Philosophical Fundamentals of Machine Learning

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Week 3

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The type of ML algorithm we use will often depend on the representation of the data we have. For example, if we are predicting real-valued data we are doing *regression* instead of *classification*. The type of data will also influence how we process the data, i.e. most ML algorithms cannot natively take category values—so we will have to convert it to a better format.

Storing and Manipulating Data

We typically operate with data in ML as lists of *vectors*. Each data point is called an *observation* or *sample*. For example, the j-th sample in a dataset with n features is stored as the row vector:

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A dataset of m samples, $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$, is stored as a (m, n) matrix, $\mathbf{X} \in S^{m \times n}$, where each row is a sample and each column is feature:

$$\mathbf{X} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & \dots & x_n^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \dots & x_n^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{(m)} & x_2^{(m)} & \dots & x_n^{(m)} \end{bmatrix}$$

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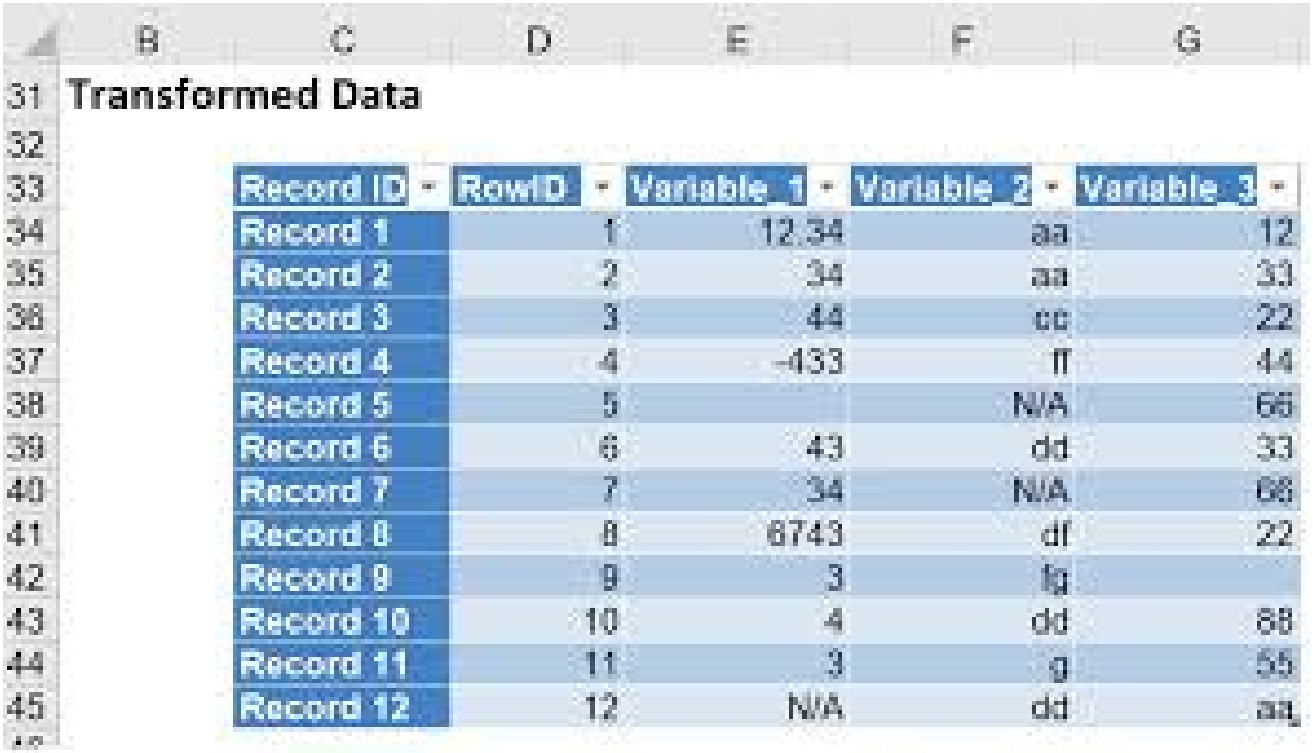

Transformed Data

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Record 2	2	34	aa	33
Record 3	3	44	cc	22
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Record 5	5		N/A	66
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1. Drop the sample.
2. Drop the feature.
3. Fill in with a dummy.

