Praktische Optimierung Blatt 08

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In [ ]:
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.linear_model import LinearRegression
from sklearn.preprocessing import PolynomialFeatures
from sklearn.pipeline import Pipeline
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF, Matern, ExpSineSquared
from gplearn.genetic import SymbolicRegressor
import graphviz
```

In [ ]:
```
np.random.seed(0)
```

Aufgabe 8.1 a)

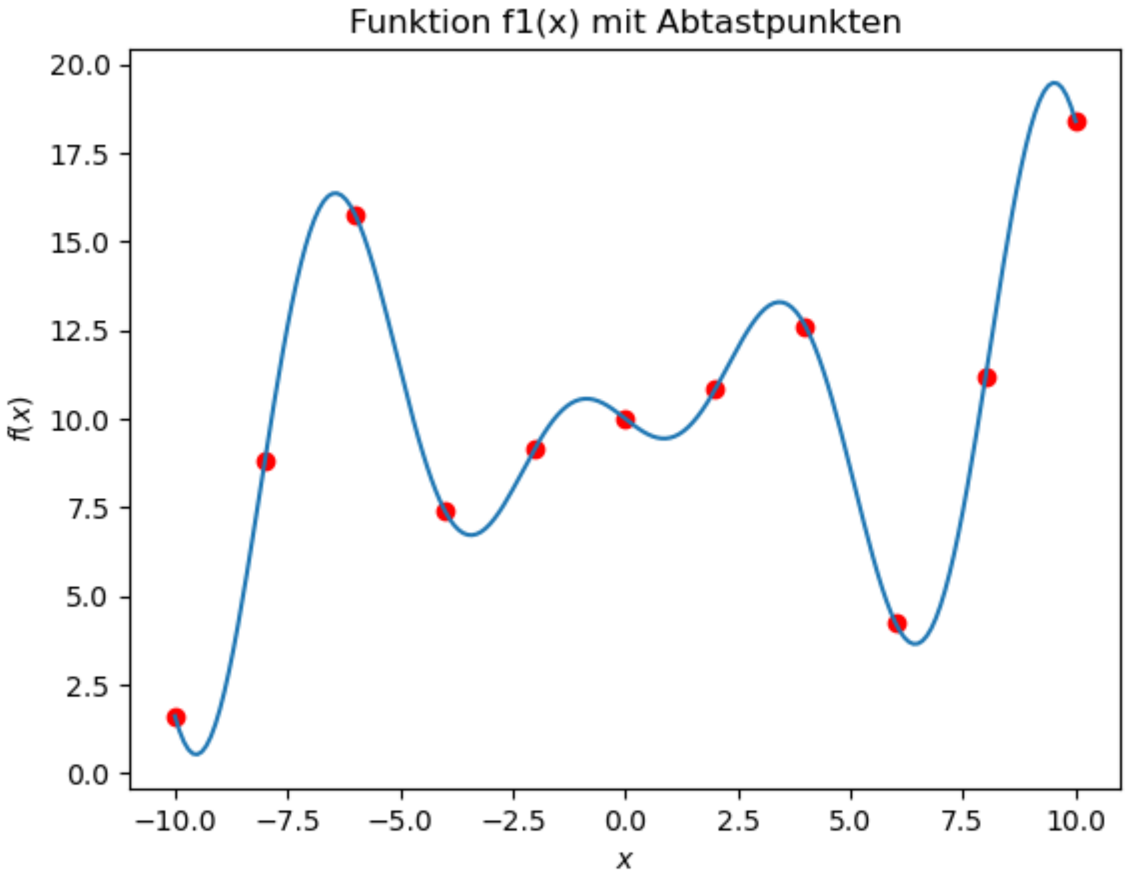
In [ ]:
```
def f1(x): return 10 - x * np.cos(x)

LOWER = -10
UPPER = 10
```

In [ ]:
```
X = np.linspace(LOWER, UPPER, 11).reshape(11, 1)
```

In [ ]:
```
X_Achse = np.linspace(LOWER, UPPER, 201)
plt.plot(X_Achse, f1(X_Achse), label="Übersicht")
plt.title("Funktion f1(x) mit Abtastpunkten")
plt.scatter(X, f1(X), c="red")
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
```

Out[ ]:
```
Text(0, 0.5, '$f(x)$')
```



(1) Polynomielle Modelle

In [ ]:
```
def poly_model_generator(func, deg, xs=X, ys=None, dim=1):
    poly_feat = PolynomialFeatures(degree=deg, include_bias=True)
    lin_reg = LinearRegression()
    pipe = Pipeline([("polynomial_features", poly_feat), ("linear_regress
    pipe.fit(xs, ys)
    return lambda x: pipe.predict(np.array(x).reshape(-1, dim)).flatten()
```

In [ ]:
```
poly_1 = poly_model_generator(f1, 1, ys=f1(X))
poly_2 = poly_model_generator(f1, 2, ys=f1(X))
poly_5 = poly_model_generator(f1, 5, ys=f1(X))
poly_10 = poly_model_generator(f1, 10, ys=f1(X))
poly_15 = poly_model_generator(f1, 15, ys=f1(X))
```

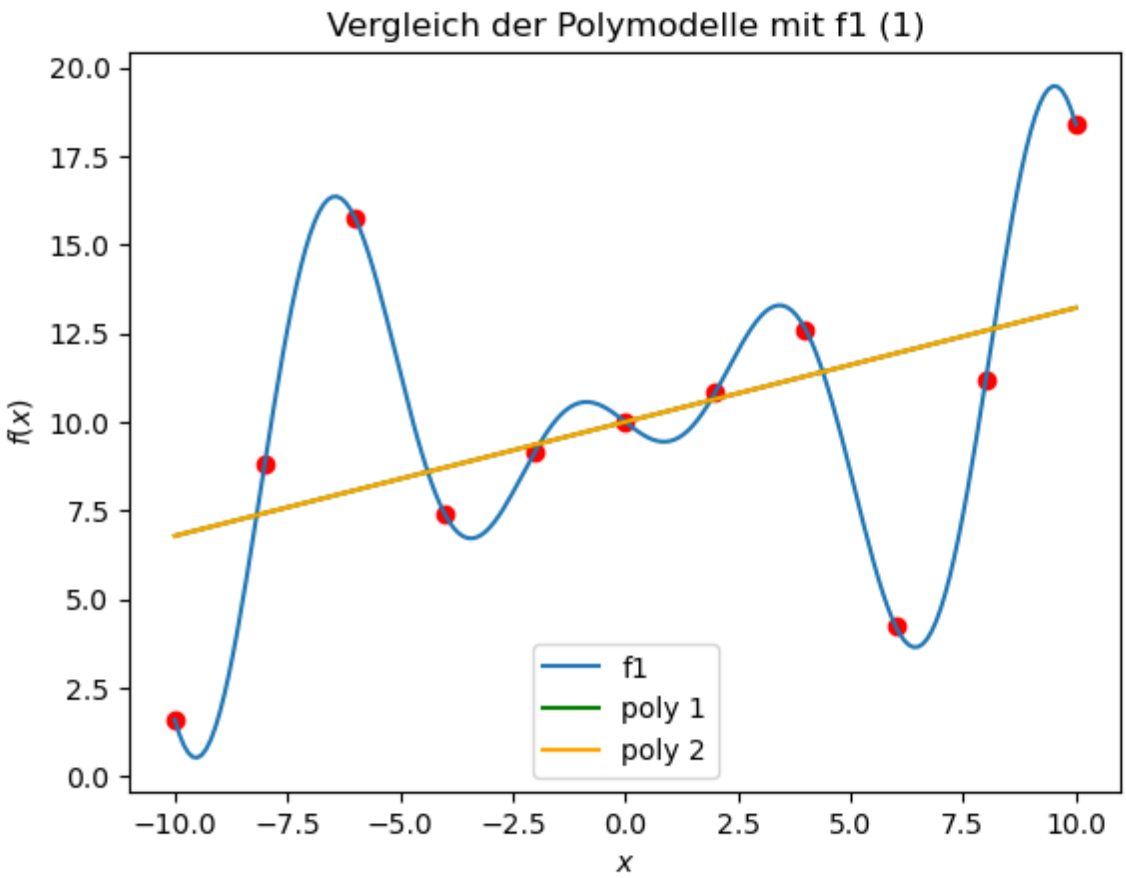
In [ ]:
```
degrees = [1, 2, 5, 10, 15]
X_test = np.linspace(LOWER, UPPER, 201)
comp_vals = f1(X_test)
for d in degrees:
    poly_model = poly_model_generator(f1, d, ys=f1(X))
    model_vals = poly_model(X_test)
    total_diff = np.abs(model_vals - comp_vals)
    total_mean = total_diff.mean()
    squared_mean = (total_diff**2).mean()
    print(f'Grade: {d}\tmittlere totale Abweichung: {total_mean : .2f}\tm
```

```
Grade: 1        mittlere totale Abweichung:  3.25       mittlere quadrati
sche Abweichung:  18.02
Grade: 2        mittlere totale Abweichung:  3.25       mittlere quadrati
sche Abweichung:  18.02
Grade: 5        mittlere totale Abweichung:  2.38       mittlere quadrati
sche Abweichung:  8.66
Grade: 10       mittlere totale Abweichung:  2.45       mittlere quadrati
sche Abweichung:  22.20
Grade: 15       mittlere totale Abweichung:  1920.82    mittlere quadrati
sche Abweichung:  24090766.49
```

In [ ]:

