DATA 3464: Fundamentals of Data Processing

Numeric Data Transformations

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Topic overview

- Why transformations are necessary
- Common transformations
- Dimensionality reduction

Resources used:

- Feature Engineering Chapter 6
- Hands on Machine Learning with Scikit-Learn and Tensorflow/PyTorch, Chapter 4. Available at MRU Library
- Scikit-learn user guide: Chapter 7
- Introduction to Machine Learning with Python. Available at MRU Library

Common 1:1 transformations

> *"Most models work best when each feature (and in regression also the target) is loosely Gaussian distributed" -- Introduction to Machine Learning with Python*

- Scaling: normalization or standardization
- Nonlinear transforms: log, square root, polynomial
- Fancier methods: Box-Cox, Yeo-Johnson

A brief intro to gradient descent

- Many linear models minimize some cost function through **gradient descent**
- The **gradient** is a vector of partial derivatives

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}$$

for some scalar-valued $f(\mathbf{x})$

Descending the gradient

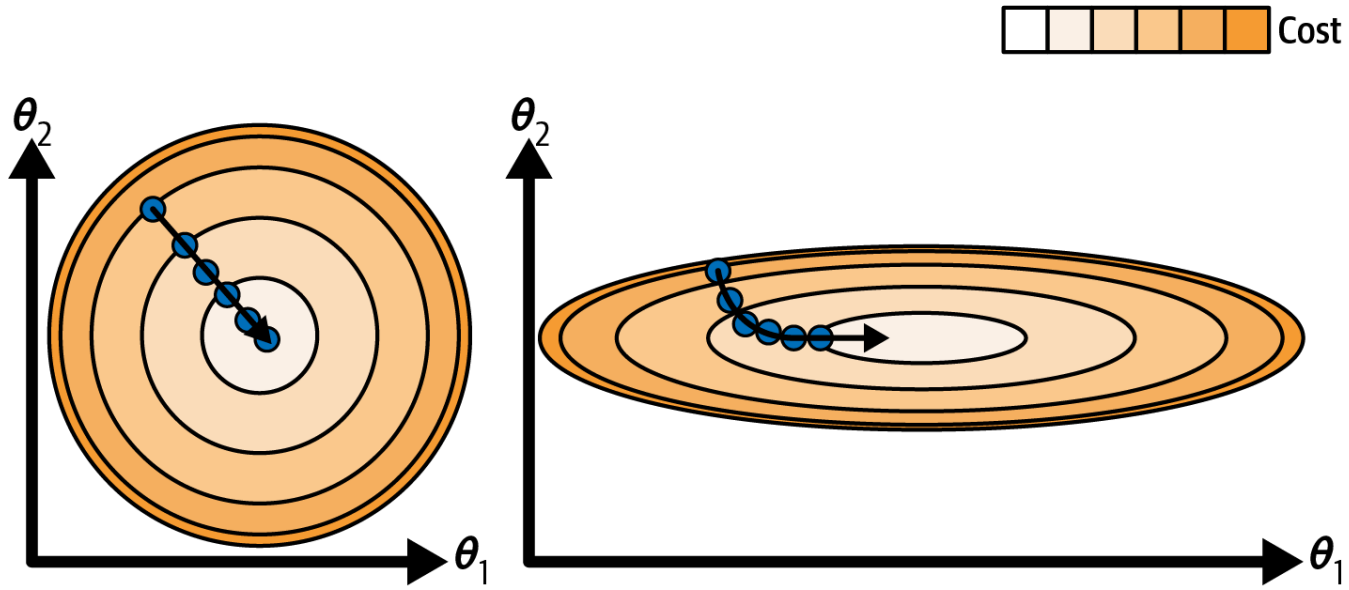
For a loss (or cost) function such as $MSE(\theta) = \frac{1}{m}(\mathbf{X}\theta - \mathbf{y})^T(\mathbf{X}\theta - \mathbf{y})$

1. Start with a random θ
2. Calculate the gradient ∇_θ for the current θ
3. Update θ as $\theta = \theta - \eta\nabla_\theta$
4. Repeat 2-3 until some stopping criterion is met

   where η is the **learning rate**, or the size of step to take in the direction opposite the gradient.

