Introduction to Machine Learning and Artificial Neural Networks (CS554)

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Non-Linear Dimensionality Reduction

(Polynomial Regression & KNN Regression & MLP Regression)

1. Introduction

In this assignment, we test three different algorithms (polynomial regression, k-th nearest neighbor and multi-layer perceptron) on a custom data set. Training and test data contains 25 samples for each, and given in the CSV format where each line represent one sample, the first value is independent variable *x*, and the second one is dependent variable *y*.

2. Methodology

- Implement Polynomial Regressor where the degree is a hyper-parameter
- Implement KNN Regressor where K is a hyper-parameter
- Implement Multi-layer Perceptron where number of hidden units is a hyper-parameter
- Train these 3 algorithms with train set
- Choose best model for each algorithm by using validation set
- Plot the best model for each algorithm with the test set
- Report mean-squared error of the best model for each algorithm on the test set
- For MLP case, with the best model, plot the learned lines, the output of each hidden unit and the actual output

3. Code

```
import csv
import numpy as np
import matplotlib.pyplot as plt


def read_data(fname):
    x, y = list(), list()
    with open(fname, 'rt') as file:
        lines = csv.reader(file)
        for line in lines:
            x.append(float(line[0]))
            y.append(float(line[1]))
    return np.array(x), np.array(y)


train_x, train_y = read_data('./data/train25.csv')
val_x, val_y = read_data('./data/validation25.csv')
test_x, test_y = read_data('./data/test25.csv')


print("---------------------------------------------")
```

```
print("TASK: Polynomial Regression")


def vectorize_poly(x, degree):
    vector = list()
    for d in range(degree, -1, -1):
        vector.append(x**d)
        # print(vector)
    return np.array(vector).transpose()


def poly_reg_lse_solver(x, y):
    return np.dot(np.dot(np.linalg.inv(np.dot(x.transpose(), x)),
x.transpose()), y)


def mse_loss(y_true, y_pred):
    return np.square(np.subtract(y_true, y_pred)).mean()


def validate(x, w, y):
    y_hat = np.dot(x, w)
    return mse_loss(y, y_hat)


def cross_validate(x_train, y_train, x_val, y_val, max_degree=10):
    losses = list()
    for degree in range(1, max_degree+1):
        vec_x_train = vectorize_poly(x_train, degree)
        vec_x_val = vectorize_poly(x_val, degree)

        assert vec_x_train.shape == (25, degree+1)
        assert vec_x_val.shape == (25, degree+1)

        w_hat = poly_reg_lse_solver(vec_x_train, y_train)

        losses.append((degree, validate(vec_x_val, w_hat, y_val), w_hat))
    return losses


losses = cross_validate(train_x, train_y, val_x, val_y)
best_degree, _, best_w_hat = min(losses, key=lambda l: l[1])

# print(best_degree)
# print(best_w_hat)

vec_x_test = vectorize_poly(test_x, best_degree)
best_model = np.dot(vec_x_test, best_w_hat)

plt.plot(test_x, test_y, "b+", test_x, best_model, "r")
plt.xlabel("X")
plt.ylabel("Value")
# plt.savefig('./images/poly_reg_best_model_fit_on_test.png')
plt.show()
print("MSE Error on Test set: {}".format(validate(vec_x_test, best_w_hat,
test_y)))
print("-----------------------------------------")


print("TASK: K-Nearest Neighbour Regression")
```