```
X_Achse = np.linspace(LOWER, UPPER, 201)
plt.plot(X_Achse, f1(X_Achse))
plt.plot(X_Achse, poly_1(X_Achse), c="green")
plt.plot(X_Achse, poly_2(X_Achse), c="orange")
plt.title("Vergleich der Polymodelle mit f1 (1)")
plt.scatter(X, f1(X), c="red")
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
plt.legend(labels=['f1', 'poly 1', 'poly 2'])
```

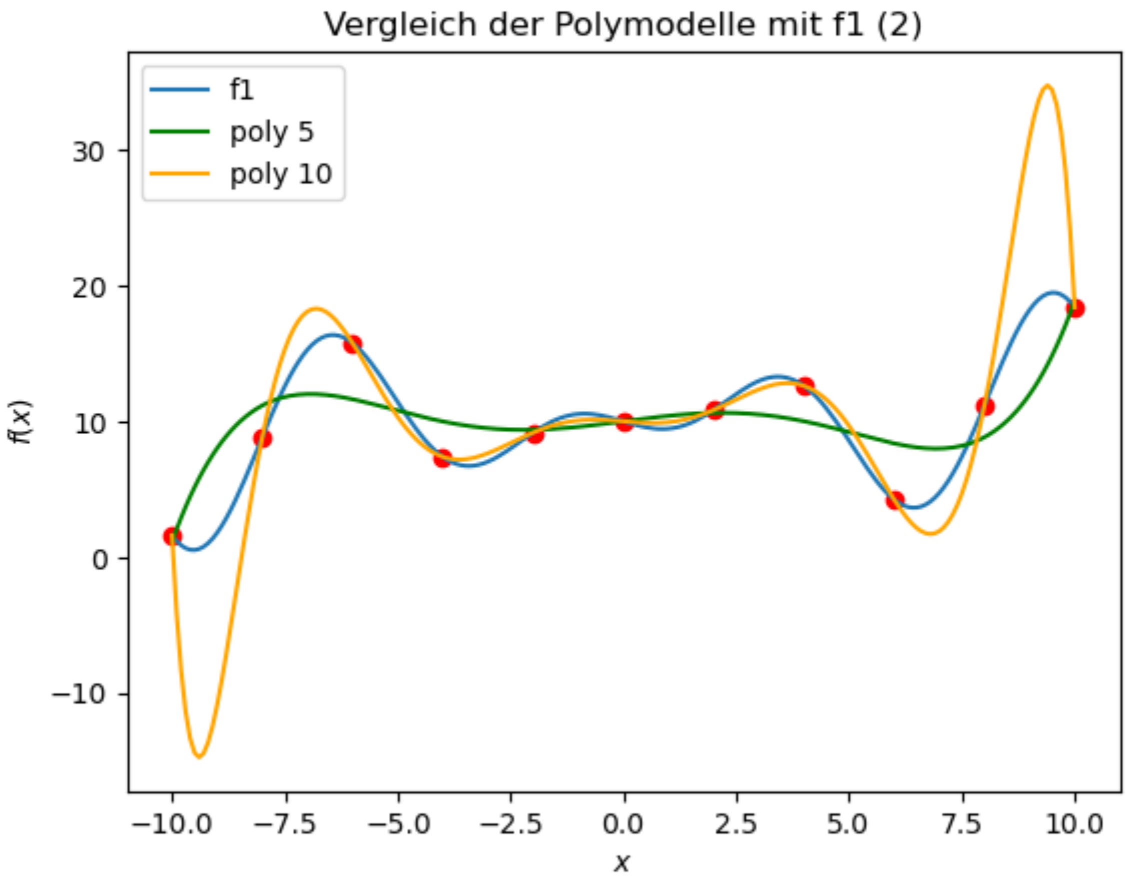
Out[ ]: <matplotlib.legend.Legend at 0x7f7ae57e2e50>



In [ ]:

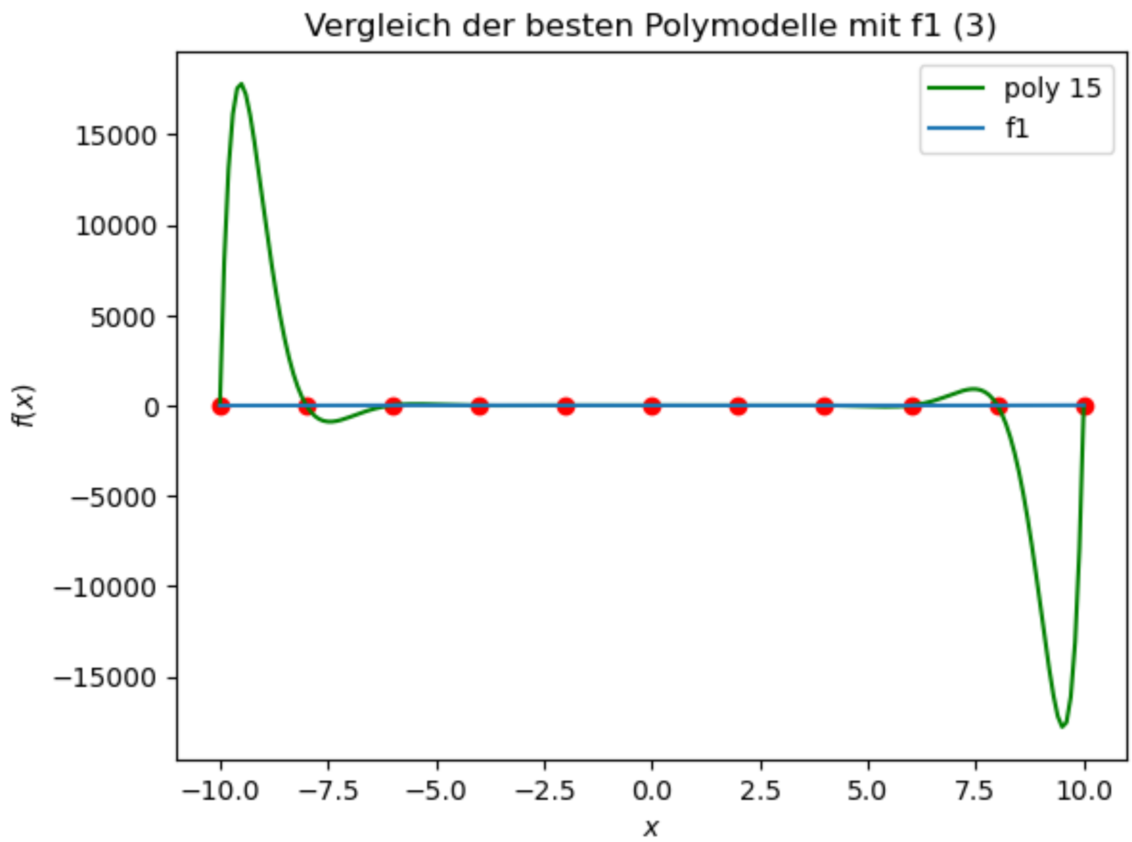
```
X_Achse = np.linspace(LOWER, UPPER, 201)
plt.plot(X_Achse, f1(X_Achse))
plt.plot(X_Achse, poly_5(X_Achse), c="green")
plt.plot(X_Achse, poly_10(X_Achse), c="orange")
plt.title("Vergleich der Polymodelle mit f1 (2)")
plt.scatter(X, f1(X), c="red")
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
plt.legend(labels=['f1', 'poly 5', 'poly 10'])
```

Out[ ]: <matplotlib.legend.Legend at 0x7f7ae5721fa0>



In [ ]:
```
X_Achse = np.linspace(LOWER, UPPER, 201)
plt.plot(X_Achse, poly_15(X_Achse), c="green")
plt.plot(X_Achse, f1(X_Achse))
plt.title("Vergleich der besten Polymodelle mit f1 (3)")
plt.scatter(X, f1(X), c="red")
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
plt.legend(labels=['poly 15', 'f1'])
```

Out[ ]: <matplotlib.legend.Legend at 0x7f7ae56472e0>



Es ist zu erkennen, dass das polynomielle Regressionsmodell mit $Grad = 5$ die geringste mittlere Abweichung zu der Ursprungsfunktion aufweist. Das nächst beste Modell bzgl. der totalen Abweichung ist das Modell mit $Grad = 10$. In Plot (2) ist zu erkennen, dass das Modell mit $Grad = 10$ in allen Abtastpunkten genau der Funktion f_1 entspricht. Allerdings in der Region $[-10, -8]$ und $[8, 10]$ eine starke Abweichung von f_1 aufweist. Das Modell mit $Grad = 5$ stimmt nicht in allen Abtastpunkten mit f_1 überein, allerdings weicht es auch nicht so stark von f_1 ab. Daher weißt es insgesamt eine geringere mittlere Abweichung auf. Die Modelle mit $Grad = 1$ und $Grad = 2$ scheinen identisch zu sein (siehe Plot (1)), also eine Regressionsgerade. Das Modell mit $Grad = 15$ ist deutlich am schlechtesten. Auch dieses weißt erneut eine sehr hohe Abweichung in den Regionen $[-10, -8]$ und $[8, 10]$ auf (siehe Plot (3)).

(2) Kriging

In [ ]:

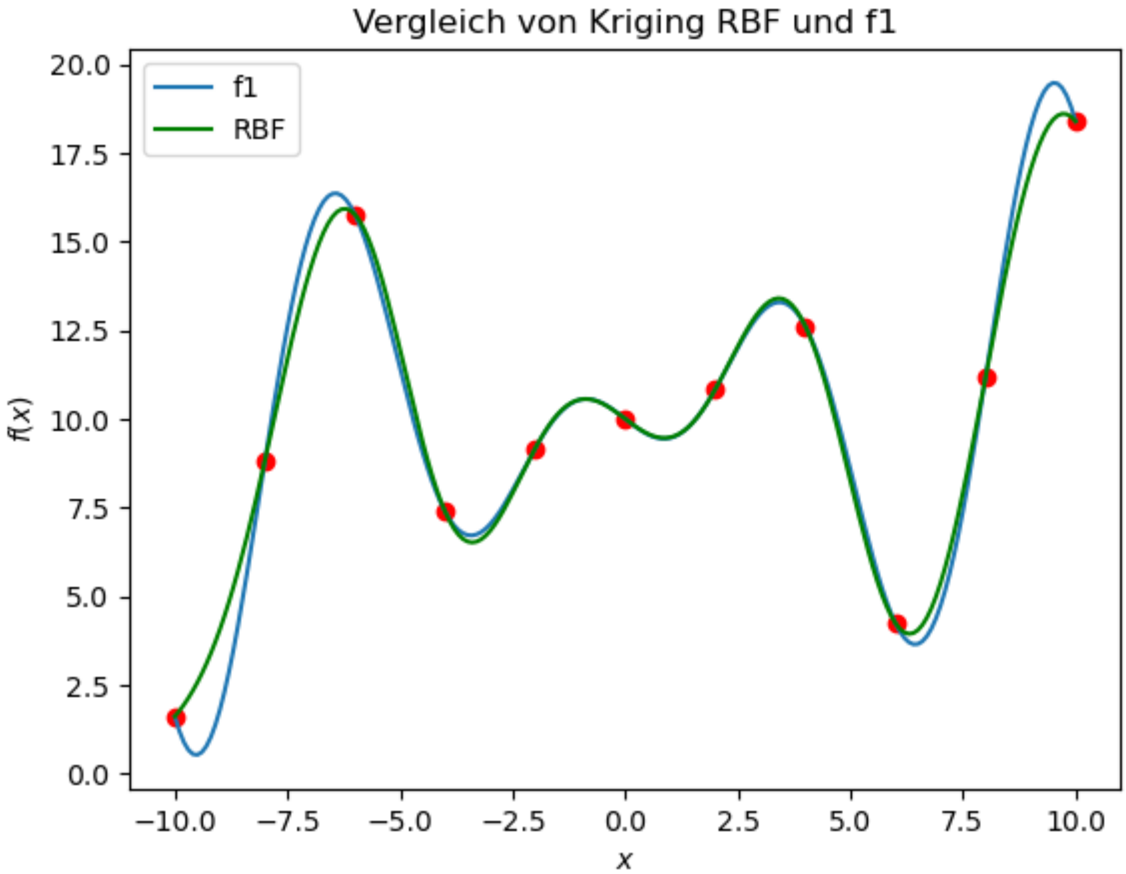
```
gpr_rbf = GaussianProcessRegressor(RBF())
gpr_rbf.fit(X, f1(X))
```

Out[ ]:

```
▾                GaussianProcessRegressor
GaussianProcessRegressor(kernel=RBF(length_scale=1))
```

In [ ]:
```
X_Achse = np.linspace(LOWER, UPPER, 201)
plt.plot(X_Achse, f1(X_Achse))
plt.plot(X_Achse, gpr_rbf.predict(X_Achse.reshape(201, 1)), c="green")
plt.title("Vergleich von Kriging RBF und f1")
plt.scatter(X, f1(X), c="red")
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
plt.legend(labels=['f1', 'RBF'])
```

Out[ ]: <matplotlib.legend.Legend at 0x7f7ae55ed730>



In [ ]:
```
total_diff_rbf = np.abs(gpr_rbf.predict(X_test.reshape(201, 1)) - comp_va
total_mean_rbf = total_diff_rbf.mean()
squared_mean_rbf = (total_diff_rbf**2).mean()
```

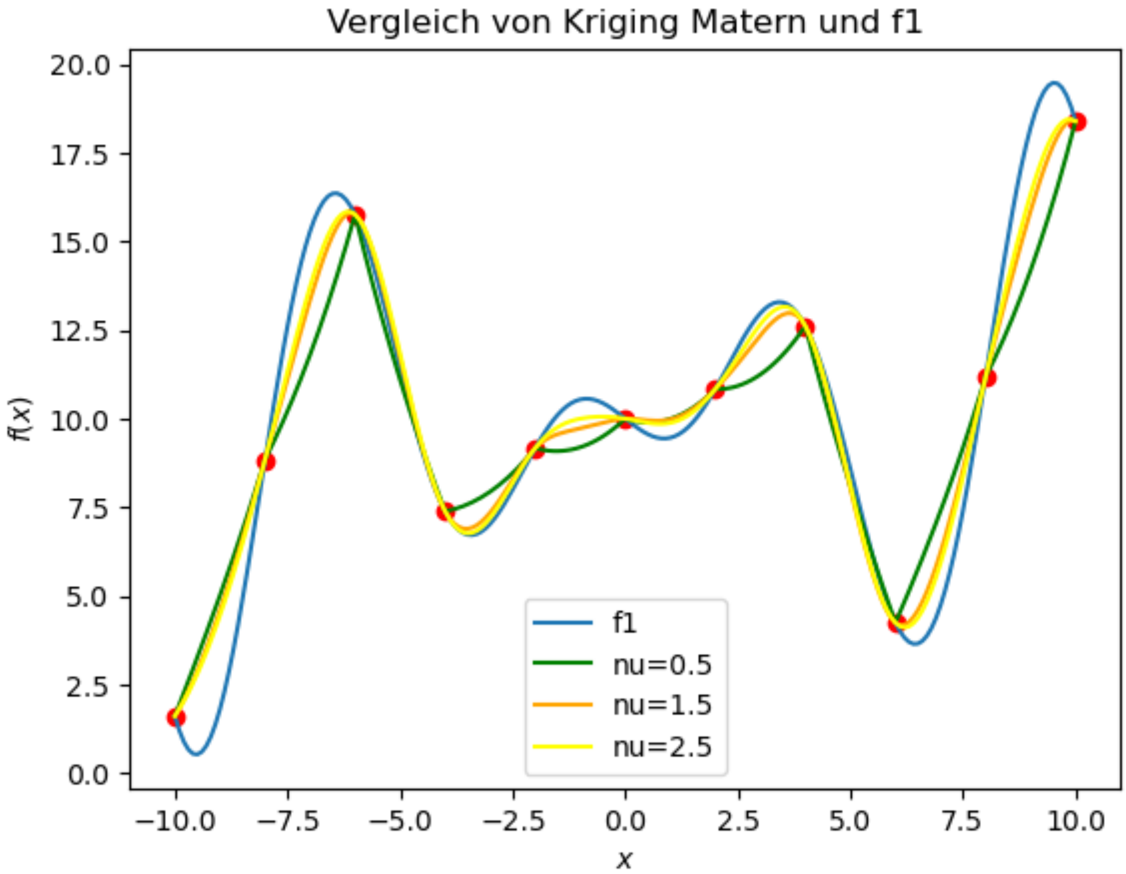
In [ ]:
```
gpr_mat0 = GaussianProcessRegressor(Matern(nu=0.5))
gpr_mat1 = GaussianProcessRegressor(Matern(nu=1.5))
gpr_mat2 = GaussianProcessRegressor(Matern(nu=2.5))

gpr_mat0.fit(X, f1(X))
gpr_mat1.fit(X, f1(X))
gpr_mat2.fit(X, f1(X))
```

Out[ ]:
```
▾ GaussianProcessRegressor
GaussianProcessRegressor(kernel=Matern(length_scale=1, nu=2.5))
```

In [ ]:
```
X_Achse = np.linspace(LOWER, UPPER, 201)
plt.plot(X_Achse, f1(X_Achse))
plt.plot(X_Achse, gpr_mat0.predict(X_Achse.reshape(201, 1)), c="green")
plt.plot(X_Achse, gpr_mat1.predict(X_Achse.reshape(201, 1)), c="orange")
plt.plot(X_Achse, gpr_mat2.predict(X_Achse.reshape(201, 1)), c="yellow")
plt.title("Vergleich von Kriging Matern und f1")
plt.scatter(X, f1(X), c="red")
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
plt.legend(labels=['f1', 'nu=0.5', 'nu=1.5', 'nu=2.5'])
```

Out[ ]: <matplotlib.legend.Legend at 0x7f7ae0039700>



In [ ]:
```
total_diff_mat0 = np.abs(gpr_mat0.predict(X_test.reshape(201, 1)) - comp_
total_diff_mat1 = np.abs(gpr_mat1.predict(X_test.reshape(201, 1)) - comp_
total_diff_mat2 = np.abs(gpr_mat2.predict(X_test.reshape(201, 1)) - comp_

total_mean_mat0   = total_diff_mat0.mean()
squared_mean_mat0 = (total_diff_mat0**2).mean()

