## Introduction

Forecasting demand is important in many practial applications including food, retail, energy and finance. The goal of this project is to predict how many food items (num_orders) will be ordered from different distribution centers (center_id) serving different types of meals (meal_id). The objective is to predict the number of orders (num_orders) for the next 10 time-steps (week 146 to 155) minimizing the total root-mean-squared-error (RMSE). Thanks to Analytics Vidhya for providing this dataset. More information can be found here: https://datahack.analyticsvidhya.com/contest/genpact-machine-learning-hackathon-1/

Gradient boosting machine (LightGBM: https://lightgbm.readthedocs.io/en/stable/Python-Intro.html) was used. Various aspects including: exploratory data analysis, visualization, feature engineering, feature importance/selection and hyperparameter optimization relevant to time-series forecasting with LightGBM are presented. The RMSE obtained for the submitted answers was 50.8 which ranks 88 out of 1861 submissions (on 2024-05-23): https://datahack.analyticsvidhya.com/contest/genpact-machine-learning-hackathon-1/#LeaderBoard

```
In [32]: import sys
         import numpy as np
         import pandas as pd
         import ml_vis_eda
         from matplotlib import pyplot as plt
         import matplotlib as mpl
         import os
         import pickle
         import lightgbm as lgb
         pd.set_option('display.max_columns', None)  # displays all columns (wrap-
```

```
In [33]: # files needed for this dataset
         df_name = 'foodDemand_train/train.csv'  # training data filename
         df_test_name = 'foodDemand_train/food_Demand_test.csv'  # features for th
         df_sample_name = 'foodDemand_train/sample_submission.csv'  # example (fea
         df_predictions_name = 'foodDemand_train/kaggle_submission.csv'  # final s
         Additional_merge_dfs = {'foodDemand_train/fulfilment_center_info.csv': 'c
```

**run_mode** variable is used to validate the entire code right from the start.

Normally to submit predictions with **run_mode=0**, the code runs on the entire train data file (weeks 1 to 145) and makes forecasts using the test file (weeks 146 to 155).

Alternatively, with **run_mode=1**, the train file is separated into a new train file (weeks 1 to 135) and new test file (weeks 136 to 145). Then using **run_mode=2**, the code can run on the new files end-to-end to evaluate the quality of the forecasts.

```
In [34]: run_mode = 0  # How to run this program
         # run_mode = 0: Use base file-names above and write final predictions for
         # run_mode = 1: use base file-names above and write new files for validat
         # run_mode = 2: use new files (from run_mode=1) and run end-to-end, then
         test_time = None  # for run_mode=1 only: number of time-steps to use for
         file_name_ext = '_virtual'  # string to append to validateion base filena
```

Variables for plotting and algorithms used are provided. Confidence intervals are determined using quantile regression (quantile_alphas):

```
In [35]: algorithms = ['mean value', 'LightGBM']
         default_algorithm = 'LightGBM'
         plot_ts = 5 # number of individual time-series with targets, predictions
         lgb_model_str = 'lightGBM_opt_pickles/lgb_model'  # prefix for data/model
         quantile_alphas = [0.05, 0.5, 0.95]  # predict quantiles for the predicti
```

Variable names (depend on the dataset). Categorical variables have more than two categories.

```
In [38]: target_feature = 'num_orders'  # this is what we will fit and predict
         categorical_features = ['center_id', 'meal_id', 'category', 'cuisine', 'c
         t_var = 'week'  # unit of 'time' (the column name in df)
         id_var = 'id'  # common column to identify submission data and training d
         unique_cols = ['center_id', 'meal_id']  # required columns to identify ti
         quantile_alphas = [0.05, 0.5, 0.95]  # predict quantiles for the predicti
```

The target variable **num_orders** is a non-negative integer (count-like), and therefore *poisson* loss function is used for the objective. This fits the data better than using least squares or RMSE (L2) loss for regression. Note that during validation, the *number of boosters* (**early_stopping_round**) is determined by L2 loss since **first_metric_only: True**, as the goal of the project is to minimize L2 for the predictions.

```
In [39]: nfold = 5  # number of cross-validation folds
         use_important_features = 4  # start with this many current features
         param_vals = {'num_leaves':None, 'learning_rate':0.05, 'max_depth':None,
                 'metric':['l2', 'poisson'], 'early_stopping_round':1000, 'num_ite
                 'min_split_gain': 0., 'min_child_weight': 1e-3, 'reg_alpha': 0.,
                 'subsample': 1.0, 'subsample_freq': 10, 'boosting_type': 'gbdt',
```

Below are the sequence of steps including: feature importances/relevance, feature engineering, hyperparameter optimization, and saving results. Each step depends on the previous one. It is good practice to check the results, accuracy and performance after each step before proceeding to the next. The file **data_and_scripts**/ **lightgbm_order_forecasting.py** in the project directory gives more details for each step including running lightGBM https://github.com/microsoft/LightGBM. Edit each step as necessary before running and check results after running it. Set the step you are working on to 'True' to run and test the results of that step.

