Hyperparameter-Tuned Estimation of Popcorn Kernel Popping Rates

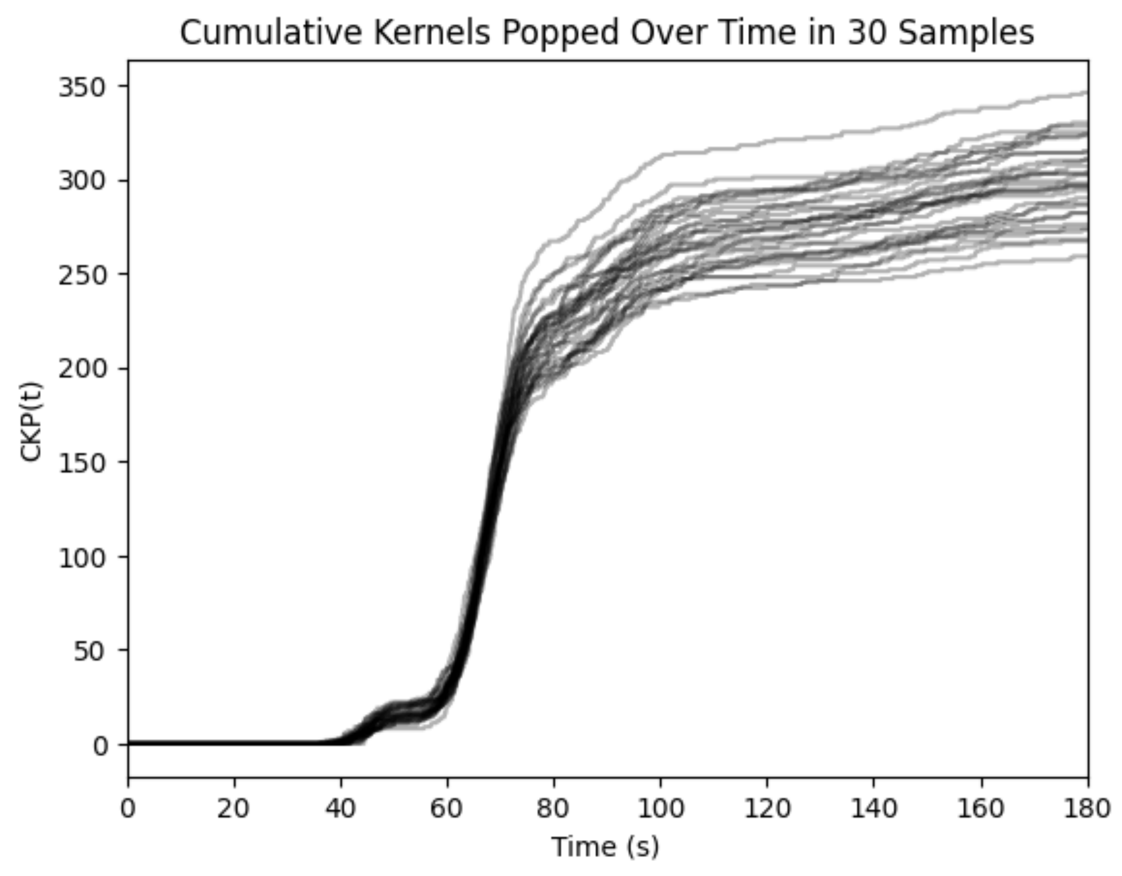
In [4]:
```
import pandas as pd
import numpy as np
seed = 42
df = pd.read_csv('./Data/popcorn_pops_custom.csv') # data is computer-generated by ChatGPT under the following assumptions:
    # most kernels pop between 60-75 seconds
    ## some pop earlier ~30-60 seconds
    ### some pop late ~75-120 seconds
df['pop_time_seconds'] = df['pop_time_seconds'].apply(lambda x: np.random.normal(150,20) if x < 20 else x) # Replace popping times <20 with > 120
df['trial'] = df['trial'] + 1
```