total_mean_mat1   = total_diff_mat1.mean()
squared_mean_mat1 = (total_diff_mat1**2).mean()

total_mean_mat2   = total_diff_mat2.mean()
squared_mean_mat2 = (total_diff_mat2**2).mean()
```

In [ ]:
```
gpr_exp4 = GaussianProcessRegressor(ExpSineSquared(periodicity=4))
gpr_exp6 = GaussianProcessRegressor(ExpSineSquared(periodicity=6))
gpr_exp8 = GaussianProcessRegressor(ExpSineSquared(periodicity=8))

gpr_exp4.fit(X, f1(X))
gpr_exp6.fit(X, f1(X))
gpr_exp8.fit(X, f1(X))
```

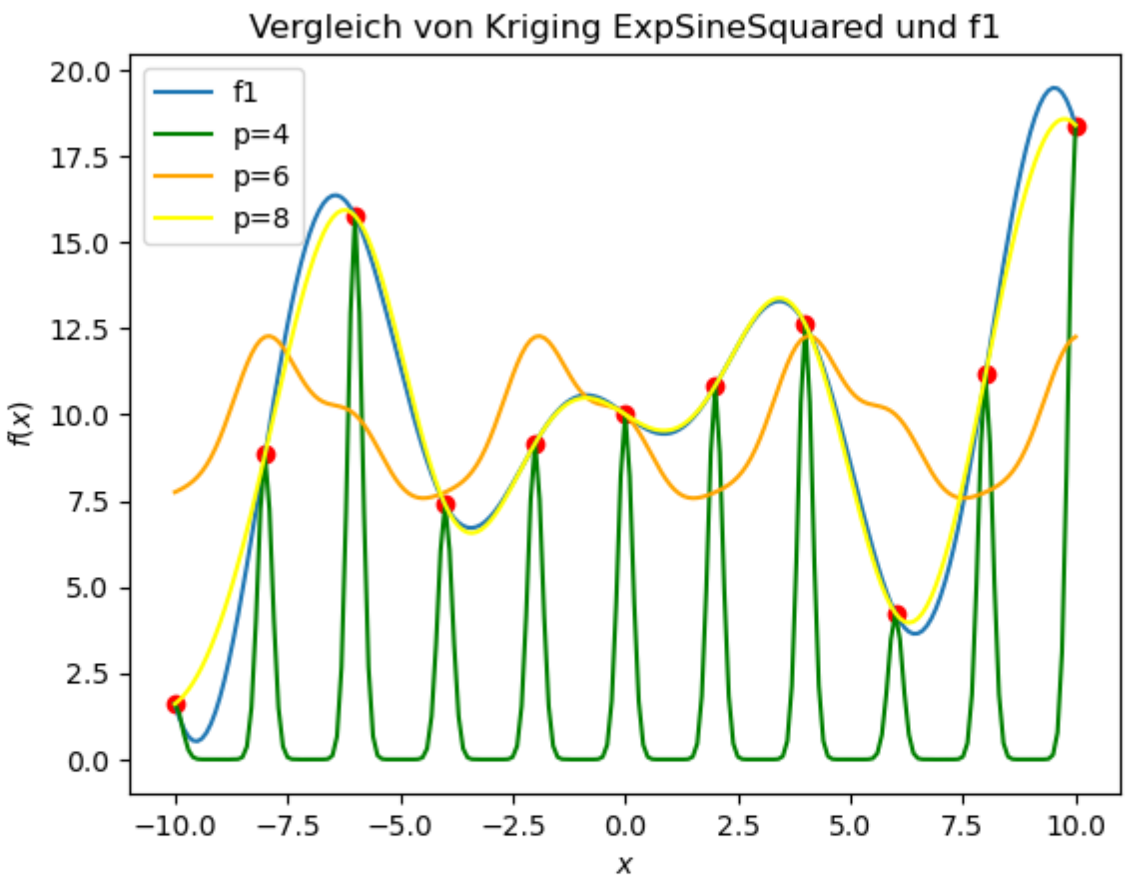
```
/home/tobi/anaconda3/envs/PO/lib/python3.8/site-packages/sklearn/gaussian
_process/kernels.py:420: ConvergenceWarning: The optimal value found for
dimension 0 of parameter length_scale is close to the specified lower bou
nd 1e-05. Decreasing the bound and calling fit again may find a better va
lue.
  warnings.warn(
/home/tobi/anaconda3/envs/PO/lib/python3.8/site-packages/sklearn/gaussian
_process/kernels.py:430: ConvergenceWarning: The optimal value found for
dimension 0 of parameter periodicity is close to the specified upper boun
d 100000.0. Increasing the bound and calling fit again may find a better
value.
  warnings.warn(
```

Out[ ]:
```
▾ GaussianProcessRegressor

GaussianProcessRegressor(kernel=ExpSineSquared(length_scale=1, pe
riodicity=8))
```

In [ ]:
```
X_Achse = np.linspace(LOWER, UPPER, 201)
plt.plot(X_Achse, f1(X_Achse))
plt.plot(X_Achse, gpr_exp4.predict(X_Achse.reshape(201, 1)), c="green")
plt.plot(X_Achse, gpr_exp6.predict(X_Achse.reshape(201, 1)), c="orange")
plt.plot(X_Achse, gpr_exp8.predict(X_Achse.reshape(201, 1)), c="yellow")
plt.title("Vergleich von Kriging ExpSineSquared und f1")
plt.scatter(X, f1(X), c="red")
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
plt.legend(labels=['f1', 'p=4', 'p=6', 'p=8'])
```

Out[ ]:
```
<matplotlib.legend.Legend at 0x7f7adbb6cfd0>
```



In [ ]:
```
total_diff_exp4 = np.abs(gpr_exp4.predict(X_test.reshape(201, 1)) - comp_
total_diff_exp6 = np.abs(gpr_exp6.predict(X_test.reshape(201, 1)) - comp_
total_diff_exp8 = np.abs(gpr_exp8.predict(X_test.reshape(201, 1)) - comp_

total_mean_exp4   = total_diff_exp4.mean()
squared_mean_exp4 = (total_diff_exp4**2).mean()

total_mean_exp6   = total_diff_exp6.mean()
squared_mean_exp6 = (total_diff_exp6**2).mean()

total_mean_exp8   = total_diff_exp8.mean()
squared_mean_exp8 = (total_diff_exp8**2).mean()
```

In [ ]:
```
print(f'Kernel: RBF \t\t\tmtA: {total_mean_rbf : .2f}\tmqA: {squared_mean_

print(f'Kernel: Matern\t nu: 0.5\tmtA: {total_mean_mat0 : .2f}\tmqA: {squ
print(f'Kernel: Matern\t nu: 1.5\tmtA: {total_mean_mat1 : .2f}\tmqA: {squ
print(f'Kernel: Matern\t nu: 2.5\tmtA: {total_mean_mat2 : .2f}\tmqA: {squ

print(f'Kernel: ESS\t  p: 4\t\tmtA: {total_mean_exp4 : .2f}\tmqA: {square
print(f'Kernel: ESS\t  p: 6\t\tmtA: {total_mean_exp6 : .2f}\tmqA: {square
print(f'Kernel: ESS\t  p: 8\t\tmtA: {total_mean_exp8 : .2f}\tmqA: {square
```

```
Kernel: RBF                     mtA:  0.41      mqA:  0.45

Kernel: Matern   nu: 0.5        mtA:  1.23      mqA:  2.73
Kernel: Matern   nu: 1.5        mtA:  0.74      mqA:  1.07
Kernel: Matern   nu: 2.5        mtA:  0.61      mqA:  0.79

Kernel: ESS       p: 4          mtA:  7.97      mqA:  88.71
Kernel: ESS       p: 6          mtA:  3.46      mqA:  18.13
Kernel: ESS       p: 8          mtA:  0.41      mqA:  0.44
```

Das wohl beste Modell ist hier Kriging mit dem ExpSineSquared Kernel mit Parameter p=8. Nahezu identische Abweichungen weißt das Modell mit RBF-Kernel auf. Diese Beiden Modelle nähern die Funktion f_1 sehr gut an.
Beim ExpSineSquared Kernel ist zu beobachten, dass das Modell mit $p = 4$ stets den Wert 0 annimmt bis sich der X-Wert an einen Abstastpunkt annähert. Dann steigt die Modellfunktion an bis diese ein lokales Maximum im Abtastpunkt annimmt. Anschließend sinkt die Funktion wieder auf 0 herab. Daher ergeben sich sehr hohe Abweichungen der Werte für alle Punkte, die kein Abtastpunkt sind. Für $p = 6$ nähert die Modellfunktion das Verhalten von f_1 schon besser an, allerdings liegen die Wert häufig noch überhalb bzw. unterhalb der Funktion.
Die Modelle des Matern-Kernels weichen deutlich weniger von einander ab. Hier ist zu beobachten, dass die Funktionswert des Modells mit $\nu = 2.5$ stets zwischen der Funktion f_1 und der Modellfunktion des Modells mit Paramter $\nu = 0.5$ liegen. Alle drei Modelle laufen allerdings genau durch die Abtastpunkte.

(3) Symbolische Regression

Funktion der Parameter:

- Population Size: steht für die Anzahl Programme in jeder Generation.
- Tournament Size: Steht für die Anzahl der Programme, die im Turnier um das Weiterkommen in die nächste Generation teilnehmen.
- Generations: Anzahl Generationen, die erstellt werden.
- Stoppkiterium: Minimaler Wert der Genauigkeitsmetrik, ab dem die Evolution gestoppt und das Programm angenommen wird, welches einen Genuigkeitswert kleiner oder gleich diesem Wert hat.

In [ ]:
```
func_sets = [['add', 'sub'] , ['mul', 'div'], ['add','mul'], ['add', 'sub
```

In [ ]:
```
mean_total_diffs = np.zeros((8, 10))
mean_squared_diffs = np.zeros((8, 10))
for j in range(10):
    for i, fs in enumerate(func_sets):
        sym_reg = SymbolicRegressor(population_size=500, tournament_size=
                                    generations=25, stopping_criteria=0.0
                                    n_jobs=-1, function_set=fs)
        sym_reg.fit(X, f1(X))
        preds = sym_reg.predict(X_test.reshape(201, 1))
        total_diff = np.abs(preds - comp_vals)
        mean_total_diffs[i][j] = total_diff.mean()
        mean_squared_diffs[i][j] = (total_diff**2).mean()
```