For demonstration and simplicity, these steps are skipped, instead perform some exploratory data analysis, load the final model results and view them.

```python
In [40]: find_relevant_raw_features = False  # find relevant raw features
         find_relevant_eng_features = False  # feature engineering / find relevant
         do_recurrent_opt = False  # do recurrent feature selection if files do no
         do_recurrent_opt_force = False  # always overwrite existing files
         write_new_model = False  # this creates the final model with the recurren
         write_new_data = False  # this runs the final model to generate the data

         # optional parameters or hyperparameter optimization in some of the above
         find_recurrent_features = True  # feature engineering: temporally lagged
         use_average_target_properties = False  # use temporal average statistics
         do_lr_opt = False  # optimize learning rate for gradient boosting
         do_pars_opt = False  # optimize hyperparameters for gradient boosting
         test_recurrent = True  # check if recurrent features improve test and CV
```

Load the raw data file and tabulate some statistics.

```python
In [41]: # functions to create new file-names for end-to-end testing predictions (
         def new_file_name(fname: str, ext_in: str, ext_out: str) -> str:
             return fname.split(ext_in)[0] + ext_out + ext_in
         def new_file_names(fnames: 'list(str)', ext_in: str, ext_out: str) -> 'li
             return [new_file_name(fname, ext_in, ext_out) for fname in fnames]
         if run_mode == 2:  # get virtual file names to read
             df_name, df_test_name, df_sample_name = new_file_names(
                 [df_name, df_test_name, df_sample_name], '.csv', file_name_ext)

         # read in the data
         df = ml_vis_eda.pd_read_csv_stats_describe(df_name)
```

```
foodDemand_train/train.csv - data in first 10 rows
        id  week  center_id  meal_id  checkout_price  base_price  \
0  1379560     1         55     1885          136.83      152.29
1  1466964     1         55     1993          136.83      135.83
2  1346989     1         55     2539          134.86      135.86
3  1338232     1         55     2139          339.50      437.53
4  1448490     1         55     2631          243.50      242.50
5  1270037     1         55     1248          251.23      252.23
6  1191377     1         55     1778          183.36      184.36
7  1499955     1         55     1062          182.36      183.36
8  1025244     1         55     2707          193.06      192.06
9  1054194     1         55     1207          325.92      384.18


   emailer_for_promotion  homepage_featured  num_orders
0                      0                  0         177
1                      0                  0         270
2                      0                  0         189
3                      0                  0          54
4                      0                  0          40
5                      0                  0          28
6                      0                  0         190
7                      0                  0         391
8                      0                  0         472
9                      0                  1         676


foodDemand_train/train.csv - summary of column statistics
                          count          mean             std          min
\
id                     456548.0  1.250096e+06  144354.822378  1000000.00
week                   456548.0  7.476877e+01      41.524956        1.00
center_id              456548.0  8.210580e+01      45.975046       10.00
meal_id                456548.0  2.024337e+03     547.420920     1062.00
checkout_price         456548.0  3.322389e+02     152.939723        2.97
base_price             456548.0  3.541566e+02     160.715914       55.35
emailer_for_promotion  456548.0  8.115247e-02       0.273069        0.00
homepage_featured      456548.0  1.091999e-01       0.311890        0.00
num_orders             456548.0  2.618728e+02     395.922798       13.00


                             25%         50%         75%         max  \
id                     1124998.75  1250183.50  1375140.25  1499999.00
week                         39.00       76.00      111.00      145.00
center_id                    43.00       76.00      110.00      186.00
meal_id                    1558.00     1993.00     2539.00     2956.00
checkout_price              228.95      296.82      445.23      866.27
base_price                  243.50      310.46      458.87      866.27
emailer_for_promotion         0.00        0.00        0.00        1.00
homepage_featured             0.00        0.00        0.00        1.00
num_orders                   54.00      136.00      324.00    24299.00


                       zero count  nan count  unique count
id                              0          0        456548
week                            0          0           145
center_id                       0          0            77
meal_id                         0          0            51
checkout_price                  0          0          1992
base_price                      0          0          1907
emailer_for_promotion      419498          0             2
homepage_featured          406693          0             2
num_orders                      0          0          1250
```

```
foodDemand_train/train.csv - correlation matrix (numeric columns only)
                        id  week  center_id  meal_id  checkout_price  \
id                     1.0  0.00       0.00     0.00            0.00
week                   0.0  1.00      -0.00     0.02            0.03
center_id              0.0 -0.00       1.00     0.01            0.00
meal_id                0.0  0.02       0.01     1.00            0.01
checkout_price         0.0  0.03       0.00     0.01            1.00
base_price             0.0  0.03       0.00     0.00            0.95
emailer_for_promotion  0.0 -0.00       0.01     0.01            0.00
homepage_featured      0.0 -0.01      -0.01     0.02           -0.06
num_orders             0.0 -0.02      -0.05     0.01           -0.28

                       base_price  emailer_for_promotion  homepage_feature
d  \
id                           0.00                   0.00               0.0
0
week                         0.03                  -0.00              -0.0
1
center_id                    0.00                   0.01              -0.0
1
meal_id                      0.00                   0.01               0.0
2
checkout_price               0.95                   0.00              -0.0
6
base_price                   1.00                   0.17               0.0
6
emailer_for_promotion        0.17                   1.00               0.3
9
homepage_featured            0.06                   0.39               1.0
0
num_orders                  -0.22                   0.28               0.2
9

                       num_orders
id                           0.00
week                        -0.02
center_id                   -0.05
meal_id                      0.01
checkout_price              -0.28
base_price                  -0.22
emailer_for_promotion        0.28
homepage_featured            0.29
num_orders                   1.00
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 456548 entries, 0 to 456547
Data columns (total 9 columns):
 #   Column                 Non-Null Count   Dtype
---  ------                 --------------   -----
 0   id                     456548 non-null  int64
 1   week                   456548 non-null  int64
 2   center_id              456548 non-null  int64
 3   meal_id                456548 non-null  int64
 4   checkout_price         456548 non-null  float64
 5   base_price             456548 non-null  float64
 6   emailer_for_promotion  456548 non-null  int64
 7   homepage_featured      456548 non-null  int64
 8   num_orders             456548 non-null  int64
dtypes: float64(2), int64(7)
memory usage: 31.3 MB
```