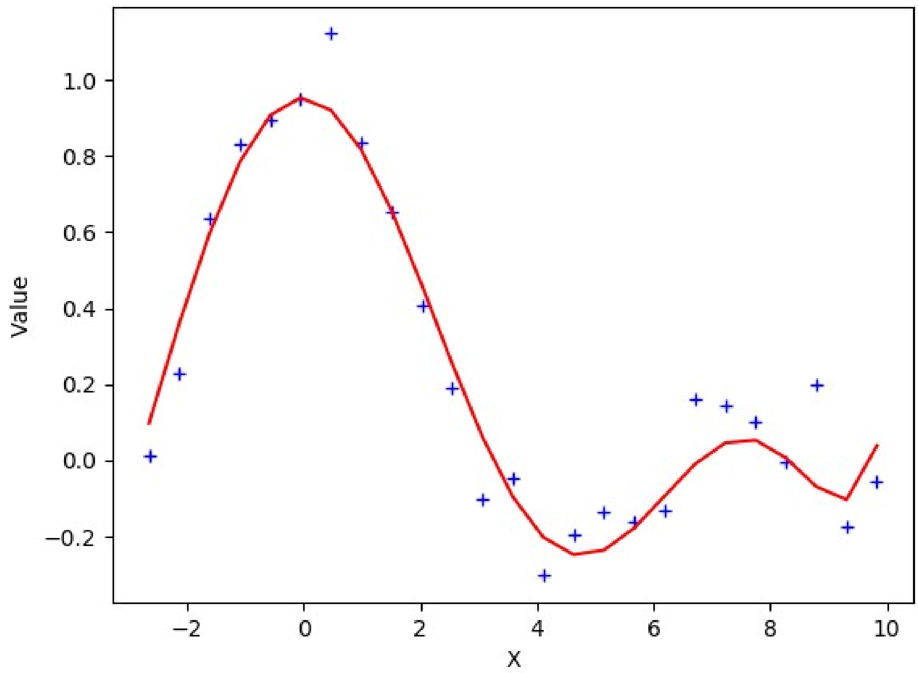
```python
def calc_dist(x1, x2):
    return (x1 - x2)**2


def knn_regressor(k, x_train, y_train, x_val):
    y_pred = list()
    for x_v in x_val:
        distances = list()
        for x_t, y_t in zip(x_train, y_train):
            distances.append((y_t, calc_dist(x_v, x_t)))
        distances = sorted(distances, key=lambda d: d[1])
        distances = distances[:k]

        y_pred.append(sum([d[0] for d in distances]) / k)
    return y_pred


def find_best_k(x_train, y_train, x_val, y_val, max_k=10):
    losses = list()
    for k in range(1, max_k+1):
        y_pred = knn_regressor(k, x_train, y_train, x_val)
        losses.append((k, mse_loss(y_val, y_pred)))
    return min(losses, key=lambda l: l[1])[0]


best_k = find_best_k(train_x, train_y, val_x, val_y)
y_pred = knn_regressor(best_k, train_x, train_y, test_x)

plt.plot(test_x, test_y, "b+", test_x, y_pred, "r")
plt.xlabel("X")
plt.ylabel("Value")
# plt.savefig('./images/knn_reg_best_model_fit_on_test.png')
plt.show()
print("MSE Error on Test set: {}".format(mse_loss(test_y, y_pred)))
print("--------------------------------------------")


print("TASK: Multilayer Perceptron")
NUM_EPOCH = 10
LR = 0.00001


def init_weights(in_channel, out_channel):
    epsilon = np.sqrt(2.0 / (in_channel * out_channel))
    w = epsilon * np.random.randn(out_channel, in_channel)
    return w.transpose()


def init_bias():
    return 0


def run_mlp(num_hidden_unit, X, y, weights=None, bias=None, is_train=True):
    if weights is None:
        w1 = init_weights(1, num_hidden_unit)
        w2 = init_weights(num_hidden_unit, 1)
    else:
        w1, w2 = weights
```

```
    if bias is None:
        b1 = init_bias()
        b2 = init_bias()
    else:
        b1, b2 = bias

    def _sigmoid(x):
        return 1 / (1 + np.exp(-x))

    def _derivative_sigmoid(x):
        return x * (1 - x)

    def forward(X_):
        z1 = np.dot(X_, w1) + b1
        a1 = _sigmoid(z1)
        z2 = np.dot(a1, w2) + b2
        return z1, z2

    def step(X_, y_, z1_, z2_, w1_, w2_):  # TODO
        layer2_error = y_ - z2_
        layer2_delta = layer2_error * _derivative_sigmoid(z2_)
        layer1_error = np.dot(layer2_delta, w2_.transpose())
        layer1_delta = layer1_error * _derivative_sigmoid(z1_)

        layer1_adjustment = np.dot(X_.transpose(), layer1_delta)
        layer2_adjustment = np.dot(z1_.transpose(), layer2_delta)

        # Adjust the weights.
        w1_ += LR * layer1_adjustment
        w2_ += LR * layer2_adjustment
        return w1_, w2_

    if is_train:
        losses = list()
        for _ in range(NUM_EPOCH):
            z1, z2 = forward(X)
            losses.append(0.5 * np.square(y - z2).mean())
            w1, w2 = step(X, y, z1, z2, w1, w2)
        final_loss = losses[-1]
    else:
        _, z2 = forward(X)
        final_loss = 0.5 * np.square(y - z2).mean()

    return (w1, w2), (b1, b2), final_loss, z2


model_lst = list()
for i in range(1, 101):
    weights, bias, _, _ = run_mlp(i, np.expand_dims(train_x, axis=-1),
np.expand_dims(train_y, axis=-1))
    _, _, val_loss, _ = run_mlp(i, np.expand_dims(val_x, axis=-1),
                             np.expand_dims(val_y, axis=-1),
weights=weights, bias=bias, is_train=False)
    model_lst.append((i, weights, bias, val_loss))

best_mlp_model = min(model_lst, key=lambda m: m[3])
best_num_hidden_unit, best_weights, best_bias, _ = best_mlp_model

_, _, test_loss, y_pred = run_mlp(best_num_hidden_unit,
np.expand_dims(test_x, axis=-1),
```