```
/home/tobi/anaconda3/envs/PO/lib/python3.8/site-packages/sklearn/utils/va
lidation.py:1143: DataConversionWarning: A column-vector y was passed whe
n a 1d array was expected. Please change the shape of y to (n_samples, ),
for example using ravel().
  y = column_or_1d(y, warn=True)
/home/tobi/anaconda3/envs/PO/lib/python3.8/site-packages/sklearn/utils/va
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```

```
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```

In [ ]:
```
fig, ax = plt.subplots(8, sharex=True)
fig.suptitle('Boxplots der mtA der Symbolischen Regression')
fig.tight_layout(pad=1.5)
plt.xlabel('mittlere absolute Abweichung')
ax[0].set_title('add sub')
ax[0].boxplot(mean_total_diffs[0], vert=False)
ax[1].set_title('mul div')
ax[1].boxplot(mean_total_diffs[1], vert=False)
ax[2].set_title('add mul')
ax[2].boxplot(mean_total_diffs[2], vert=False)
ax[3].set_title('add sub mul div')
ax[3].boxplot(mean_total_diffs[3], vert=False)
ax[4].set_title('sin cos')
ax[4].boxplot(mean_total_diffs[4], vert=False)
ax[5].set_title('add mul sin')
ax[5].boxplot(mean_total_diffs[5], vert=False)
ax[6].set_title('sub mul cos')
ax[6].boxplot(mean_total_diffs[6], vert=False)
ax[7].set_title('add sub mul div cos sin')
ax[7].boxplot(mean_total_diffs[7], vert=False)
```

Out[ ]:
```
{'whiskers': [<matplotlib.lines.Line2D at 0x7f553a37deb0>,
  <matplotlib.lines.Line2D at 0x7f553a308190>],
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  <matplotlib.lines.Line2D at 0x7f553a3086d0>],
 'boxes': [<matplotlib.lines.Line2D at 0x7f553a37dc10>],
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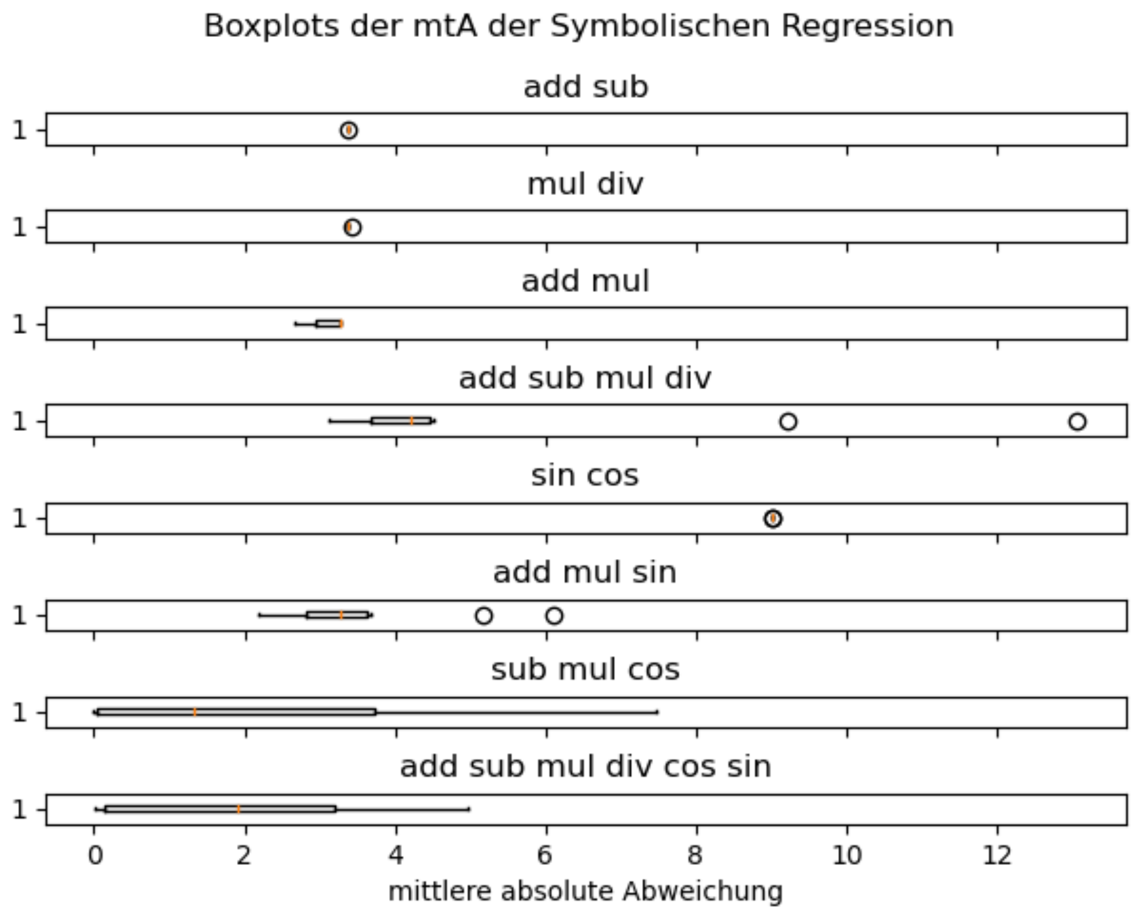
 'fliers': [<matplotlib.lines.Line2D at 0x7f553a308c10>],
 'means': []}
```



In [ ]:
```
fig, ax = plt.subplots(8, sharex=True)
fig.suptitle('Boxplots der mqA der Symbolischen Regression')
fig.tight_layout(pad=1.5)
plt.xlabel('mittlere quadratische Abweichung')
plt.xlim(0, 200)
ax[0].set_title('add sub')
ax[0].boxplot(mean_squared_diffs[0], vert=False)
ax[1].set_title('mul div')
ax[1].boxplot(mean_squared_diffs[1], vert=False)
ax[2].set_title('add mul')
ax[2].boxplot(mean_squared_diffs[2], vert=False)
ax[3].set_title('add sub mul div')
ax[3].boxplot(mean_squared_diffs[3], vert=False)
ax[4].set_title('sin cos')
ax[4].boxplot(mean_squared_diffs[4], vert=False)
ax[5].set_title('add mul sin')
ax[5].boxplot(mean_squared_diffs[5], vert=False)
ax[6].set_title('sub mul cos')
ax[6].boxplot(mean_squared_diffs[6], vert=False)
ax[7].set_title('add sub mul div cos sin')
ax[7].boxplot(mean_squared_diffs[7], vert=False)
```

Out[ ]:
```
{'whiskers': [<matplotlib.lines.Line2D at 0x7f5538fbd2e0>,
  <matplotlib.lines.Line2D at 0x7f5538fbd580>],
 'caps': [<matplotlib.lines.Line2D at 0x7f5538fbd820>,
  <matplotlib.lines.Line2D at 0x7f5538fbdac0>],
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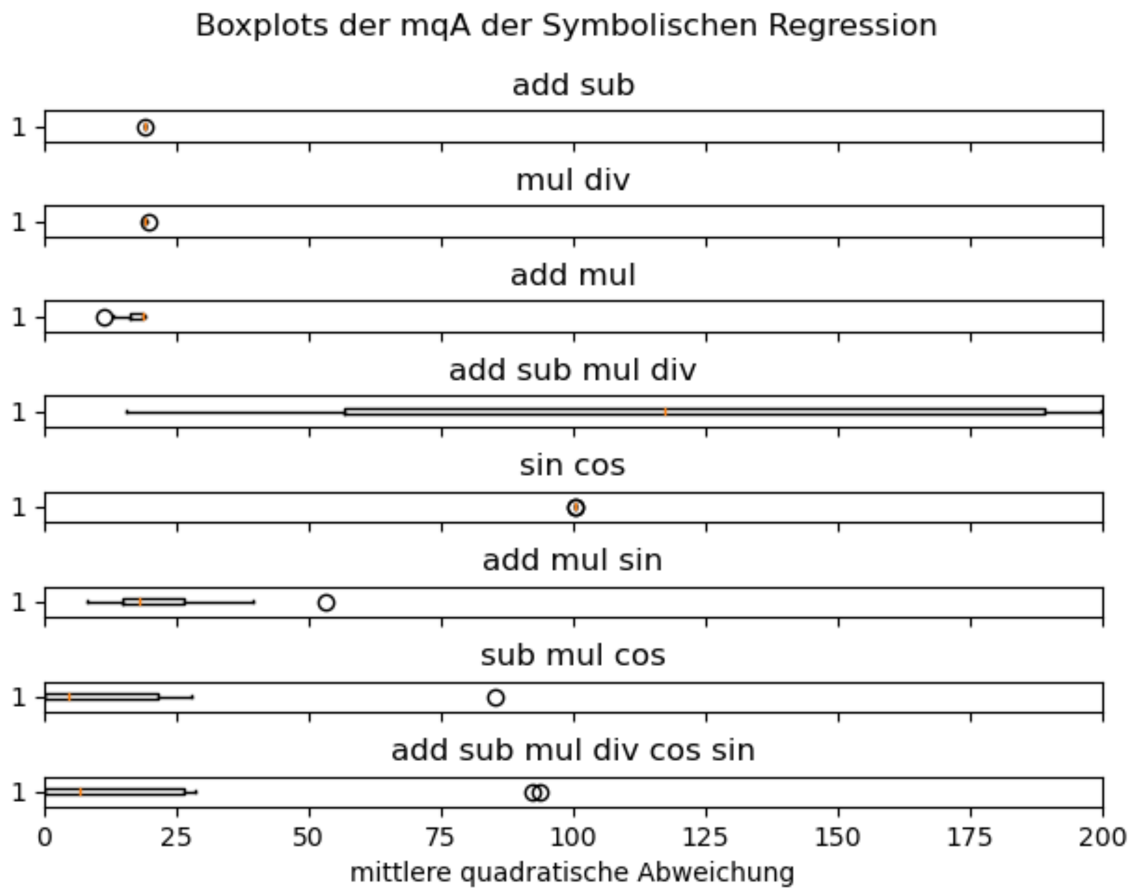


