Bias/variance of non-parametric models

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```
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

from sklearn.tree import DecisionTreeRegressor
from sklearn.neighbors import KNeighborsRegressor
```

Generate data

We will generate data from the true function

$$t(x) = e^{-x^2} + 1.5e^{-(x-2)^2}$$

in the range $-5 < x < 5$.

To this we will add Gaussian noise ϵ so that

$$y = t(x) + \epsilon$$

We will use this data for *all* of the models trained in this notebook.

```
# Utility functions to generate data
def f(x):
    x = x.ravel()
    return np.exp(-x ** 2) + 1.5 * np.exp(-(x - 2) ** 2)

def generate(n_samples, noise, n_repeat=1):
    X = np.random.rand(n_samples) * 10 - 5
    X = np.sort(X)
    if n_repeat == 1:
        y = f(X) + np.random.normal(0.0, noise, n_samples)
    else:
        y = np.zeros((n_samples, n_repeat))
        for i in range(n_repeat):
            y[:, i] = f(X) + np.random.normal(0.0, noise, n_samples)

    X = X.reshape((n_samples, 1))
    return X, y
```

Set up simulation

```
# Simulation settings
n_repeat = 500       # Number of iterations for computing expectations
n_train  = 500        # Size of the training set
n_test   = 1000       # Size of the test set
noise    = 0.15       # Standard deviation of the noise
np.random.seed(4)
```

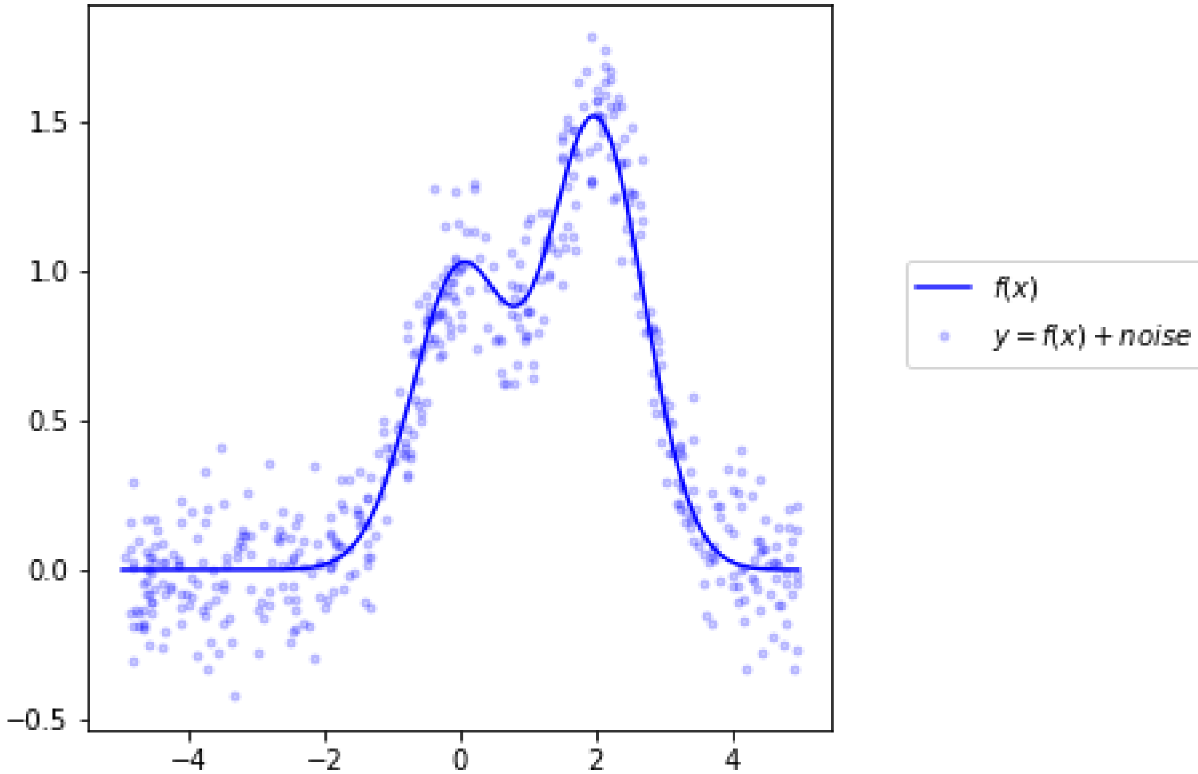
```python
def plot_simulation(estimators):

  n_estimators = len(estimators)
  plt.figure(figsize=(5*n_estimators, 10))