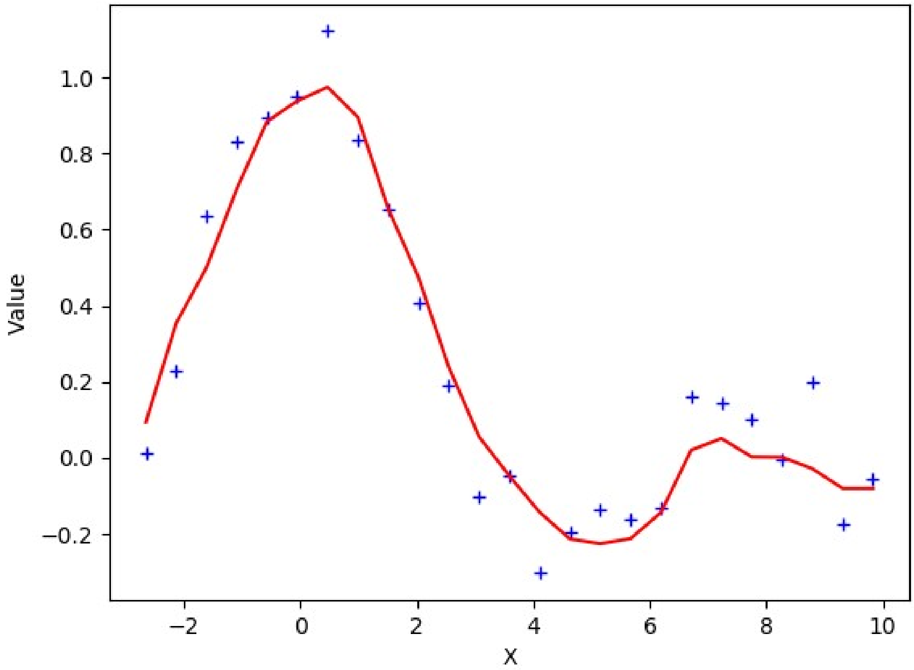
```
                                    np.expand_dims(test_y, axis=-1),
weights=best_weights,
                                    bias=best_bias, is_train=False)

plt.plot(test_x, test_y, "b+", test_x, y_pred, "r")
plt.xlabel("X")
plt.ylabel("Value")
# plt.savefig('./images/mlp_best_model_fit_on_test.png')
plt.show()
print("MSE Error on Test set: {}".format(test_loss))
print("--------------------------------------------")

# plt.plot(train_x, train_y, "b+", train_x, y_pred, "r")
# plt.xlabel("X")
# plt.ylabel("Value")
# # plt.savefig('./images/mlp_best_model_fit_on_test.png')
# plt.show()
# print("MSE Error on Test set: {}".format(test_loss))
# print("--------------------------------------------")
```

4. Results

- ***Best model fitted on test set for Polynomial Regression***



- ***Best model fitted on test set for KNN Regression***



- ***Best model fitted on test set for MLP Regression***