In den Boxplots ist zu erkennen, dass die Funktionsmenge $[sub, mul, cos]$ im mittel die geringste mittlere absolute und quadratische Abweichung aufweißt. Dabei handelt es sich um die Funktionsmenge die benötigt wird, um die Funktion f_1 genau nachbauen zu können. Die nächst beste Funktionsmenge ist $[add, sub, mul, div, sin, cos]$. Dies liegt daran, dass alle Funktionen die für eine genau rekonstruktion von f_1 benötigt werden in dieser Menge enthalten sind. Allerdings ist diese Menge im mittel etwas schlechter als die zuvor betrachtete, da auch Funktionen enthalten sind, welche nicht benötigt werden.

In [ ]:
```
best_sym_reg = SymbolicRegressor(population_size=500, tournament_size=10,
                                 generations=25, stopping_criteria=0.0
                                 n_jobs=-1, function_set=['sub', 'mul'
best_sym_reg.fit(X, f1(X))
```

```
/home/tobi/anaconda3/envs/PO/lib/python3.8/site-packages/sklearn/utils/va
lidation.py:1143: DataConversionWarning: A column-vector y was passed whe
n a 1d array was expected. Please change the shape of y to (n_samples, ),
for example using ravel().
  y = column_or_1d(y, warn=True)
```

Out[ ]:

▾ SymbolicRegressor

```
sub(sub(sub(0.900, -0.648), sub(mul(sub(-0.668, 0.513), sub(sub
(0.900, sub(mul(sub(-0.668, 0.513), sub(sub(0.900, -0.648), sub(m
ul(sub(-0.668, 0.513), cos(0.853)), 0.937))), cos(cos(cos(0.19
3))))), sub(mul(cos(sub(sub(0.900, -0.648), cos(X0))), mul(X0, 0.
882)), cos(cos(0.193))))), cos(cos(cos(0.193))))), sub(cos(cos(mu
l(mul(0.160, X0), sub(X0, X0)))), cos(0.513)))
```

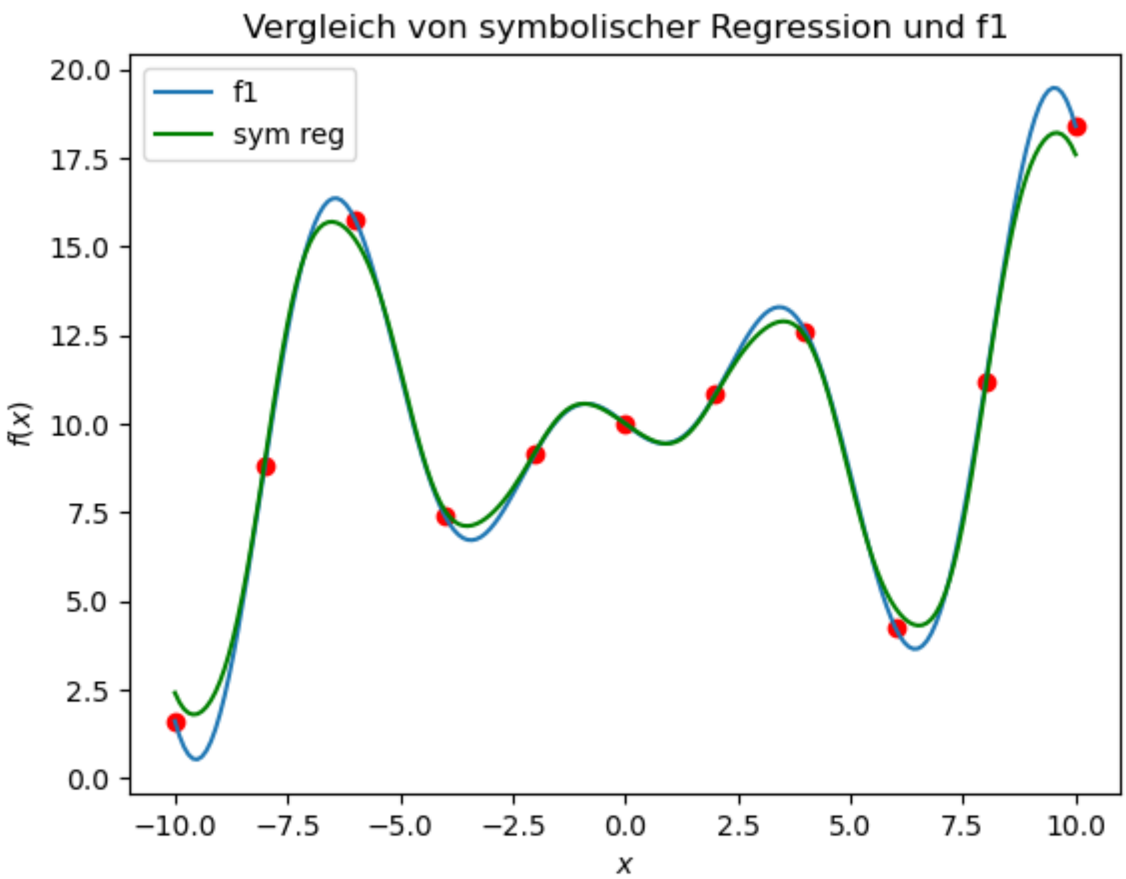
In [ ]:
```
print(best_sym_reg)
```

```
sub(sub(sub(0.900, -0.648), sub(mul(sub(-0.668, 0.513), sub(sub(0.900, su
b(mul(sub(-0.668, 0.513), sub(sub(0.900, -0.648), sub(mul(sub(-0.668, 0.5
13), cos(0.853)), 0.937))), cos(cos(cos(0.193))))), sub(mul(cos(sub(sub
(0.900, -0.648), cos(X0))), mul(X0, 0.882)), cos(cos(0.193))))), cos(cos
(cos(0.193))))), sub(cos(cos(mul(mul(0.160, X0), sub(X0, X0)))), cos(0.51
3)))
```

In [ ]:
```
# Option um den Syntaxbaum grafisch zu betrachten
graph = graphviz.Source(best_sym_reg._program.export_graphviz())
#graph
```

In [ ]:
```
X_Achse = np.linspace(LOWER, UPPER, 201)
plt.plot(X_Achse, f1(X_Achse))
plt.plot(X_Achse, best_sym_reg.predict(X_Achse.reshape(201, 1)), c="green
plt.title("Vergleich von symbolischer Regression und f1")
plt.scatter(X, f1(X), c="red")
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
plt.legend(labels=['f1', 'sym reg'])
```

Out[ ]: <matplotlib.legend.Legend at 0x7f552fa7c820>



(b)

Anmerkung: Für Kriging haben wir beim Lösen von (a) keine Funktion zur Generierung bzw. Anpassung der Modelle verwendet, also können wir diese auch nicht wieder verwenden. Daher implementieren wir diese Funktion hier erst bei (b). Diese könnte auch identisch für die Lösung von (a) verwendet werden.