  # Loop over estimators to compare
  for n, (name, estimator) in enumerate(estimators):
      # Compute predictions
      y_predict = np.zeros((n_test, n_repeat))

      for i in range(n_repeat):
          estimator.fit(X_train[i].reshape(-1,1), y_train[i])
          y_predict[:, i] = estimator.predict(X_test.reshape(-1,1))

      # Bias^2 + Variance + Noise decomposition of the mean squared error
      y_error = np.zeros(n_test)

      for i in range(n_repeat):
          for j in range(n_repeat):
              y_error += (y_test[:, j] - y_predict[:, i]) ** 2

      y_error /= (n_repeat * n_repeat)

      y_noise = np.var(y_test, axis=1)
      y_bias = (f(X_test) - np.mean(y_predict, axis=1)) ** 2
      y_var = np.var(y_predict, axis=1)

      # Plot figures
      plt.subplot(2, n_estimators, n + 1)
      plt.plot(X_test, f(X_test), "b", label="$f(x)$")
      plt.plot(X_train[0], y_train[0],  ".b", alpha=0.2, label="$y = f(x)+noise$")

      for i in range(20):
          if i == 0:
              plt.plot(X_test, y_predict[:, i], "r", label=r"$\^y(x)$")
          else:
              plt.plot(X_test, y_predict[:, i], "r", alpha=0.1)

      plt.plot(X_test, np.mean(y_predict, axis=1), "c",
              label=r"$E[ \^y(x)]$")

      plt.xlim([-5, 5])
      plt.title(name)

      if n == n_estimators - 1:
          plt.legend(loc=(1.1, .5))

      plt.subplot(2, n_estimators, n_estimators + n + 1)
      plt.plot(X_test, y_noise, "c", label="$noise(x)$", alpha=0.3)
      plt.plot(X_test, y_bias, "b", label="$bias^2(x)$", alpha=0.6),
      plt.plot(X_test, y_var, "g", label="$variance(x)$", alpha=0.6),
      plt.plot(X_test, y_error, "r", label="$error(x)$", alpha=0.4)
      plt.title("{0:.4f} (error) = {1:.4f} (bias^2) \n"
```

```
            " + {2:.4f} (var) + {3:.4f} (noise)".format( np.mean(y_error),
                                                        np.mean(y_bias),
                                                        np.mean(y_var),
                                                        np.mean(y_noise)))

      plt.xlim([-5, 5])
      plt.ylim([0, 0.1])

      if n == n_estimators - 1:

          plt.legend(loc=(1.1, .5))

  plt.subplots_adjust(right=.75)
```

```
X_test, y_test = generate(n_samples=n_test, noise=noise, n_repeat=n_repeat)
```

```
X_train = np.zeros(shape=(n_repeat, n_train))
y_train = np.zeros(shape=(n_repeat, n_train))

for i in range(n_repeat):
    X, y = generate(n_samples=n_train, noise=noise)
    X_train[i] = X.ravel()
    y_train[i] = y
```

