 \times 0.667}{0.8+0.667} \approx 0.727$

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  - x_4 represents the Entropy of the image.

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  - If $P(\text{authentic}) \geq 0.5$, the model predicts the banknote as authentic (Class 1)
  - If $P(\text{authentic}) < 0.5$, the model predicts the banknote as not authentic (Class 0)

Application of logistic regression: Results

Pls verify confusion matrix, precision, recall.... by hand after class

```
   Variance  Skewness  Curtosis  Entropy  Class
0   3.62160    8.6661   -2.8073 -0.44699      0
1   4.54590    8.1674   -2.4586 -1.46210      0
2   3.86600   -2.6383    1.9242  0.10645      0
3   3.45660    9.5228   -4.0112 -3.59440      0
4   0.32924   -4.4552    4.5718 -0.98880      0
Accuracy: 0.98
Confusion Matrix:
[[144   4]
 [  2 125]]
Classification Report:
              precision    recall  f1-score   support

           0       0.99      0.97      0.98       148
           1       0.97      0.98      0.98       127

    accuracy                           0.98       275
   macro avg       0.98      0.98      0.98       275
weighted avg       0.98      0.98      0.98       275
```

Statsmodels: Python package

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- Statsmodels includes modules for performing hypothesis tests, constructing confidence intervals, and fitting different types of statistical models with an emphasis on providing detailed statistical information.
- Statsmodels is commonly used in academic research, econometrics, and any scenario where a detailed statistical analysis is required.

Statsmodels: Linear regression example

```python
import statsmodels.api as sm
import numpy as np

# Generate some random data for demonstration
np.random.seed(42)
X = np.random.rand(100, 2)
y = 3 * X[:, 0] + 2 * X[:, 1] + 1 + 0.1 * np.random.randn(100)

# Add a constant term to the independent variable
X = sm.add_constant(X)

# Create a linear model
model = sm.OLS(y, X)
results = model.fit()

# Print detailed statistical summary
print(results.summary())
```

Statsmodels: output

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.991
Model:                            OLS   Adj. R-squared:                  0.991
Method:                 Least Squares   F-statistic:                     5655.
Date:                Thu, 21 Dec 2023   Prob (F-statistic):          3.86e-101
Time:                        10:50:14   Log-Likelihood:                 89.304
No. Observations:                 100   AIC:                            -172.6
Df Residuals:                      97   BIC:                            -164.8
Df Model:                           2
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const          0.9772      0.026     37.651      0.000       0.926       1.029
x1             3.0339      0.033     91.615      0.000       2.968       3.100
x2             2.0355      0.035     57.426      0.000       1.965       2.106
==============================================================================
Omnibus:                        5.986   Durbin-Watson:                   2.104
Prob(Omnibus):                  0.050   Jarque-Bera (JB):                5.624
Skew:                           0.439   Prob(JB):                       0.0601
Kurtosis:                       3.761   Cond. No.                         5.22
==============================================================================
```

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- Use Cases: Scikit-learn is widely used in industry for building and deploying machine learning models in areas such as image recognition, natural language processing, and predictive analytics.