In [ ]:
```
import random
random.seed(42)

# 3:1 train/test split
sample = random.sample(range(1, 40), 30)
train = pd.DataFrame()
for trial in sample:
    trial = df[df['trial'] == trial]
    train = pd.concat([train,trial])

test = pd.DataFrame()
for i in range(max(df['trial'])):
    if i not in sample:
        trial = df[df['trial'] == i ]
        test = pd.concat([test,trial])
```

In [140…
```
# CDF of Popped Kernels for Training Set
time = np.arange(0, 180.01, 0.01)
pops = np.zeros((len(sample), len(time)))

for i, trial in enumerate(sample):
    pop_times = df[df['trial'] == trial]['pop_time_seconds'].values
    # Sort pop times for cumulative counting
    pop_times = np.sort(pop_times)

    # Count how many pop times are ≤ each time point
    pops[i] = np.searchsorted(pop_times, time, side='right')
```

Out[140…
```
array([[  0.,   0.,   0., ..., 276., 276., 276.],
       [  0.,   0.,   0., ..., 282., 282., 282.],
       [  0.,   0.,   0., ..., 330., 330., 330.],
       ...,
       [  0.,   0.,   0., ..., 259., 259., 259.],
       [  0.,   0.,   0., ..., 346., 346., 346.],
       [  0.,   0.,   0., ..., 290., 290., 290.]], shape=(30, 18001))
```

In [190…
```
## Discrete Cumulative Disitrubtion Function (CDF) of Popped Kernels
import matplotlib.pyplot as plt
from matplotlib.lines import Line2D
for i in range(len(pops)):
    plt.plot(time, pops[i], alpha = 0.3, color = "black")
plt.xlabel("Time (s)")
plt.ylabel("CKP(t)")
plt.xlim(0,180)
plt.title("Cumulative Kernels Popped Over Time in 30 Samples")
plt.show()
```



Now that we've split our data into a 3:1 training/test, we'll tune a spline model onto our training data, adjusting the smoothness hyperparameter s. Within the training set, leave-one-out cross validation (LOOCV) across trials in our training set. Once we've constructed and validated our spline model, we'll use it to predict exit times for kernel popping.

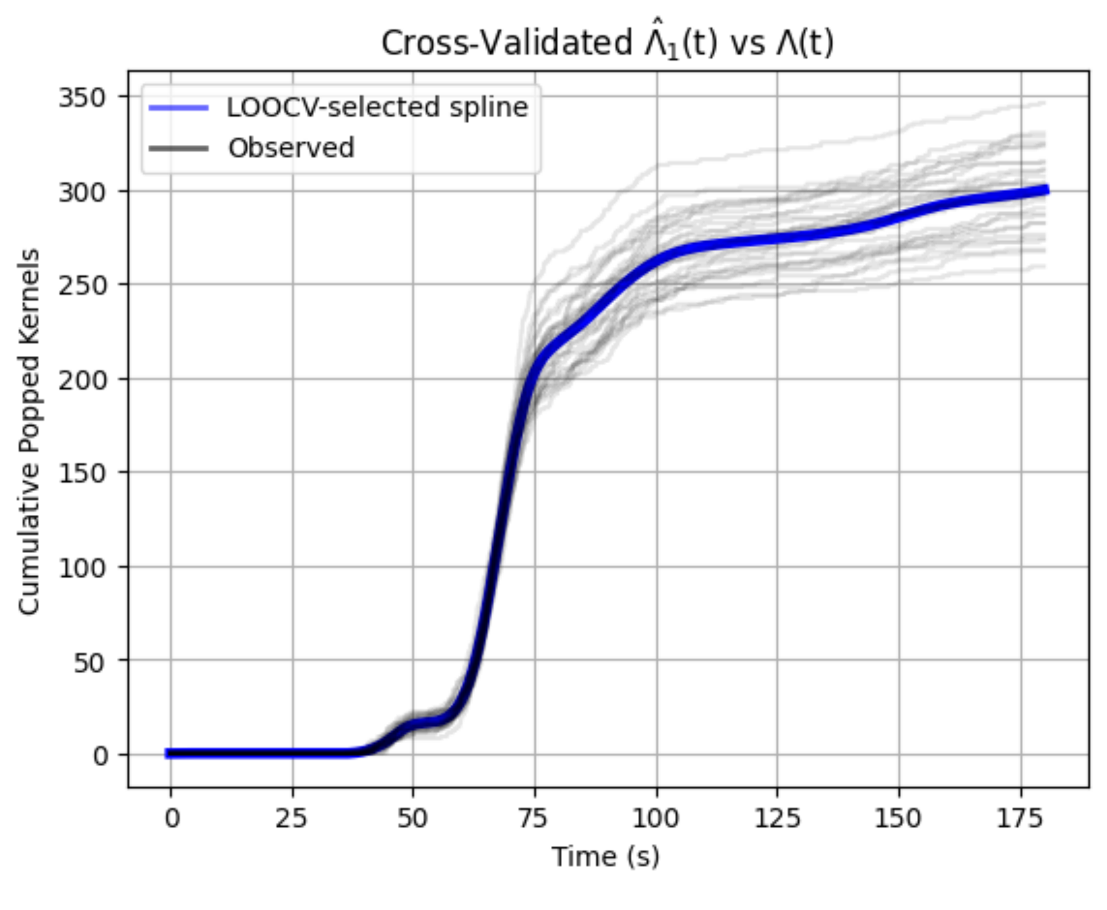
In [177…
```
import statsmodels.api as sm
from scipy.stats import t
import scipy.stats as stats
from itertools import combinations
from scipy.interpolate import UnivariateSpline
from sklearn.metrics import mean_squared_error
from tqdm import tqdm
```