In [ ]:
```
def f2(x): return 5 * np.min(x, axis=0) - 3 * x[0]

LOWER_X = 0
UPPER_X = 100
LOWER_Y = 30
UPPER_Y = 70
```

In [ ]:
```
x = np.linspace(0, 100, 101)
y = np.random.normal(50, 7, size=100)

X, Y = np.meshgrid(x, y)
Z = 5 * np.min([X, Y], axis=0) - 3 * X
```

In [ ]:
```
x_Achse = np.linspace(LOWER_X, UPPER_X, 101)
y_Achse = np.linspace(LOWER_Y, UPPER_Y, 41)

X_Achse, Y_Achse = np.meshgrid(x_Achse, y_Achse)
X_test = np.array(list(zip(X_Achse.flatten(), Y_Achse.flatten())))
comp_vals = 5 * np.min([X_Achse, Y_Achse], axis=0) - 3 * X_Achse
```

(1) ploynomielle Regression

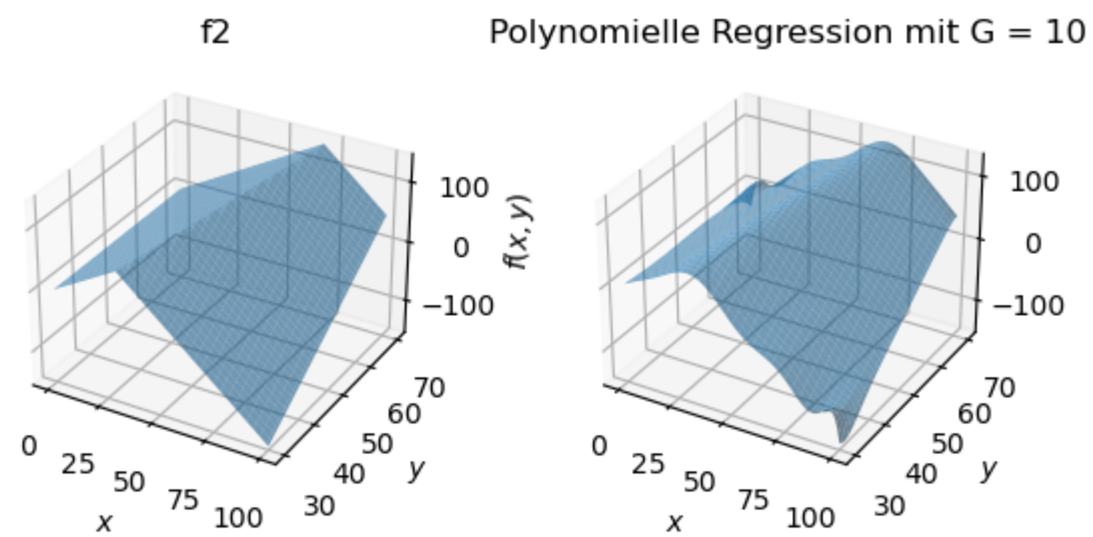
In [ ]:
```
poly_1  = poly_model_generator(f2, 1,  xs=np.array(list(zip(X.flatten(),
poly_2  = poly_model_generator(f2, 2,  xs=np.array(list(zip(X.flatten(),
poly_5  = poly_model_generator(f2, 5,  xs=np.array(list(zip(X.flatten(),
poly_10 = poly_model_generator(f2, 10, xs=np.array(list(zip(X.flatten(),
poly_15 = poly_model_generator(f2, 15, xs=np.array(list(zip(X.flatten(),
```

In [ ]:
```
degrees = [1, 2, 5, 10, 15]
for d in degrees:
    poly_model = poly_model_generator(f1, d, xs=np.array(list(zip(X.flatt
    model_vals = poly_model(X_test)
    total_diff = np.abs(model_vals - comp_vals.flatten())
    total_mean = total_diff.mean()
    squared_mean = (total_diff**2).mean()
    print(f'Grade: {d}\tmittlere totale Abweichung: {total_mean : .2f}\tm
```

```
Grade: 1        mittlere totale Abweichung:  35.05      mittlere quadrati
sche Abweichung:  1760.89
Grade: 2        mittlere totale Abweichung:  9.40       mittlere quadrati
sche Abweichung:  136.97
Grade: 5        mittlere totale Abweichung:  4.96       mittlere quadrati
sche Abweichung:  42.24
Grade: 10       mittlere totale Abweichung:  2.00       mittlere quadrati
sche Abweichung:  11.47
Grade: 15       mittlere totale Abweichung:  10.04      mittlere quadrati
sche Abweichung:  1143.05
```

In [ ]:
```
fig = plt.figure()
ax1 = fig.add_subplot(121, projection='3d')
ax2 = fig.add_subplot(122, projection='3d')

ax1.set_title('f2')
ax1.set_xlabel('$x$')
ax1.set_ylabel('$y$')
ax1.set_zlabel('$f(x,y)$')
ax2.set_title('Polynomielle Regression mit G = 10')
ax2.set_xlabel('$x$')
ax2.set_ylabel('$y$')
ax1.set_axisbelow(True)
ax2.set_axisbelow(True)
ax1.plot_surface(X_Achse, Y_Achse, comp_vals, alpha=0.6)
ax2.plot_surface(X_Achse, Y_Achse, poly_10(X_test.reshape(-1,2)).reshape(
fig.tight_layout(pad=5)
```



Grafisch ist zu erkennen, dass das polynomielle Regressionsmodell die Funktion f_2 annähernd rekonstruiert hat. Allerdings weißt die Funktion f_2 eine Spitze auf, welche beim Regressionsmodell abgerundet ist. Außerdem liegen an den Rändern der Wertebereich bei diesem erneut Schwankungen vor (wie bereits bei (a) beobachtet). Das Modell weißt eine mittlere quadratische Abweichung von 11.47 auf und ist somit etwas schlechter als das beste polynomielle Regressionsmodell in (a). Außerdem ist zu beobachten, dass das beste Modell in (a) den Grad 5 verwendet hat, während das beste Modell hier den Grad 10 aufweist.

(2) Kriging

In [ ]:
```
# Wenn dim=1, dann kann diese Funktion für (a) verwendet werden
def kriging_model_generator(xs, ys, kernel, dim=2, **kwargs):
    gpr_model = GaussianProcessRegressor(kernel(**kwargs))
    gpr_model.fit(xs, ys)
    return lambda x: gpr_model.predict(np.array(x).reshape(-1, dim)).flat
```

In [ ]:
```
def find_best_kriging(xs, ys):
    best_abs_diff = np.Inf
    best_sq_diff = np.Inf
    best_kernel = None
    best_param = None

    x_Achse = np.linspace(LOWER_X, UPPER_X, 101)
    y_Achse = np.linspace(LOWER_Y, UPPER_Y, 41)
    X_Achse, Y_Achse = np.meshgrid(x_Achse, y_Achse)
    X_test = np.array(list(zip(X_Achse.flatten(), Y_Achse.flatten())))

    comp_vals = 5 * np.min([X_Achse, Y_Achse], axis=0) - 3 * X_Achse

    try: # RBF
        current_kernel = "RBF"
        model = kriging_model_generator(xs, ys, kernel=RBF)

        preds = model(X_test)
        abs_diff = np.abs(comp_vals.flatten() - preds)
        mean_abs_diff = abs_diff.mean()
        mean_sq_diff = (abs_diff**2).mean()
        if mean_abs_diff < best_abs_diff:
            best_abs_diff = mean_abs_diff
            best_sq_diff = mean_sq_diff
            best_kernel = current_kernel

    except np.linalg.LinAlgError:
        print(f'Der Kernel {current_kernel} ist nicht anwendbar')

    try: # Matern
        current_kernel = "Matern"
        nus = [0.5, 1.5, 2.5]
        for nu in nus:
            model = kriging_model_generator(xs, ys, kernel=Matern, nu=nu)

            preds = model(X_test)
            abs_diff = np.abs(comp_vals.flatten() - preds)
            mean_abs_diff = abs_diff.mean()
            mean_sq_diff = (abs_diff**2).mean()
            if mean_abs_diff < best_abs_diff:
                best_abs_diff = mean_abs_diff
                best_sq_diff = mean_sq_diff
                best_kernel = current_kernel
                best_param = nu

    except np.linalg.LinAlgError:
        print(f'Der Kernel {current_kernel} ist nicht anwendbar')

    try: # ExpSineSquared
        current_kernel = "ExpSineSquared"
        ps = [4, 6, 8]
        for p in ps:
            model = kriging_model_generator(xs, ys, kernel=ExpSineSquared

            preds = model(X_test)
            abs_diff = np.abs(comp_vals.flatten() - preds)
            mean_abs_diff = abs_diff.mean()
            mean_sq_diff = (abs_diff**2).mean()
            if mean_abs_diff < best_abs_diff:
                best_abs_diff = mean_abs_diff
```

```
                best_sq_diff = mean_sq_diff
                best_kernel = current_kernel
                best_param = p

    except np.linalg.LinAlgError:
        print(f'Der Kernel {current_kernel} ist nicht anwendbar')

    return {'kernel' : best_kernel, 'param' : best_param, 'mtA' : best_ab
```

In [ ]:

```
find_best_kriging(np.array(list(zip(X.flatten(), Y.flatten()))), Z.flatte
```

```
/home/tobi/anaconda3/envs/PO/lib/python3.8/site-packages/sklearn/gaussian
_process/kernels.py:420: ConvergenceWarning: The optimal value found for
dimension 0 of parameter length_scale is close to the specified lower bou
nd 1e-05. Decreasing the bound and calling fit again may find a better va
lue.
  warnings.warn(
/home/tobi/anaconda3/envs/PO/lib/python3.8/site-packages/sklearn/gaussian
_process/_gpr.py:629: ConvergenceWarning: lbfgs failed to converge (statu
s=2):
ABNORMAL_TERMINATION_IN_LNSRCH.

Increase the number of iterations (max_iter) or scale the data as shown i
n:
    https://scikit-learn.org/stable/modules/preprocessing.html
  _check_optimize_result("lbfgs", opt_res)
Der Kernel ExpSineSquared ist nicht anwendbar
```

Out[ ]:

```
{'kernel': 'Matern',
 'param': 0.5,
 'mtA': 0.677539140590192,
 'msA': 5.331582559737829}
```

Der ExpSineSquared Kernel kann nicht verwendet werden. Das beste Kriging-Modell für f_2 verwendet den Matern Kernel mit dem Parameter $\nu = 0.5$.