None

Supporting needed files are loaded and prepared.

```
In [42]:  df_test = pd.read_csv(df_test_name)
          df_sample = pd.read_csv(df_sample_name)
          df_predictions = df_sample.copy()
          df_predictions[target_feature] = np.nan  # to make sure all get filled in
          assert all(df_test[id_var].sort_values() == df_sample[id_var].sort_values
          assert df_test[t_var].min() > df[t_var].max() # check that the data to pr
          if run_mode == 2:
              lgb_model_str = lgb_model_str + file_name_ext
```

For **run_mode=1**, new csv files are written and then program is terminated. Then restart
program with **run_mode=2** for testing forecasts end-to-end.

```
In [43]:  if run_mode == 1: # overwrite df and df_test data to test the whole code
              end_time = df[t_var].max()  # last valid sample for testing
              if test_time_len is None:
                  test_time_len = df_test[t_var].max() - end_time
              test_time = end_time - test_time_len
              # modify the dataframes
              df_test = df[df[t_var] > test_time]
              df_sample = df_test[[id_var, target_feature]]
              df = df[df[t_var] <= test_time]
              df_name, df_test_name, df_sample_name = new_file_names(
                  [df_name, df_test_name, df_sample_name], '.csv', file_name_ext)
              # write the modified csvs
              df.to_csv(df_name, index=False)
              df_test[target_feature] = np.nan
              df_test.to_csv(df_test_name, index=False)
              df_sample.to_csv(df_sample_name, index=False)
              sys.exit(f'Files written: {df_name}, {df_test_name}, {df_sample_name}
```

Set up the time intervals that define the training/validation, test and prediction data.

```
In [44]:  start_time = df[t_var].min()  # first sample
          end_time = df_test[t_var].max()  # last sample to predict
          test_time = df[t_var].max()  # last valid sample
          tstep = end_time - test_time
          df = pd.concat((df, df_test), axis=0)  # avoids errors later if manipulat
          train_time = test_time - tstep
```