Visualizing in 2D

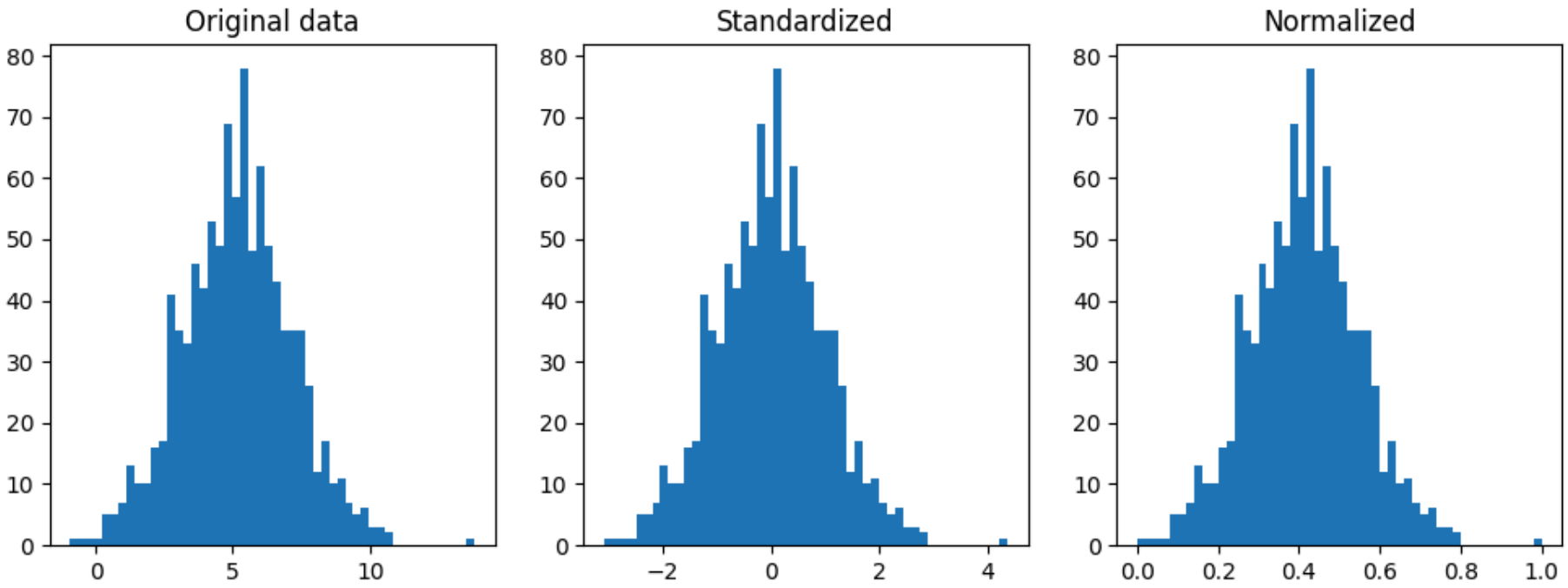
- The gradient has $m + 1$ dimensions, where m is the number of features
- step size η is a scalar parameter



> *Main takeaway: feature should be more or less on the same scale*

Figure 4-7 from Hands-on Machine Learning

Approaches to scaling



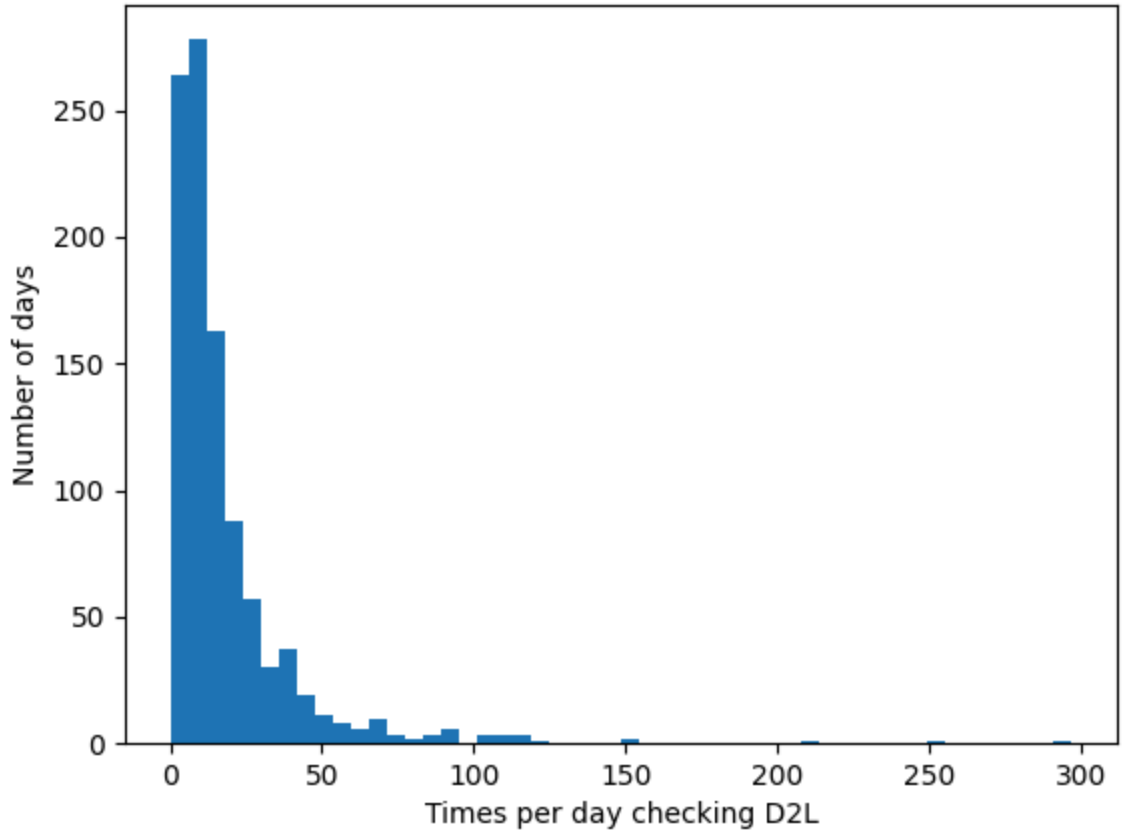
Standardize: $x_{scaled} = \dfrac{x - \mu_x}{\sigma_x}$