```
plt.figure(figsize=(5,5))
plt.plot(X_test, f(X_test), "b", label="$f(x)$");
plt.plot(X_train[0], y_train[0],  ".b", alpha=0.2, label="$y = f(x)+noise$");
plt.legend(loc=(1.1, .5));
```

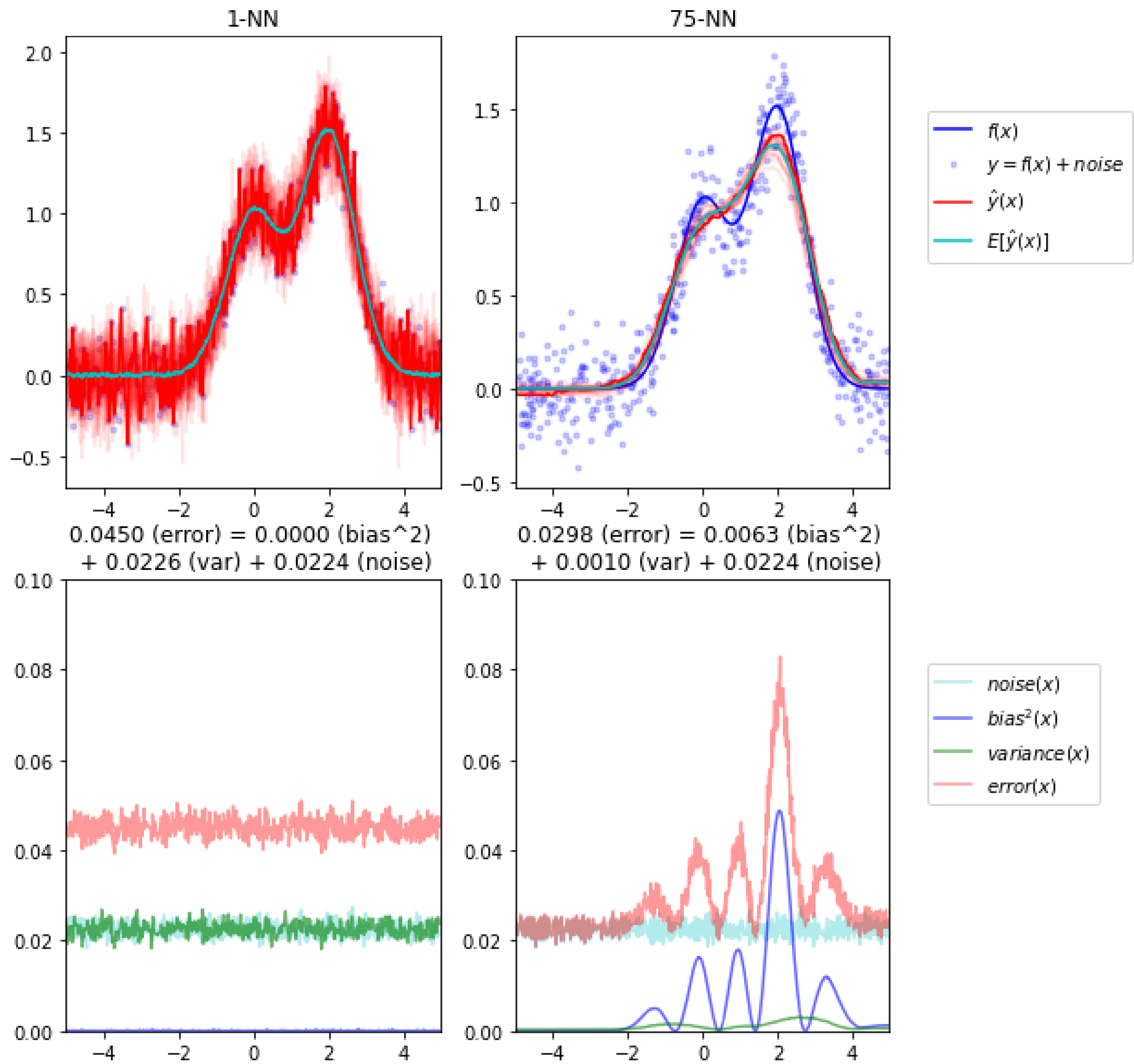


K Nearest Neighbors

Consider the following KNN regression models. Which model will have more bias? Which model will have more variance?

- **Model A**: K = 1
- **Model B**: K = 75

```
estimators = [("1-NN", KNeighborsRegressor(n_neighbors=1)),
              ("75-NN", KNeighborsRegressor(n_neighbors=75))]

