In [ ]:
```
!pip install biopython
!pip install matplotlib
```

In [18]:
```
from Bio import Entrez, SeqIO
from Bio.Align import PairwiseAligner
from Bio import pairwise2
import numpy as np
import pandas as pd
import random
import matplotlib.pyplot as plt
```

1 Dalis

Iš paieškos sąrašo: https://www.ncbi.nlm.nih.gov/nuccore?term=33175%5BBioProject%5D+OR+33317%5BBioProject%5D sekų prieigos ID yra išsaugotos 'sequence.seq' faile. Iš failo pasirenkama dvidešimt 16S sekų ID.

In [50]:
```
NUMBER_OF_SEQUENCES = 20

sequence_ids = []
with open('sequence.seq') as f:
  sequence_ids = f.readlines()
  sequence_ids = sequence_ids[:NUMBER_OF_SEQUENCES]
```

Pagal ID sekos yra gaunamos fasta formatu.

In [ ]:
```
sequences = []
for seq_id in sequence_ids:
    handle = Entrez.efetch(db="nucleotide", id=seq_id, rettype="fasta", retmode="text")
    record = SeqIO.read(handle, "fasta")
    sequences.append(record)
```

Gaunami globalūs poriniai išlyginimai.

In [52]:
```
aligner = PairwiseAligner()
aligner.mode = 'global'
alignment_table = np.empty((20, 20),dtype='int')
for i in range(NUMBER_OF_SEQUENCES):
    for j in range(i, NUMBER_OF_SEQUENCES):
```

```
        alignment_score = aligner.score(sequences[i], sequences[j])
        alignment_table[i][j] = alignment_score
        alignment_table[j][i] = alignment_score
```

Sukuriama lentelė su sekų eilės numeriais ir atitinkamomis išlyginimo kainomis.

In [53]:
```
row_col_names = ["Seka " + str(i + 1) for i in range(NUMBER_OF_SEQUENCES)]
df = pd.DataFrame(alignment_table,index = row_col_names, columns=row_col_names)
```

Atspausdinama lentelė

In [54]:
```
print(df)
```

	Seka 1	Seka 2	Seka 3	Seka 4	Seka 5	Seka 6	Seka 7	Seka 8
Seka 1	1414	1159	1115	1125	1106	893	1148	1146
Seka 2	1159	1475	1228	1243	1209	963	1324	1360
Seka 3	1115	1228	1355	1222	1238	970	1233	1219
Seka 4	1125	1243	1222	1344	1225	987	1261	1240
Seka 5	1106	1209	1238	1225	1342	981	1238	1204
Seka 6	893	963	970	987	981	1045	1045	970
Seka 7	1148	1324	1233	1261	1238	1045	1466	1349
Seka 8	1146	1360	1219	1240	1204	970	1349	1485
Seka 9	1145	1359	1218	1239	1203	970	1349	1482
Seka 10	904	1037	978	960	969	944	1030	1049
Seka 11	907	1038	981	962	967	946	1033	1070
Seka 12	899	1031	973	953	958	937	1025	1061
Seka 13	1159	1348	1248	1267	1232	982	1364	1351
Seka 14	1141	1316	1230	1235	1203	964	1284	1293
Seka 15	1086	1171	1161	1168	1145	928	1165	1164
Seka 16	1162	1364	1229	1249	1215	968	1347	1361
Seka 17	1161	1361	1227	1247	1214	968	1345	1357
Seka 18	1167	1346	1252	1319	1264	994	1380	1352
Seka 19	1147	1316	1259	1263	1313	987	1353	1327
Seka 20	1142	1314	1256	1265	1314	986	1350	1323

	Seka 9	Seka 10	Seka 11	Seka 12	Seka 13	Seka 14	Seka 15
Seka 1	1145	904	907	899	1159	1141	1086
Seka 2	1359	1037	1038	1031	1348	1316	1171
Seka 3	1218	978	981	973	1248	1230	1161
Seka 4	1239	960	962	953	1267	1235	1168
Seka 5	1203	969	967	958	1232	1203	1145
Seka 6	970	944	946	937	982	964	928
Seka 7	1349	1030	1033	1025	1364	1284	1165
Seka 8	1482	1049	1070	1061	1351	1293	1164
Seka 9	1484	1048	1069	1060	1350	1292	1164
Seka 10	1048	1122	1051	1042	1037	993	919
Seka 11	1069	1051	1120	1109	1045	985	917
Seka 12	1060	1042	1109	1110	1040	978	907
Seka 13	1350	1037	1045	1040	1539	1306	1173
Seka 14	1292	993	985	978	1306	1442	1184
Seka 15	1164	919	917	907	1173	1184	1297
Seka 16	1360	1045	1047	1040	1353	1311	1180
Seka 17	1356	1045	1046	1039	1351	1309	1179
Seka 18	1351	1034	1041	1034	1425	1305	1165
Seka 19	1326	1024	1017	1010	1373	1281	1160
Seka 20	1322	1025	1019	1011	1377	1276	1157

	Seka 16	Seka 17	Seka 18	Seka 19	Seka 20

Seka 1	1162	1161	1167	1147	1142
Seka 2	1364	1361	1346	1316	1314
Seka 3	1229	1227	1252	1259	1256
Seka 4	1249	1247	1319	1263	1265
Seka 5	1215	1214	1264	1313	1314
Seka 6	968	968	994	987	986
Seka 7	1347	1345	1380	1353	1350
Seka 8	1361	1357	1352	1327	1323
Seka 9	1360	1356	1351	1326	1322
Seka 10	1045	1045	1034	1024	1025
Seka 11	1047	1046	1041	1017	1019
Seka 12	1040	1039	1034	1010	1011
Seka 13	1353	1351	1425	1373	1377
Seka 14	1311	1309	1305	1281	1276
Seka 15	1180	1179	1165	1160	1157
Seka 16	1496	1492	1362	1326	1325
Seka 17	1492	1494	1359	1323	1322
Seka 18	1362	1359	1500	1400	1402
Seka 19	1326	1323	1400	1500	1476
Seka 20	1325	1322	1402	1476	1500

2 Dalis

Užduočiai pasirinktas ***Halopiger xanaduensis*** archėjos genomas, kurio ID: NC_012654.1. Genomo seka atsisiunčiama.