In [ ]:

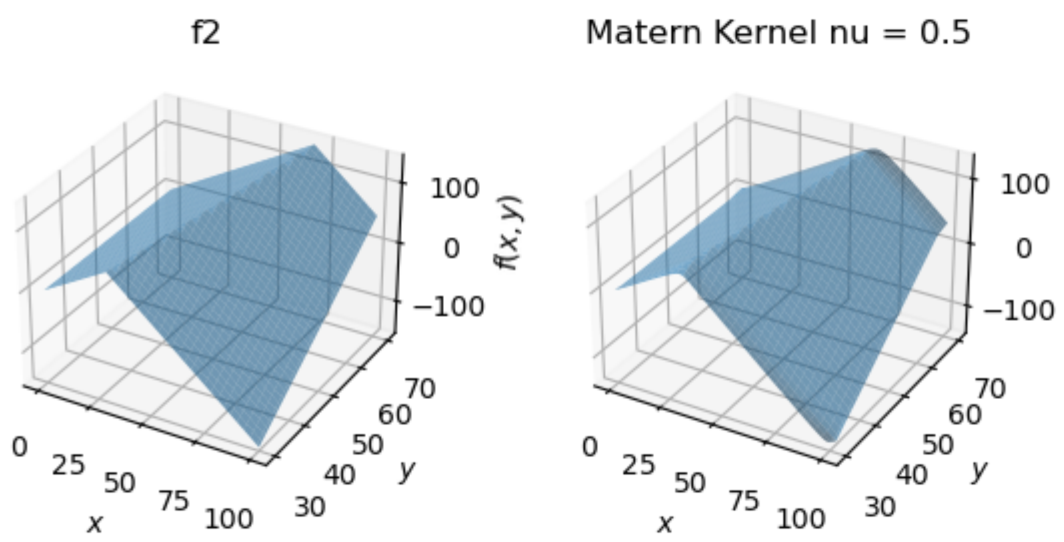
```
best_kriging_model = kriging_model_generator(np.array(list(zip(X.flatten(
                                             kernel=Matern, nu=0.5)
```

In [ ]:

```
preds = best_kriging_model(X_test)
abs_diff = np.abs(comp_vals.flatten() - preds)
mean_abs_diff = abs_diff.mean()
mean_sq_diff = (abs_diff**2).mean()
```

In [ ]:
```
fig = plt.figure()
ax1 = fig.add_subplot(121, projection='3d')
ax2 = fig.add_subplot(122, projection='3d')

ax1.set_title('f2')
ax1.set_xlabel('$x$')
ax1.set_ylabel('$y$')
ax1.set_zlabel('$f(x,y)$')
ax2.set_title('Matern Kernel nu = 0.5')
ax2.set_xlabel('$x$')
ax2.set_ylabel('$y$')
ax1.set_axisbelow(True)
ax2.set_axisbelow(True)
ax1.plot_surface(X_Achse, Y_Achse, comp_vals, alpha=0.6)
ax2.plot_surface(X_Achse, Y_Achse, best_kriging_model(X_test.reshape(-1,2
fig.tight_layout(pad=5)
```



In [ ]:
```
print(f'Kriging mit Matern Kernel mit nu = 0.5: \n')
print(f'mittlere absolute Abweichung: {mean_abs_diff : .2f}\t\tmittlere q
```

```
Kriging mit Matern Kernel mit nu = 0.5:

mittlere absolute Abweichung:  0.68		mittlere quadratische Abw
eichung: 5.33
```

Grafisch sieht die Funktionsannäherung durch Kriging recht gut aus. Allerdings ist eine durchschnittliche quadratische Abweichung von etwa 5.33 festzustellen. Kriging scheint die Funktion hier schlechter anzunähern als in (a).

(3) symbolische Regression

Ich verwende hier als Funktionsmenge $[sub, mul, min]$, da die Funktion f_2 aus genau diesen drei Funktion zusammengesetzt ist. In (a) hat sich für f_1 gezeigt, dass die beste Funktionsmenge genau aus den Funktionen bestand, die benötigt werden um f_1 rekonstruieren zu können. Daher nehme ich das selbe für f_2 an.

In [ ]:
```
func_set = ['sub', 'mul', 'min']
best_sym_reg = SymbolicRegressor(population_size=1000, tournament_size=10
                                 generations=50, stopping_criteria=0.0
                                 n_jobs=-1, function_set=func_set)
best_sym_reg.fit(np.array(list(zip(X.flatten(), Y.flatten()))), Z.flatten
```

Out[ ]:

▾ SymbolicRegressor

```
min(sub(sub(min(X0, X1), sub(X0, sub(min(X0, X1), sub(X0, sub(min
(X0, X1), sub(X0, min(X1, X0))))))), sub(mul(0.414, mul(mul(0.66
3, X0), sub(X0, X0))), min(X1, X0))), mul(X0, X1))
```

In [ ]:
```
print(best_sym_reg)
```

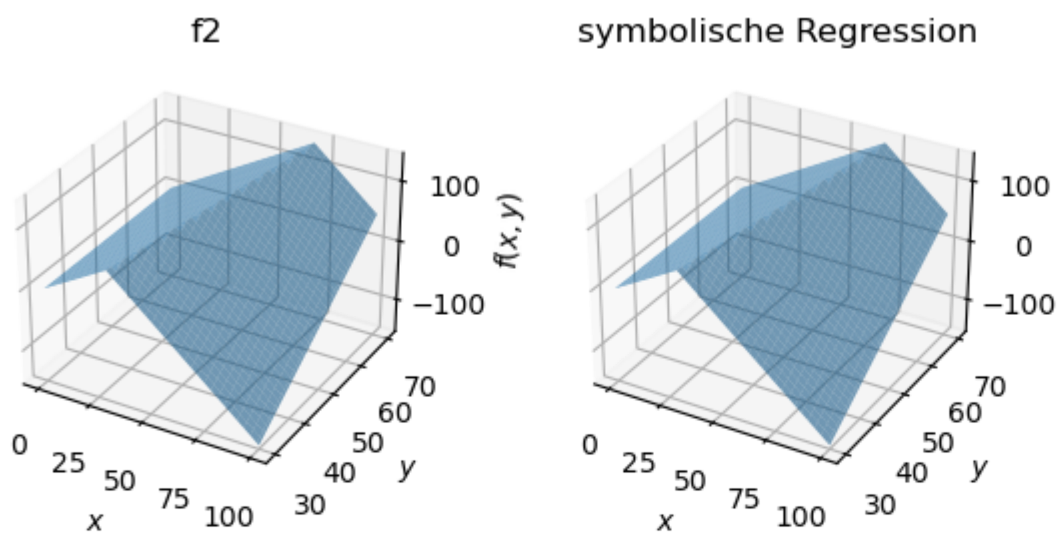
```
min(sub(sub(min(X0, X1), sub(X0, sub(min(X0, X1), sub(X0, sub(min(X0, X
1), sub(X0, min(X1, X0))))))), sub(mul(0.414, mul(mul(0.663, X0), sub(X0,
X0))), min(X1, X0))), mul(X0, X1))
```

In [ ]:
```
total_diff = np.abs(best_sym_reg.predict(X_test.reshape(-1, 2)) - comp_va

mean_absolute_diff = total_diff.mean()
mean_squared_diff  = (total_diff**2).mean()
```

In [ ]:
```
fig = plt.figure()
ax1 = fig.add_subplot(121, projection='3d')
ax2 = fig.add_subplot(122, projection='3d')

ax1.set_title('f2')
ax1.set_xlabel('$x$')
ax1.set_ylabel('$y$')
ax1.set_zlabel('$f(x,y)$')
ax2.set_title('symbolische Regression')
ax2.set_xlabel('$x$')
ax2.set_ylabel('$y$')
ax1.set_axisbelow(True)
ax2.set_axisbelow(True)
ax1.plot_surface(X_Achse, Y_Achse, comp_vals, alpha=0.6)
ax2.plot_surface(X_Achse, Y_Achse, best_sym_reg.predict(X_test.reshape(-1
fig.tight_layout(pad=5)
```



In [ ]:
```
print(f'Symbolische Regression mit population_size = 1000 und generations
print(f'mittlere absolute Abweichung: {mean_absolute_diff : .2f}\t\tmittl
```

```
Symbolische Regression mit population_size = 1000 und generations = 50:

mittlere absolute Abweichung:  0.00		mittlere quadratische Abw
eichung: 0.00
```

Die symbolische Regression mit der Funktionsmenge $[sub, mult, min]$ und einer population_size von 1000 und einer Anzahl von Generationen von 50 kann die Funktion f_2 nahezu perfekt simulieren.