Data Statistics and Visualization

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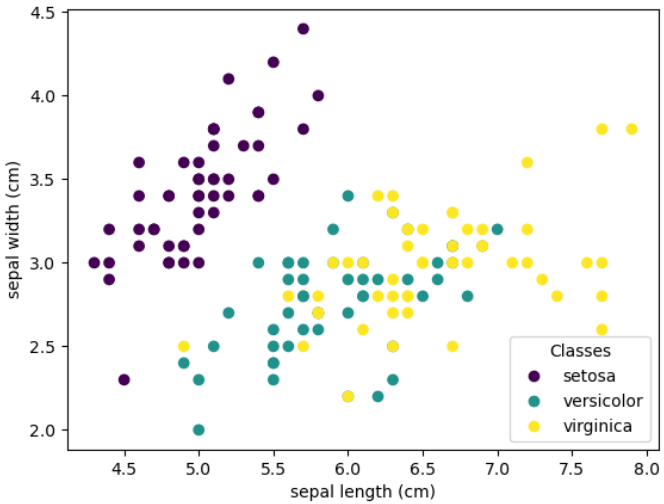
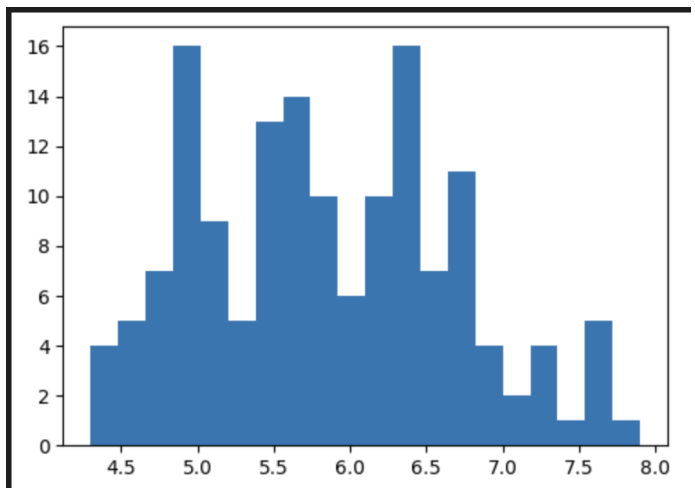


(a) Scatter Plot



(b) Histogram

Figure: Examples of scatter plots and histograms from Iris dataset.

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An example rescaling strategy is the *min-max* rescaler, where we rescale each feature x_i as follows:

$$x_i^* = \frac{x_i - \min x_i}{\max x_i - \min x_i}$$

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Rescaling transforms the data features to make them more manageable for certain algorithms without changing the *distribution* of values in those features. In contrast, *normalization* changes the distribution of feature values so that the features are normally distributed.

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This can be really useful if the data is high variance. For example, if half of the data values cluster around 0 but the other half cluster around 1000, our ML models will tend to ignore the former and focus on the latter when learning and making predictions. We want our ML models to learn patterns in data instead of ignoring certain data.

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Note that rescaling doesn't normally fix this: if we rescaled the prior example, we would still have either our values be 0 or 1, and so our model would largely ignore the former still.

One-Hot Vectors

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Instead, if we want the various feature values to be independent of one another, we use a *one-hot* or *dummy variable* encoding where each category is encoded as an element in binary vectors. For example, if we have categories "red", "blue", and "green", we can encode it as a binary, 3-length vectors:

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$$red = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad blue = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \quad green = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

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To prevent this, what we do is make sure that our samples are balanced, e.g. we would have training data where 50% survive and 50% do not survive. One technique is called *random sampling* where we randomly duplicate the minority classes of our training data until we have equal quantities. There are other techniques, such as SMOTE, that synthesize new data for balancing.