plot_simulation(estimators)
```

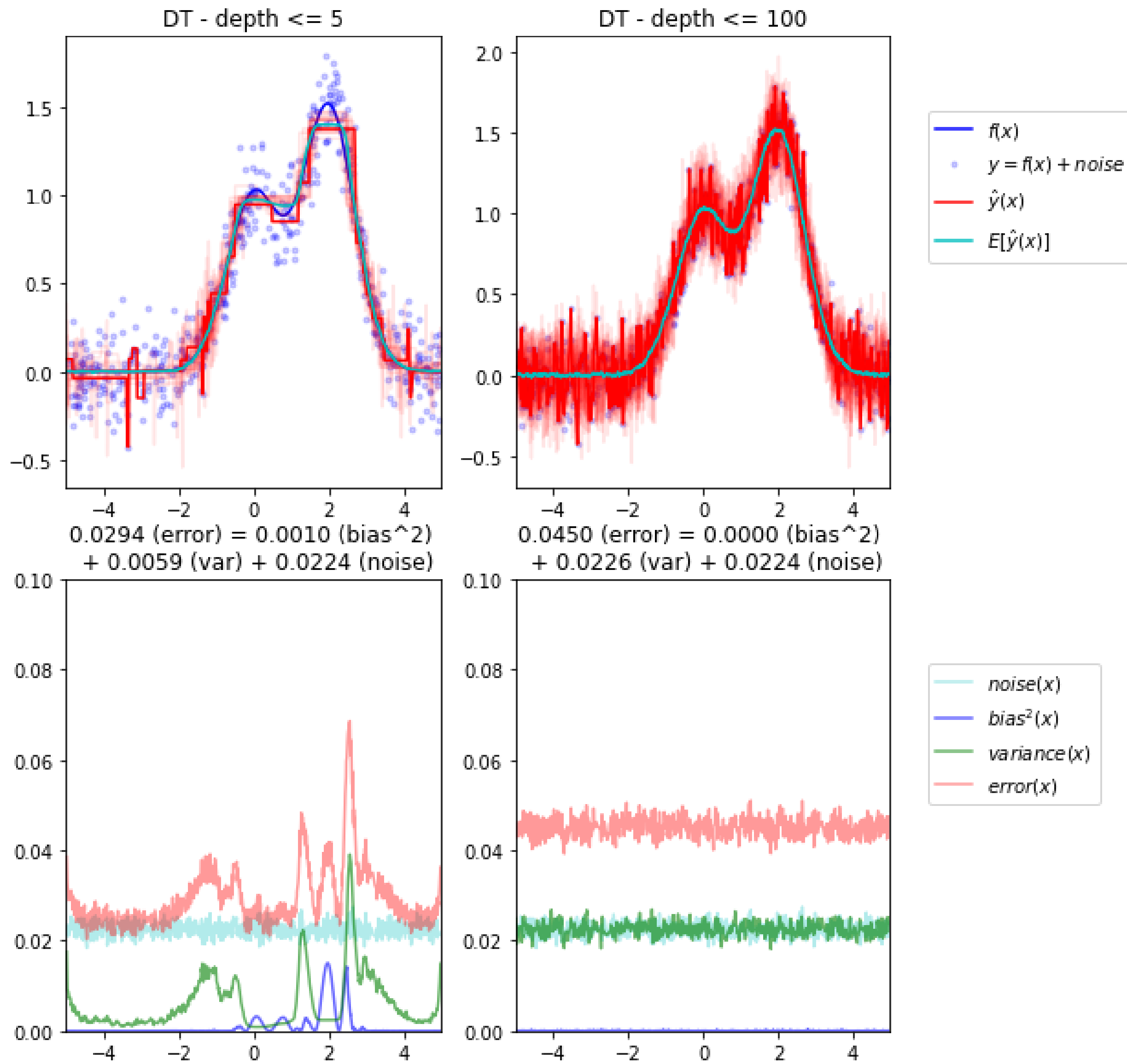


Decision tree by depth

Consider the following decision tree regression models. Which model will have more bias? Which model will have more variance?

- **Model A**: Max depth = 5
- **Model B**: Max depth = 100

```
estimators = [("DT - depth <= 5",  DecisionTreeRegressor(max_depth=5)),
              ("DT - depth <= 100", DecisionTreeRegressor(max_depth=100))]

plot_simulation(estimators)
```



Decision tree by pruning parameter

Suppose we use cost complexity tuning to train the decision tree that minimizes

$$\sum_{m=1}^{|T|}\sum_{x_i}^{R_m}(y_i - \hat{y}_{R_m})^2 + \alpha|T|$$

Consider the following decision tree regression models. Which model will have more bias? Which model will have more variance?

- **Model A**: $\alpha = 0.00001$
- **Model B**: $\alpha = 0.001$

```
estimators = [("DT -   = 10e-6",   DecisionTreeRegressor(ccp_alpha=10e-6)),
              ("DT -   = 10e-4", DecisionTreeRegressor(ccp_alpha=10e-4))]
```

```
plot_simulation(estimators)
```