Normalize:

$$x_{scaled} = \frac{x - \min(x)}{\max(x) - \min(x)}$$

Nonlinear transforms

- Common case: count data
- Example: Ask 1000 students how often they checked D2L that day
- Not a Gaussian distribution!
- What about the central limit theorem?



Where we left off on January 27

Transformations in training vs inference

- Define functions, e.g.

```
def standardize(X, mu, sigma):
    return (X - mu) / sigma
```

- Compute scaling parameters **on the training data**, then stash them somewhere:

```
mu = X_train.mean()
sigma = X_train.std()
# ... later on, during inference
X = standardize(X, mu, sigma)
```

> *What would happen if* `standardize` *instead computed values on the fly?*
>
> *What else am I missing here?*

Manual approach in the wild

You may run across magic numbers, e.g from the PyTorch tutorials:

```
import torch
from torchvision import transforms, datasets

data_transform = transforms.Compose([
        transforms.RandomResizedCrop(224),
        transforms.RandomHorizontalFlip(),
        transforms.ToTensor(),
        transforms.Normalize(mean=[0.485, 0.456, 0.406],
                             std=[0.229, 0.224, 0.225])
    ])
```

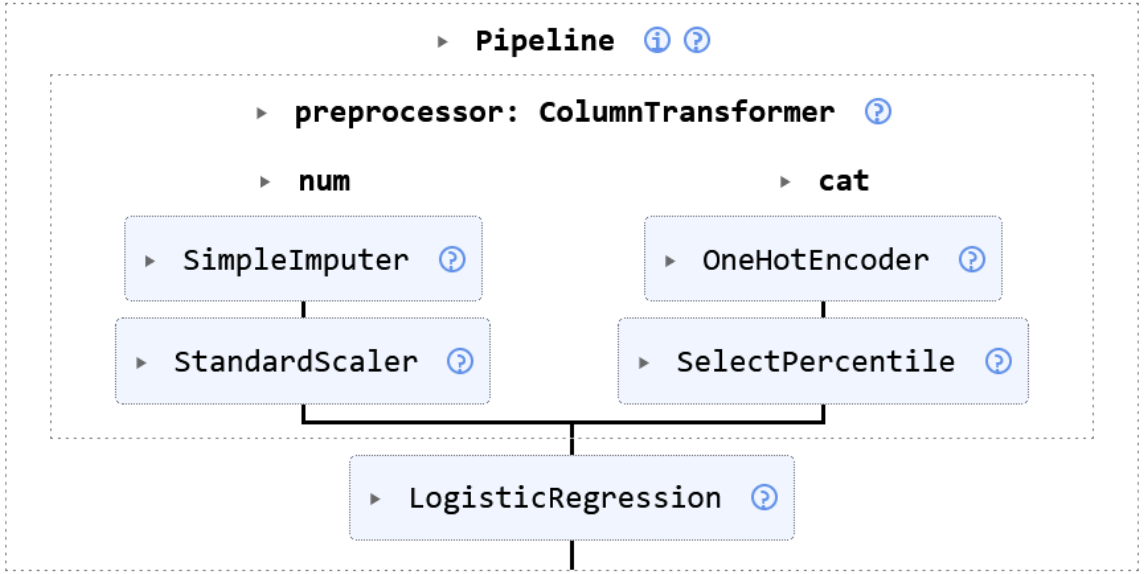
This really should have a comment! Derived from ImageNet.

An alternative solution: Scikit-learn `Pipeline`s

- Hard-coding scaling (and other) parameters is okay, provided you can **justify the choice** and **document where they came from**
- Scikit-learn has a handy Pipeline class that handles this for you
- Each step in the pipeline has a `fit` and `transform` method
  - `fit` computes parameters from the training data
  - `transform` applies the transformation
  - `fit_transform` does both -- **only use on training data!**
- You can call these functions on the whole pipeline to fit or apply all in one go

Different processing for different features

- Linear pipelines are great for doing the same thing to multiple features
- Most of the time, different features need different processing
- We can use a ColumnTransformer to split the pipeline



From Scikit-learn Column transformer example.