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IMPORTANT: you can retrain to improve performance on validation data, but you should never retrain to improve on test data.

k-Fold Cross Validation

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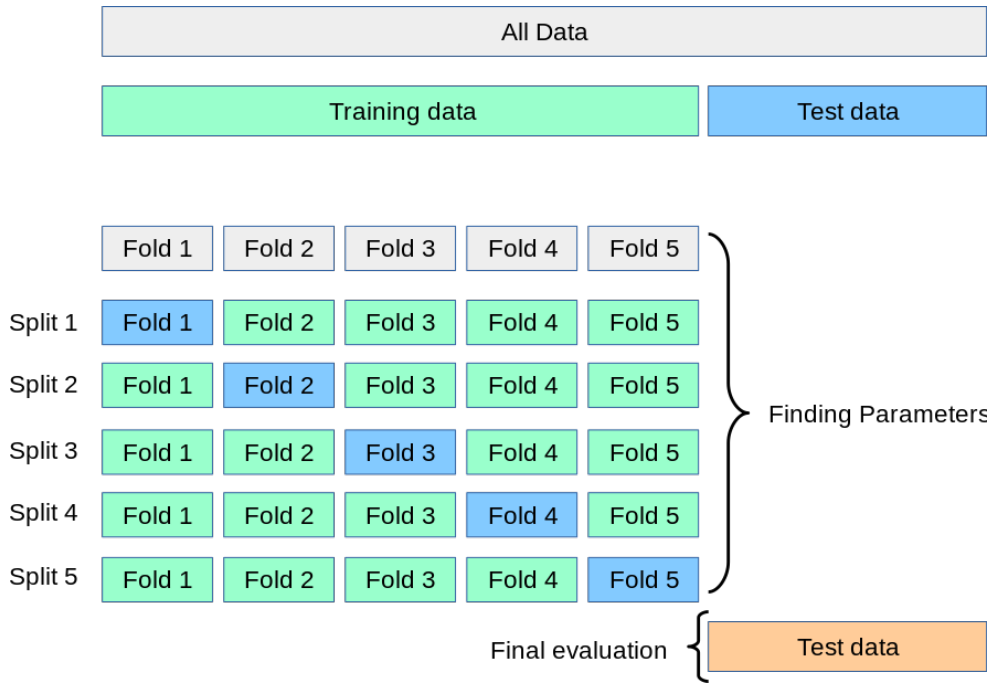

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Maximum Likelihood Estimation

Definition (Likelihood Function)

Suppose we have some data $\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}), \ldots, (\mathbf{x}^{(m)}, y^{m})\}$ that we are trying to learn with a model characterized by parameters $\theta \in \Theta$ that outputs a probabilistic prediction Pr. Then the *likelihood* for that data is defined as:

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Example

If the model is a Bernoulli distribution, then the likelihood is just the product of those Bernoullis where $\Pr(y = k | \mathbf{x}, \theta) = p^k (1-p)^{1-k}$,.

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Remark

Maximum likelihood estimation has a Bayesian interpretation. Suppose we wanted to estimate the posterior probability of $\Pr(\theta|\mathcal{D})$, and suppose we wanted the most likely model θ. This is often called the *mode* or *maximum a posteriori* (MAP) estimate. Then the maximum likelihood estimate is just the MAP in cases where we assume a *uniform* prior over possible models.

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Remark

Typically when making predictions, we take the expected value of our model, i.e $\mathbb{E}[f(\mathbf{x}; \theta)]$. Here with our linear regression, this will just be the mean of our normal distribution: $\mathbf{x}^\intercal \theta$.

Ordinary Least Squares

Mean Squared Error

When we make the assumption that our data is i.i.d. and the variance is known, we can analytically solve for the linear regression that maximizes the likelihood. We do this by finding the model that minimizes the negative log-likelihood. Let $\mathbf{X} \in \mathbb{R}^{m \times n}$ be the matrix of our data features and $\mathbf{y}$ the vector of targets from $\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}), \ldots, (\mathbf{x}^{(m)}, y^{(m)})\}$.