Plot histograms for all features.

```
In [45]:  ml_vis_eda.plot_multiple(df.values, df.columns, targets=df[target_feature
                  nbins=40, no_data=np.nan, range_targets=[0., 1500.], cmap=None)
```
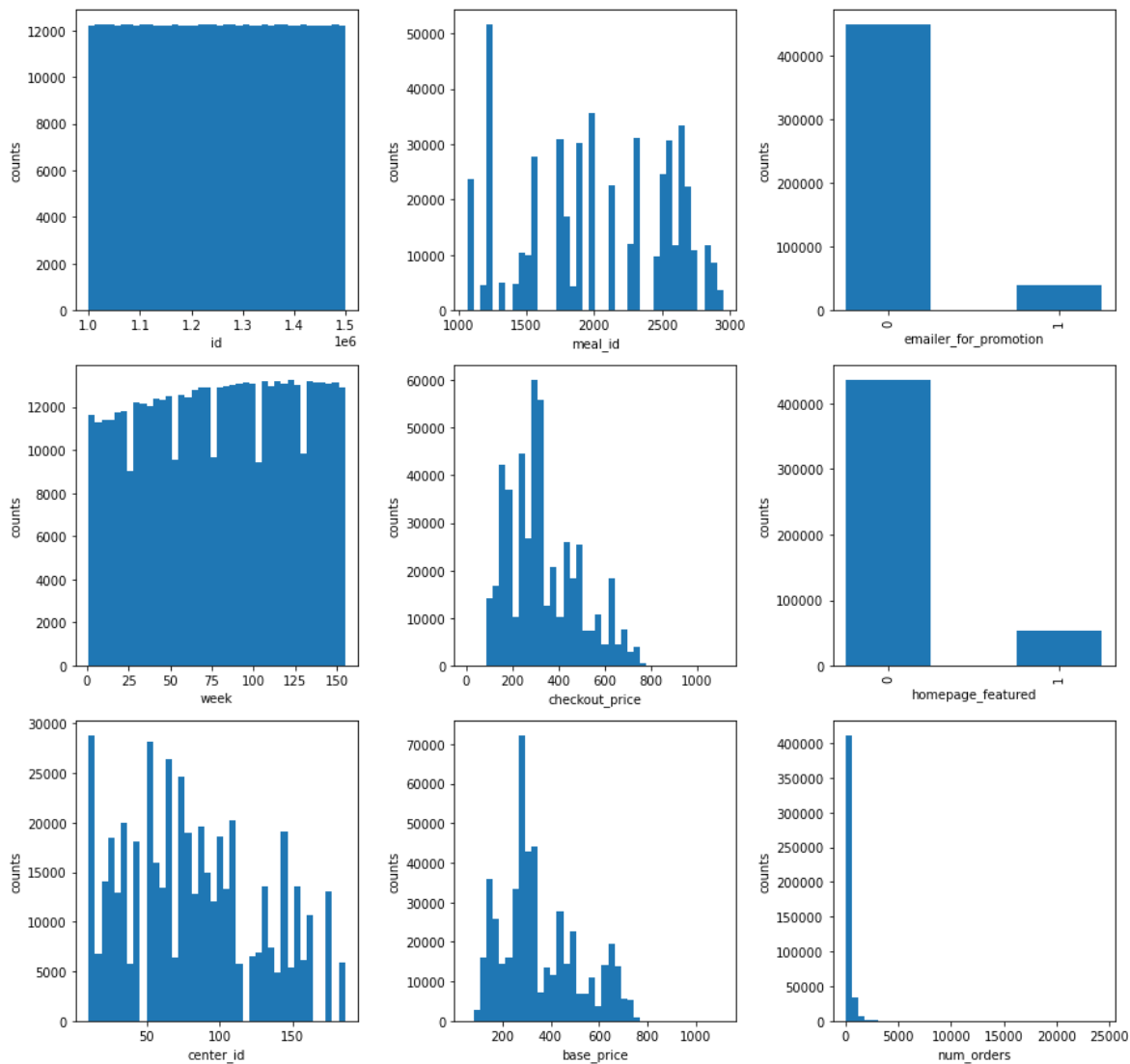
Merge the columns from all datasets to verify if there is additional information that can improve the model's accuracy.

```
In [46]:  for merge_df, merge_col in Additional_merge_dfs.items():
              df_to_merge = ml_vis_eda.pd_read_csv_stats_describe(merge_df)
              df = df.merge(df_to_merge, on=merge_col)
```

```
foodDemand_train/fulfilment_center_info.csv - data in first 10 rows
   center_id  city_code  region_code center_type  op_area
0         11        679           56      TYPE_A      3.7
1         13        590           56      TYPE_B      6.7
2        124        590           56      TYPE_C      4.0
3         66        648           34      TYPE_A      4.1
4         94        632           34      TYPE_C      3.6
5         64        553           77      TYPE_A      4.4
6        129        593           77      TYPE_A      3.9
7        139        693           34      TYPE_C      2.8
8         88        526           34      TYPE_A      4.1
9        143        562           77      TYPE_B      3.8


foodDemand_train/fulfilment_center_info.csv - summary of column statistics
             count unique     top freq        mean        std    min    25%
\
center_id     77.0    NaN     NaN  NaN   83.142857  46.090219   10.0   50.0
city_code     77.0    NaN     NaN  NaN  600.662338  66.720274  456.0  553.0
region_code   77.0    NaN     NaN  NaN   56.493506  18.126473   23.0   34.0
center_type     77      3  TYPE_A   43         NaN        NaN    NaN    NaN
op_area       77.0    NaN     NaN  NaN    3.985714   1.106406    0.9    3.5

              50%    75%    max  zero count  nan count  unique count
center_id    77.0  110.0  186.0           0          0            77
city_code   596.0  651.0  713.0           0          0            51
region_code  56.0   77.0   93.0           0          0             8
center_type   NaN    NaN    NaN           0          0             3
op_area       3.9    4.4    7.0           0          0            30


foodDemand_train/fulfilment_center_info.csv - correlation matrix (numeric
