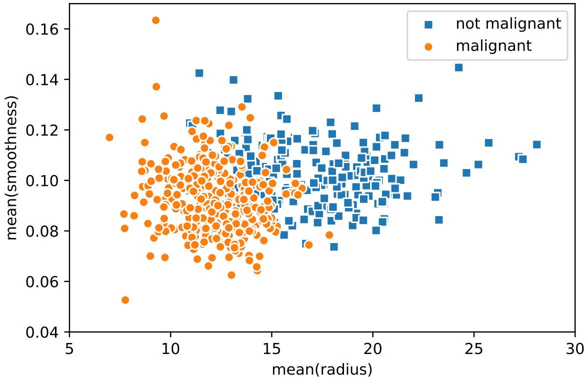
Preprocessing: Normalisation, scaling and categorical data

Herman Kamper

2024-01,

Feature normalisation example

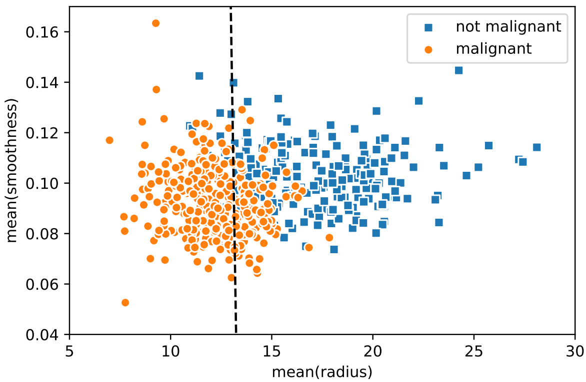
Breast cancer data:[1]



Gradients on original data (for logistic regression):

```
                                   w0        w1        w2
Iteration 1000 gradients: [ -289.919 -3694.766 -26.513 ]
Iteration 2000 gradients: [ -246.909 -3223.000 -22.423 ]
Iteration 3000 gradients: [  -93.780 -1352.985  -8.034 ]
Iteration 4000 gradients: [  -92.243 -1332.636  -7.894 ]
```

Logistic regression on original data:



[1]Data from the UCI Machine Learning Repository.

Feature normalisation

Standardise the means and variances of the data:

$$\tilde{x}_d^{(n)} = \frac{x_d^{(n)} - \hat{\mu}_d}{\hat{\sigma}_d}$$

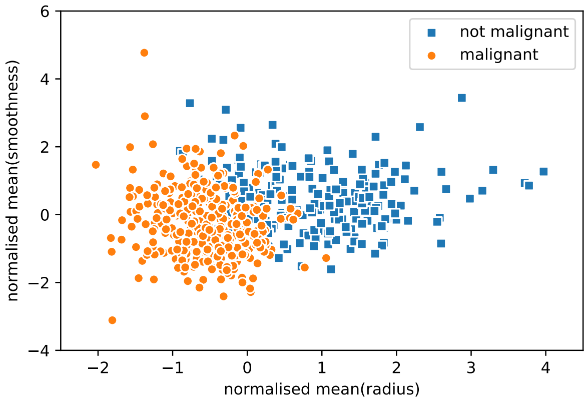
where $\hat{\mu}_d$ and $\hat{\sigma}_d^2$ are, respectively, the sample mean and variance of the dth feature.

$$\underset{\mathbf{x}^{(1)}}{\begin{bmatrix} 11 \\ 0.1 \end{bmatrix}}, \underset{\mathbf{x}^{(2)}}{\begin{bmatrix} 25 \\ 0.12 \end{bmatrix}}, \underset{\mathbf{x}^{(3)}}{\begin{bmatrix} 17 \\ 0.08 \end{bmatrix}}, \ldots, \underset{\mathbf{x}^{(N)}}{\begin{bmatrix} 6 \\ 0.07 \end{bmatrix}}$$

$$\underset{\tilde{\mathbf{x}}^{(1)}}{\begin{bmatrix} \\ \end{bmatrix}}, \underset{\tilde{\mathbf{x}}^{(2)}}{\begin{bmatrix} \\ \end{bmatrix}}, \underset{\tilde{\mathbf{x}}^{(3)}}{\begin{bmatrix} \\ \end{bmatrix}}, \ldots, \underset{\tilde{\mathbf{x}}^{(N)}}{\begin{bmatrix} \\ \end{bmatrix}}$$

Feature normalisation example

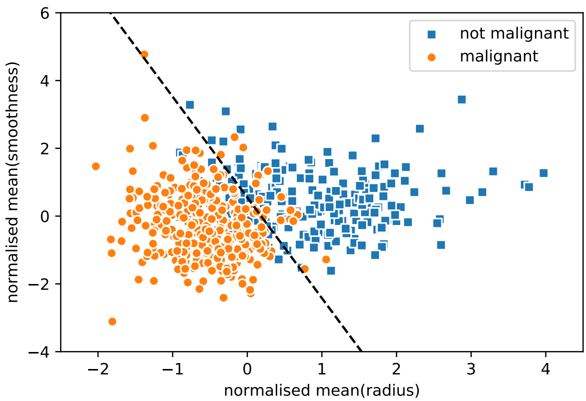
Normalised breast cancer data:



Gradients on normalised data (for logistic regression):

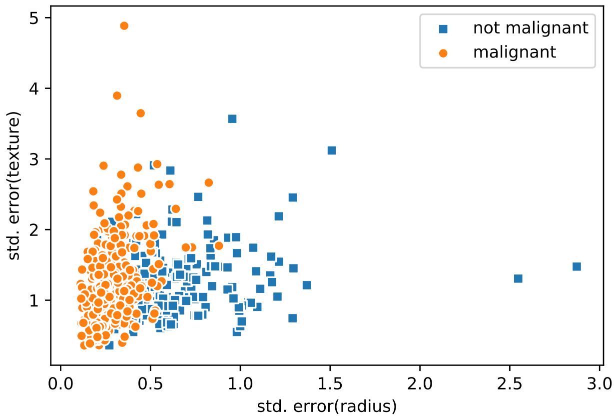
			w_0	w_1	w_2	
Iteration	1000	gradients: [	−0.525	9.179	2.472	]
Iteration	2000	gradients: [	−0.194	3.588	0.990	]
Iteration	3000	gradients: [	−0.096	1.752	0.486	]
Iteration	4000	gradients: [	−0.051	0.928	0.258	]

Logistic regression on normalised data:

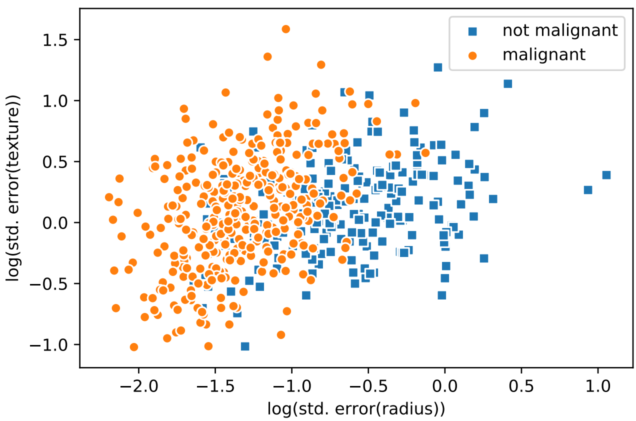


Log scaling example

Unnormalised breast cancer data:



Log-scaled breast cancer data:



Feature normalisation and scaling in practice

Feature normalisation and scaling are often a bit of an art.

You can develop an intuition as you play around with different models and optimisation algorithms.

Note: Always think about how you will apply your model to new unseen data.

Categorical output

In multiclass classification we have categorical output, i.e. $y \in \{1, 2, \ldots, K\}$.

We can just save these target values explicitly. E.g. for softmax regression, you can write the loss as:

$$J(\mathbf{W}) = -\sum_{n=1}^{N} \sum_{k=1}^{K} \mathbb{I}\{y^{(n)} = k\} \log f_k(\mathbf{x}^{(n)}; \mathbf{W})$$

Alternatively, we can encode the target output using a *one-hot* vector:

$$\mathbf{y}^{(n)} = \begin{bmatrix} 0 & 0 & \ldots & 0 & 1 & 0 & \ldots & 0 \end{bmatrix}^\top$$

E.g. for softmax regression, you can write the loss as:

$$J(\mathbf{W}) = -\sum_{n=1}^{N} \sum_{k=1}^{K} y_k^{(n)} \log f_k(\mathbf{x}^{(n)}; \mathbf{W})$$

Note that these two formulations are mathematically exactly equivalent.

Categorical input

We might have inputs that are categorical (also called *discrete* or *qualitative* features).

E.g. someone's `occupation` might be `student`, `lecturer` or `artist`. How do we represent this?

One option is to create a new feature:

$$x = \begin{cases} 0 & \text{if } \texttt{student} \\ 1 & \text{if } \texttt{lecturer} \\ 2 & \text{if } \texttt{artist} \end{cases}$$

But this implies an ordering, which might not be true. E.g. in the above represtation, `artist` is closer to `lecturer` than to `student`.

Instead use one-hot vector (also called a *one-of-K* vector) to encode input:

Sometimes such a one-hot $\mathbf{x}$ is called a *dummy variable*.

Videos covered in this note

- Preprocessing 1: Feature normalisation and scaling (14 min)
- Preprocessing 2: Categorical features and categorical output (9 min)

Reading

- ISLR 3.3.1