In [178…
```
# non-parametric regression on cumulative counts using one smoothing spline
# Hyperparameter tuning on smoothness s across each trial's CDF
# executable: train_spline_model.py stored in ./Model/spline_model.pkl
    # n_trials, n_timepoints = pops.shape
    # s_grid = np.logspace(-1, 4, 20)  # try a range of smoothing factors
    # errors = []

    # for s in tqdm(s_grid):
    #     fold_mse = []

    #     for i in range(n_trials):
    #         # Leave-one-out split
    #         train_cdfs = np.delete(pops, i, axis=0)
    #         val_cdf = pops[i]

    #         # Fit spline on mean of training trials
    #         y_train_mean = np.mean(train_cdfs, axis=0)
    #         spline = UnivariateSpline(time, y_train_mean, s=s)

    #         # Evaluate on validation trial
    #         y_pred = spline(time)
    #         mse = mean_squared_error(val_cdf, y_pred)
    #         fold_mse.append(mse)

    #     errors.append(np.mean(fold_mse))

    # best_s = s_grid[np.argmin(errors)]
    # print(f"Optimal smoothing factor: {best_s:.4f}")
```

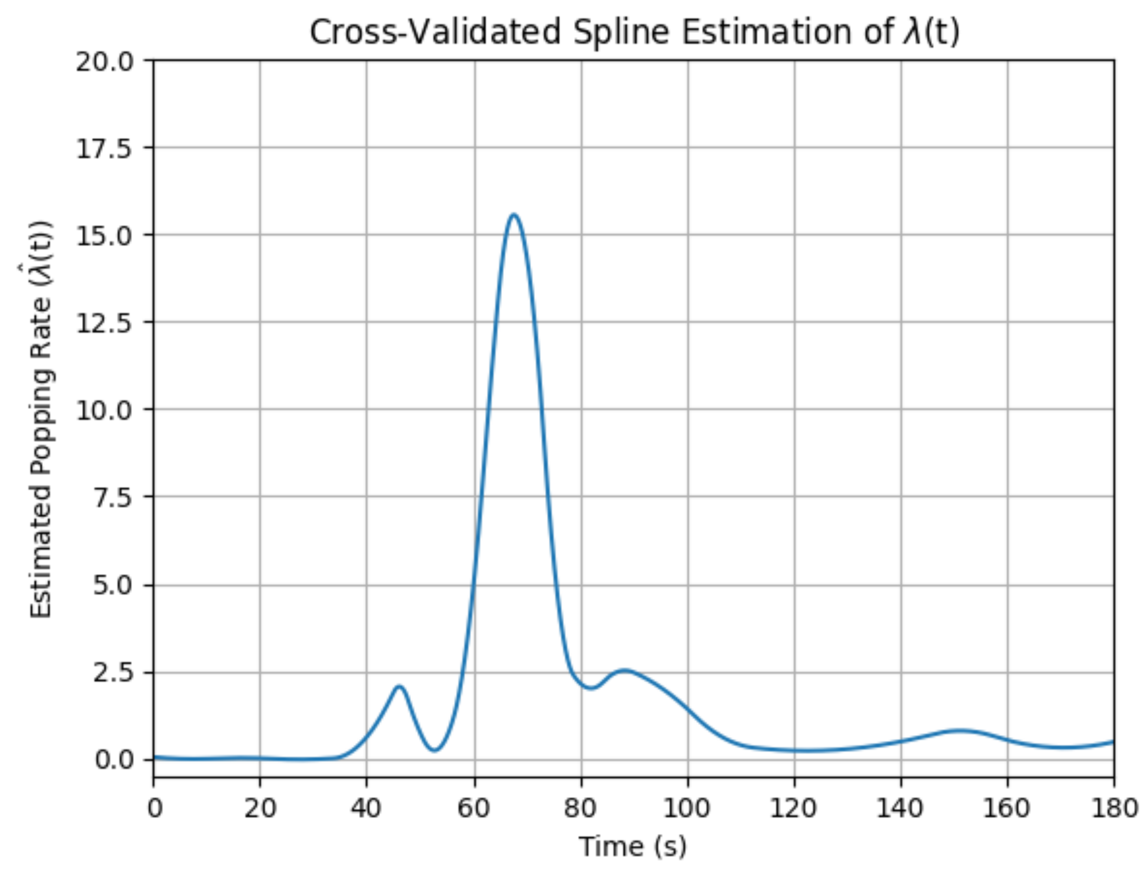
```
100%|██████████| 20/20 [14:16<00:00, 42.80s/it]
Optimal smoothing factor: 885.8668
```

In [209…
```
import joblib

# Load model
spline_model = joblib.load("./Model/spline_model.pkl")

# Predict CDF of Kernels Popped
time = np.arange(0, 180.01, 0.01)

# Plot LOOCV-selected spline
plt.plot(time, spline_model(time), 'k', linewidth=4, color = "blue")