columns only)
             center_id  city_code  region_code  op_area
center_id         1.00       0.07        -0.02    -0.11
city_code         0.07       1.00         0.03     0.13
region_code      -0.02       0.03         1.00     0.03
op_area          -0.11       0.13         0.03     1.00
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 77 entries, 0 to 76
Data columns (total 5 columns):
 #   Column       Non-Null Count  Dtype
---  ------       --------------  -----
 0   center_id    77 non-null     int64
 1   city_code    77 non-null     int64
 2   region_code  77 non-null     int64
 3   center_type  77 non-null     object
 4   op_area      77 non-null     float64
dtypes: float64(1), int64(3), object(1)
memory usage: 3.1+ KB
None


foodDemand_train/meal_info.csv - data in first 10 rows
   meal_id   category  cuisine
0     1885  Beverages     Thai
1     1993  Beverages     Thai
2     2539  Beverages     Thai
3     1248  Beverages   Indian
4     2631  Beverages   Indian
5     1311     Extras     Thai
6     1062  Beverages  Italian
```

```
7     1778  Beverages   Italian
8     1803    Extras      Thai
9     1198    Extras      Thai

foodDemand_train/meal_info.csv - summary of column statistics
          count unique       top freq       mean         std     min  \
meal_id    51.0    NaN       NaN  NaN  2013.921569  553.633555  1062.0
category     51     14  Beverages   12          NaN         NaN     NaN
cuisine      51      4      Thai   15          NaN         NaN     NaN


             25%     50%     75%     max  zero count  nan count  unique co
unt
meal_id   1550.5  1971.0  2516.5  2956.0           0          0
51
category     NaN     NaN     NaN     NaN           0          0
14
cuisine      NaN     NaN     NaN     NaN           0          0
4


foodDemand_train/meal_info.csv - correlation matrix (numeric columns only)
         meal_id
meal_id      1.0
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 51 entries, 0 to 50
Data columns (total 3 columns):
 #   Column    Non-Null Count  Dtype
---  ------    --------------  -----
 0   meal_id   51 non-null     int64
 1   category  51 non-null     object
 2   cuisine   51 non-null     object
dtypes: int64(1), object(2)
memory usage: 1.3+ KB
None
```

Move the target column to the end of the dataframe.