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$$\begin{aligned} NLL_{\mathcal{D}}^{LR}(\theta) &= \frac{1}{2\sigma^2} \sum_{i=1}^{m} (y^{(i)} - \mathbf{x}^{(i)\top}\theta)^2 \\ &= \frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\theta)^2 \end{aligned}$$

Ordinary Least Squares

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Taking the average across our m samples, this is just the classic *mean squared error*.

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If we cannot ensure the conditions for the OLS solution, we use gradient descent to find the best linear regression.

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Often when doing linear regression, we will find that our features happen to be correlated with one another. This can lead to our linear regression *overfitting*. To combat this, we use what is called a *regularizer* to make our model better at fitting to our training data.

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Regularization can be understood as changing our prior in MLE from a uniform prior to another prior. That is, we want the MAP for our linear regression. That MAP is given by the numerator in Bayes theorem. By taking the negative logarithm of that numerator we have:

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$$\begin{aligned} \Pr(\theta|\mathcal{D}) &\propto \Pr(\mathcal{D}|\theta)\Pr(\theta) \\ -\log\Pr(\theta|\mathcal{D}) &\propto -\log(\Pr(\mathcal{D}|\theta)\Pr(\theta)) \\ &NLL_{\mathcal{D}}(\theta) - \log\Pr(\theta) \end{aligned}$$

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We use this loss function when fitting our regression. The resulting model is called *ridge regression*. The parameter α is the weight penalty we give to large weights θ.

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Logistic Regression

The direct analog to linear regression for classification are linear classifiers. All linear classifiers involve the application of a linear transformation $\Phi : \mathbb{R}^n \to \mathbb{R}^d$ of $n-1$ features and d targets and apply a non-linear function to decide which class to predict.

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Let our targets $Y : \Omega \to \{0, 1\}$, $\mathbf{x} \in \mathbb{R}^n$ where $\mathbf{x} = [1, x_1, \ldots, x_{n-1}]^\intercal$. If $\theta = [\theta_0, \theta_1, \ldots, \theta_{n-1}]^\intercal$, then the *binary logistic regression* model is:

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$$
\begin{aligned}
NLL_{\mathcal{D}}^{ce} &= -\log \prod_{i=1}^{m} \text{Ber}(y^{(i)} | \sigma(\mathbf{x}^{(i)\intercal}\theta)) \\
&= \sum_{i=1}^{m} -\log(\sigma(\mathbf{x}^{(i)\intercal}\theta)^{y^{(i)}} \cdot (1 - \sigma(\mathbf{x}^{(i)\intercal}\theta))^{1-y^{(i)}}) \\
&= \sum_{i=1}^{m} -[y^{(i)} \log \sigma(\mathbf{x}^{(i)\intercal}\theta) + (1 - y^{(i)}) \log(1 - \sigma(\mathbf{x}^{(i)\intercal}\theta))]
\end{aligned}
$$

Optimizing Logistic Regression

We can extend the binary cross-entropy function to the multinomial case with the general cross-entropy loss. Unfortunately, in both cases, we cannot analytically compute the model parameters that minimize the NLL. So we have to use an optimization scheme, namely **gradient descent**.

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Intuitively, we can think of the derivate, when it exists, as giving us the *tangent* line at a specific point.

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Gradient Descent Algorithm

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Our goal is to minimize our loss function $l_{\mathcal{D}}$ with our model $f(\mathbf{x};\theta)$:

$$\min_{\theta \in \Theta} l_{\mathcal{D}}(f(\mathbf{x};\theta))$$

To do that, we essentially find the spot where our gradient is 0 by iteratively following it downhill.

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$$\theta^{(i+1)} = \theta^{(i)} - \eta_i(\nabla_\theta l_{\mathcal{D}}(f(\mathbf{x};\theta))(\theta^{(i)}))$$

The variable η_i is called the *learning rate* and so long as we choose a small enough learning rate, our algorithm will converge to a local minima.

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