# Plot a few sample trial CDFs
for i in range(len(pops)):
    plt.plot(time, pops[i], alpha = 0.1, color = "black")

custom_lines = [
    Line2D([0], [0], color='blue', lw=2, label="LOOCV-selected spline", alpha = 0.6),
    Line2D([0], [0], color='black', lw=2, label="Observed", alpha = 0.6)
]

plt.title(r'Cross-Validated $\hat{\Lambda}_{1}$(t) vs $\Lambda$(t)')
plt.xlabel("Time (s)")
plt.ylabel("Cumulative Popped Kernels")
plt.legend(handles = custom_lines)
plt.grid(True)
plt.show()
```

```
/var/folders/jc/b9r1lwld74jfg3kzdjjk6_gc0000gn/T/ipykernel_33385/2880084744.py:10: UserWarning: color is redundantly defined by the 'color' keyword arg
ument and the fmt string "k" (-> color=(0.0, 0.0, 0.0, 1)). The keyword argument will take precedence.
  plt.plot(time, spline_model(time), 'k', linewidth=4, color = "blue")
```



In [207…
```
# estimation of lambda(t) via non-parametric regression using LOOCV-spline model
Lambda_hat = spline_model(time)
lambda_hat = spline_model.derivative()(time) # differentiate Lambda(t) to get lambda(t)

plt.plot(time, lambda_hat, label=r'$\hat{\lambda}(t)$')
plt.xlabel("Time (s)")
plt.ylabel(r"Estimated Popping Rate ($\hat{\lambda}$(t))")
plt.title(r"Cross-Validated Spline Estimation of $\lambda$(t)")
plt.grid()
plt.xlim(0,180)
plt.ylim(-0.5,20)
plt.show()
```



From here, we can use this model and cross-validate on the remaining test data to see if we can accurately predict when to stop waiting for popcorn by minimizing residual unpopped kernels and burnt popcorn.