In [47]:
```python
df_targets = df.pop(target_feature)
df = df.join(df_targets)
df.head()
```

Out[47]:

|   | id | week | center_id | meal_id | checkout_price | base_price | emailer_for_promot |
|---|---------|------|-----------|---------|----------------|------------|--------------------|
| 0 | 1379560 | 1 | 55 | 1885 | 136.83 | 152.29 | |
| 1 | 1018704 | 2 | 55 | 1885 | 135.83 | 152.29 | |
| 2 | 1196273 | 3 | 55 | 1885 | 132.92 | 133.92 | |
| 3 | 1116527 | 4 | 55 | 1885 | 135.86 | 134.86 | |
| 4 | 1343872 | 5 | 55 | 1885 | 146.50 | 147.50 | |

Sort the data such that adjacent rows represent the same time-series location with increasing time.

In [48]:
```python
df = df.sort_values(by=[*tuple(unique_cols), t_var])
```

**apply_unique_ts_map** identifies rows in the pandas dataframe **df** that correspond to individual time series. This is used later for time series plotting.

In [49]:
```python
def apply_unique_ts_map(dvalues, tvalues, train_time, test_time):
    """
    identify individual time-series
    return row index indicators (start, end train set, end test set, end

    :param dvalues: (int numpy array) shape = (nrows, *) each row uniquel
    :param tvalues: (int numpy array) shape = (nrows,) each row represent
    :param train_time: (int) latest time for training data
    :param test_time: (int) latest time for test data

    return
        ts_inds_inv: [list] of size==(num_rows,) time-series index each r
        ts_inds: [int numpy array] shape=(num_ts, 4), for each time-serie
            start time, end train time, end test time, end time
    """
    nrows = dvalues.shape[0]
    ts_inds_inv = np.zeros((nrows,), dtype=int)
    last_cur = tuple(dvalues[0])
    ts_inds = [[0] * 4]
    cur_ts = 0
    def get_t_status(tvalue):
        if tvalue > test_time:
            return 2
        elif tvalue > train_time:
            return 1
        return 0
    for ind in range(nrows):
        cur = tuple(dvalues[ind])
        tvalue = tvalues[ind]
        ts_status = get_t_status(tvalue)
        if cur != last_cur:
            ts_inds[-1][3] = ind
            ts_inds.append([ind] * 4)
            cur_ts += 1
            last_cur = cur
        ts_inds[-1][ts_status+1:] = [ind+1] * (3-ts_status)
        ts_inds_inv[ind] = cur_ts
    return np.array(ts_inds), ts_inds_inv,
ts_inds, ts_inds_inv = apply_unique_ts_map(df[unique_cols].values, df[t_v
num_ts = ts_inds.shape[0]  # the number of timeseries in the dataframe
print(f'number of time series: {num_ts}')
```

number of time series: 3600

Convert all category objects to natural number values for simpler computational logic, e.g. [0, 1, 2, ..., C]

In [50]:
```python
def apply_unique_cats(df, categorical_features):
    """
    Convert a Pandas dataframe's categorical features to non-negative int

    :param df: [pandas.core.frame.DataFrame] shape = (num_rows, num_colum
    :param categorical_features: [list of str] features to modify
    return
        df_copy: [pandas.core.frame.DataFrame] shape = (num_rows, num_col
            copy of input df with non-negative integer labeling for all c
        cat_codes: [dict] keys gives each feature as str, values are orig
    """
    cat_codes = {}
    df_copy = df.copy()
    for cat_feature in categorical_features:
        df_copy[cat_feature], cat_values = df_copy[cat_feature].factorize
        cat_codes[cat_feature] = cat_values
    return df_copy, cat_codes
df_copy, cat_codes = apply_unique_cats(df, categorical_features)
# this is the one-to-one mapping for categorical features between df and
print(cat_codes)
```

```
{'center_id': Int64Index([ 10,  11,  13,  14,  17,  20,  23,  24,  26,  27
,  29,  30,  32,
             34,  36,  39,  41,  42,  43,  50,  51,  52,  53,  55,  57,  5
8,
             59,  61,  64,  65,  66,  67,  68,  72,  73,  74,  75,  76,  7
7,
             80,  81,  83,  86,  88,  89,  91,  92,  93,  94,  97,  99, 10
1,
            102, 104, 106, 108, 109, 110, 113, 124, 126, 129, 132, 137, 13
9,
            143, 145, 146, 149, 152, 153, 157, 161, 162, 174, 177, 186],
           dtype='int64'), 'meal_id': Int64Index([1062, 1109, 1198, 1207,
1216, 1230, 1247, 1248, 1311, 1438, 1445,
            1525, 1543, 1558, 1571, 1727, 1754, 1770, 1778, 1803, 1847, 18
78,
            1885, 1902, 1962, 1971, 1993, 2104, 2126, 2139, 2290, 2304, 23
06,
            2322, 2444, 2490, 2492, 2494, 2539, 2569, 2577, 2581, 2631, 26
40,
            2664, 2704, 2707, 2760, 2826, 2867, 2956],
           dtype='int64'), 'category': Index(['Beverages', 'Biryani', 'Des
ert', 'Extras', 'Fish', 'Other Snacks',
       'Pasta', 'Pizza', 'Rice Bowl', 'Salad', 'Sandwich', 'Seafood', 'Sou
p',
       'Starters'],
      dtype='object'), 'cuisine': Index(['Continental', 'Indian', 'Italian
', 'Thai'], dtype='object'), 'city_code': Int64Index([456, 461, 473, 478,
485, 515, 517, 522, 526, 541, 553, 556, 561,
            562, 576, 577, 579, 590, 593, 596, 599, 602, 604, 609, 614, 61
5,
            620, 628, 632, 638, 647, 648, 649, 651, 654, 658, 659, 675, 67
6,
            679, 680, 683, 685, 693, 695, 698, 699, 700, 702, 703, 713],
           dtype='int64'), 'region_code': Int64Index([23, 34, 35, 56, 71,
77, 85, 93], dtype='int64'), 'center_type': Index(['TYPE_A', 'TYPE_B', 'TY
PE_C'], dtype='object')}
```