In [ ]:
```
genome_id = "NC_012654.1"
handle = Entrez.efetch(db="nucleotide", id=genome_id, rettype="fasta", retmode="text")
genome = SeqIO.read(handle, "fasta")
```

In [57]:
```
genome_lenght = len(genome.seq)
T_lenght = 2000
print(genome_lenght)
```

```
270022
```

Iš genomo atsitiktinai iškerpamas 2000 bp ilgio fragmentas **T**.

In [46]:
```
cut_index = random.randint(0,genome_lenght - 2001)

T = genome[cut_index:cut_index + 2000]
genome_without_T = genome[:cut_index] + genome[cut_index + 2000:]
```

```
assert(len(genome) == len(T) + len(genome_without_T) and len(T) == 2000)
```

In [47]:
```
aligner = PairwiseAligner()
aligner.mode = 'local'
aligner.match_score = 1
aligner.mismatch_score = -1
aligner.gap_score = -2
```

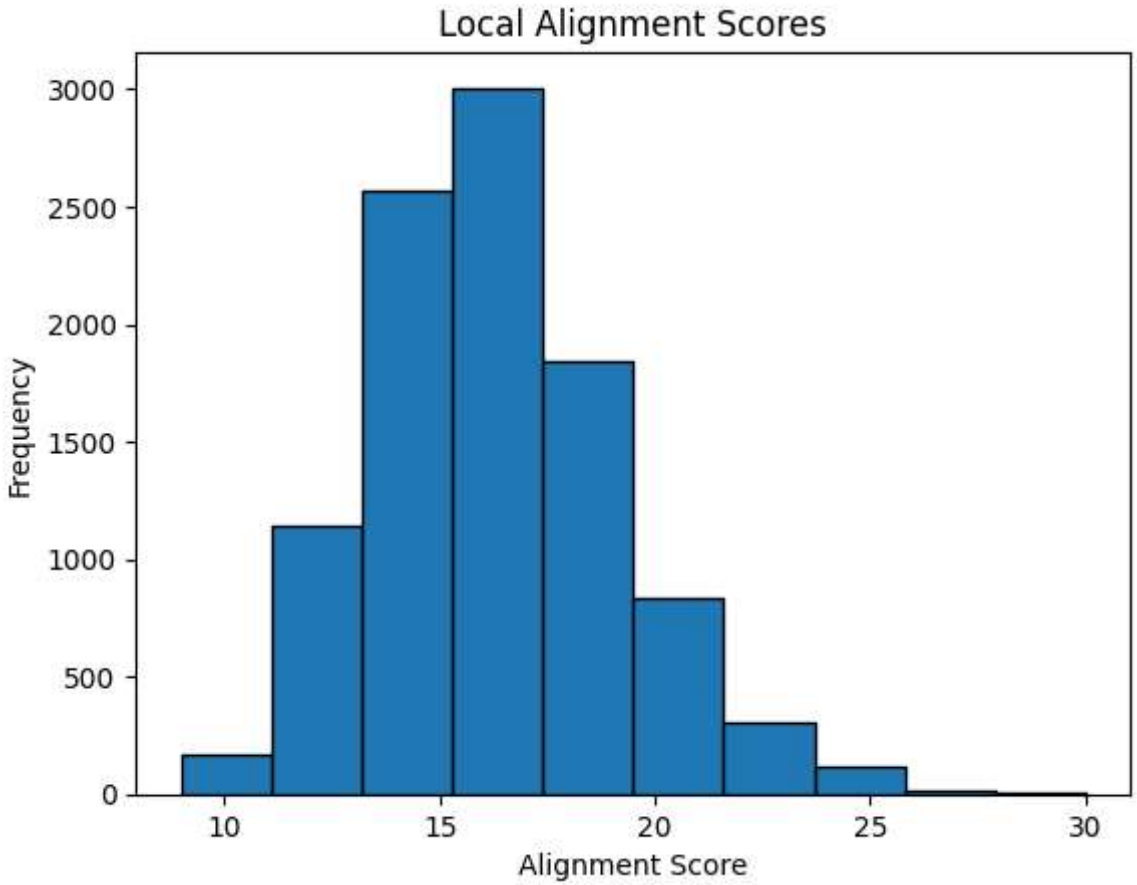
Iš likusio genomo 10_000 kartų atsitiktinai parenkami 100 bp fragmentai, ir atliekami lokalūs išlyginimai su **T**.

In [48]:
```
alignment_scores = np.empty((10000),dtype='int')
genome_without_T_lenght  = len(genome_without_T)

for i in range(10000):
  fragment_index = random.randint(0,genome_without_T_lenght - 101)
  fragment = genome_without_T[fragment_index:fragment_index + 100]
  alignment_scores[i] = aligner.score(fragment,T)
```

Pavaizduojama išlyginimų kainų histograma

In [49]:
```
plt.hist(alignment_scores, edgecolor='black')
plt.xlabel('Alignment Score')
plt.ylabel('Frequency')
plt.title('Local Alignment Scores')
plt.show()
```


Local Alignment Scores
Frequency
Alignment Score
0
500
1000
1500
2000
2500
3000
10
15
20
25
30