Frequency histograms show how the feature distributions are related to the target feature **num_orders**. The heights of the bars (*counts*) are the frequency of occurence for a given feature over the entire dataset (e.g. the sum of the heights of the bars is equal to the number of rows in the dataframe). The color of each bar represents the average value of **num_orders** in that bar.
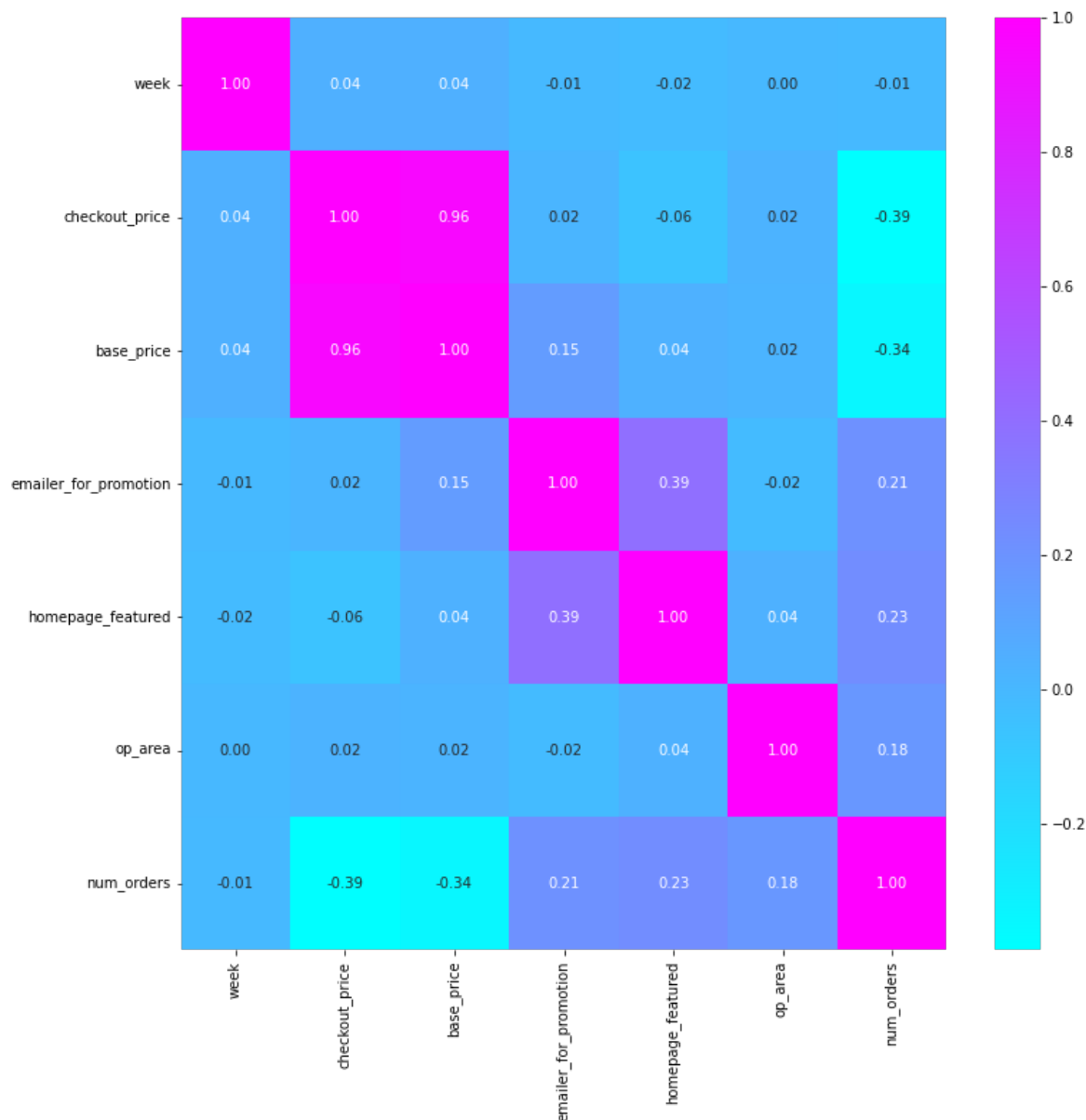
In [51]: `ml_vis_eda.plot_multiple(df_copy[df_copy.columns].values, df_copy.columns`
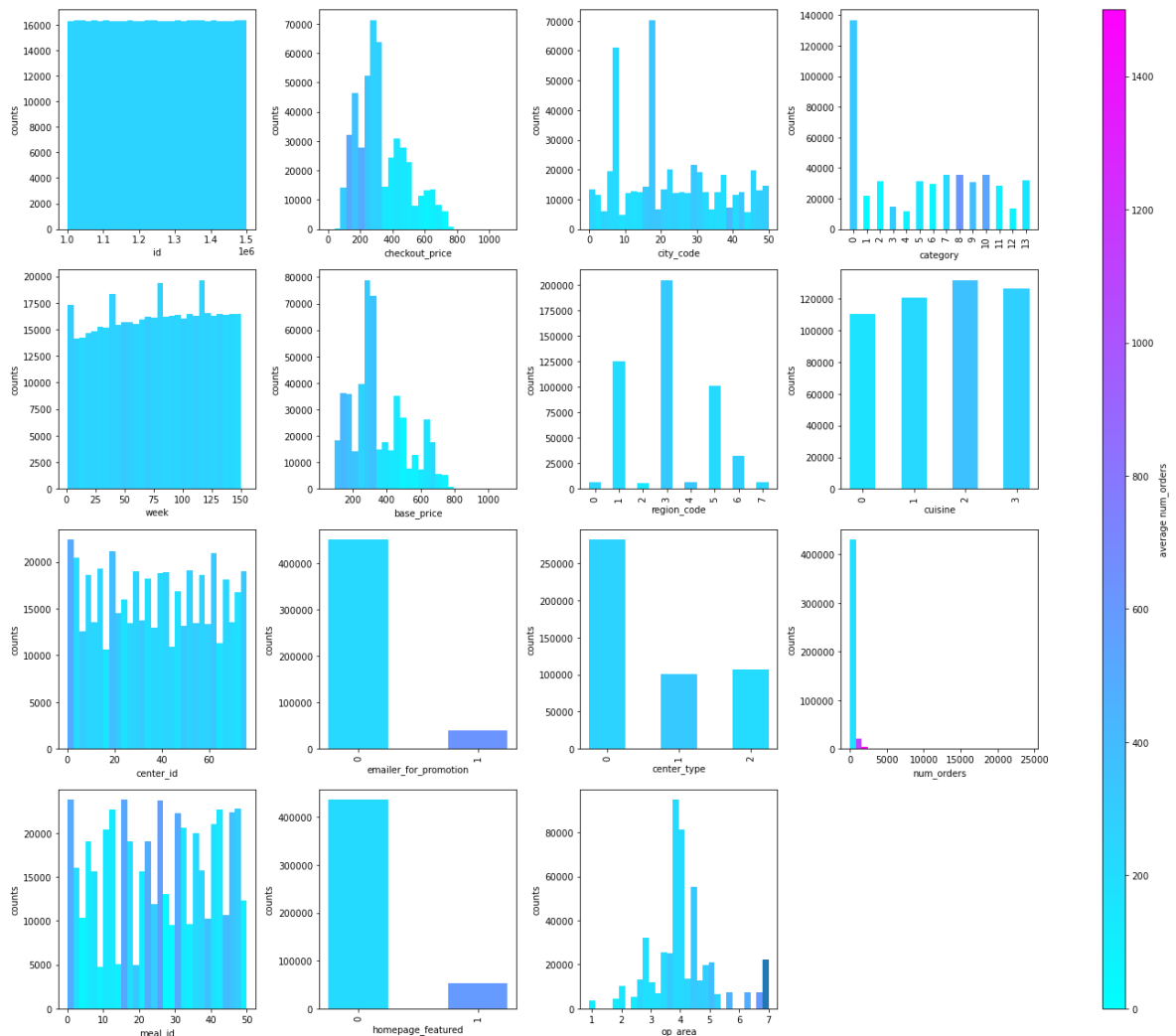


The color variation indicates that **num_orders** depends on **emailer_for_promotion**, **homepage_featured**, **base_price**, **checkout_price** and **op_area**.

The relationship between features is shown below using *spearman ranking* correlation coefficient. This makes sense for all variables that can be ordered including numerical and binary categorical features, but not categorical variables with more than one category.

In [52]: `ordered_features = ['week', 'checkout_price', 'base_price', 'emailer_for_`
`ml_vis_eda.plot_corr(df_copy[ordered_features], method='spearman')`

The correlation heatmap indicates that **checkout_price** and **base_price** are strongly correlated (R^2=0.96) meaning that together they do not add nearly any new information.

Based on the heatmap correlations, **checkout_price** is plotted below against all other features in scatter plots. These show that the targets **num_orders** depends on **checkout price** for a few of the *meal_id* categories.

```
In [53]: ml_vis_eda.plot_multiple(df_copy[df_copy.columns].values, df_copy.columns
                    target_label=target_feature, nbins=30, no_data=-1, range_targ
```
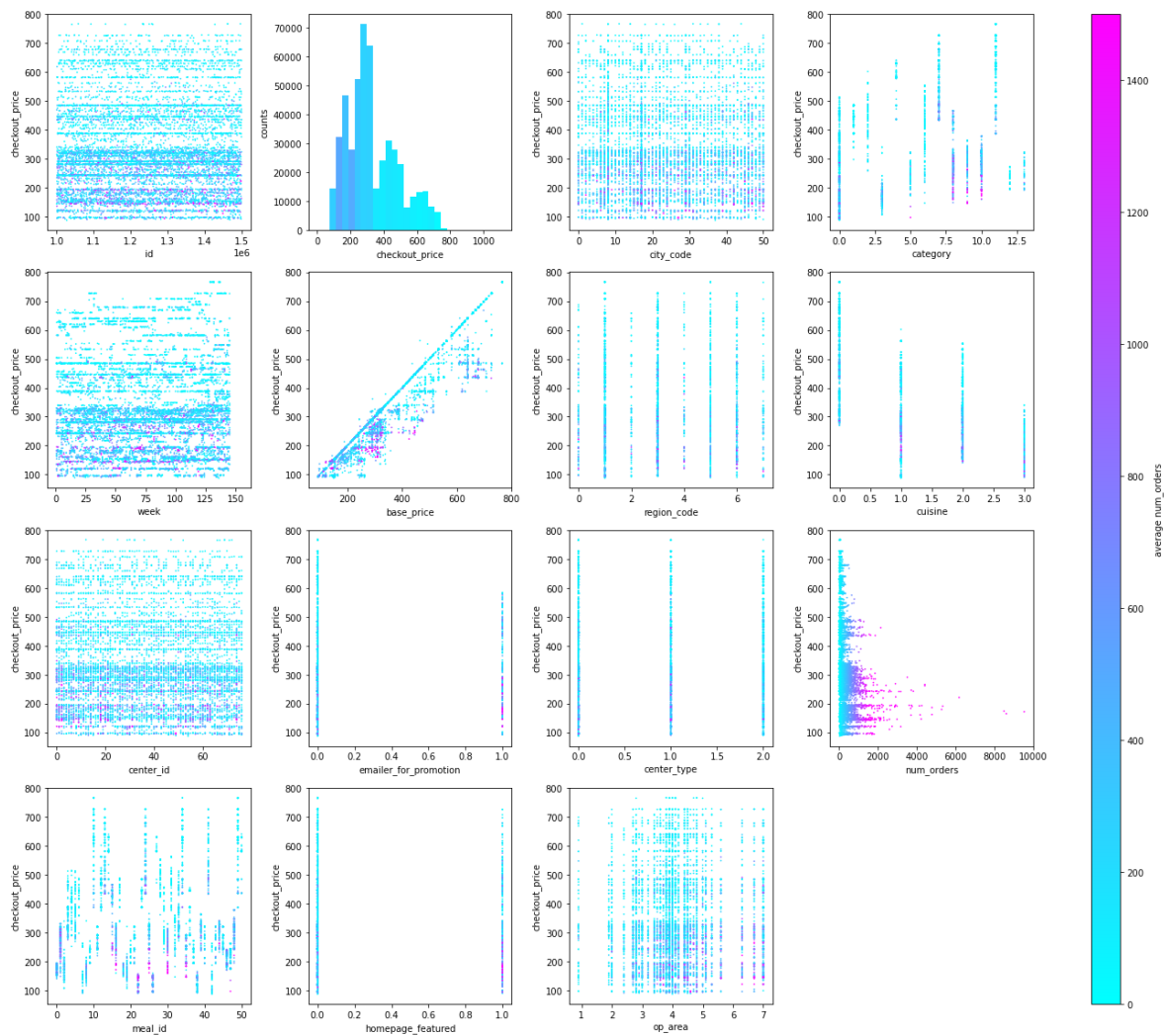
Feature engineering is used to create additional features:

```
In [54]: df_tree = df_copy.copy()

         def add_merged_feature(df_tree, columns, merge_col_name, mean_col_name=No
                 median_col_name=None, sum_col_name=None, any_col_name=None):
             if mean_col_name is not None:  # gets mean by group
                 grpby_df = df_tree.groupby(columns)[mean_col_name].mean().reset_i
             elif count_col_name is not None:  # gets valid count by group
                 grpby_df = df_tree.groupby(columns)[count_col_name].count().reset
             elif median_col_name is not None:
                 grpby_df = df_tree.groupby(columns)[median_col_name].median().res
             elif sum_col_name is not None:
                 grpby_df = df_tree.groupby(columns)[sum_col_name].sum().reset_ind
             elif any_col_name is not None:
                 grpby_df = df_tree.groupby(columns)[any_col_name].any().reset_ind
             columns2 = list.copy(columns)
             columns2.append(merge_col_name)
             grpby_df.columns= columns2
             df_tree = df_tree.merge(grpby_df, on=columns, how='left')
             return df_tree

         relevant_eng_features_fname = lgb_model_str + '_relevant_eng_features.pkl

         # start with these base features
         selectable_features = [['center_id'], ['meal_id'], ['checkout_price'], ['
             ['homepage_featured'], ['city_code'], ['region_code'], ['center_type'
         selectable_features.append([t_var])

         # get temporal feature mean -- these inputs are known for future predicti
         eng_cat_features = ['base_price', 'checkout_price', 'emailer_for_promotio
         for eng_cat_feature in eng_cat_features:
             grp = df_tree.sort_values(t_var).groupby(['center_id', 'meal_id'])[en
             feature_name = eng_cat_feature + '_mean_ts'
             df_tree[feature_name] = grp.transform(lambda x: x.expanding().mean())
             selectable_features.append([feature_name, eng_cat_feature])

         # add some engineered features
         eng_cat_features = ['center_id', 'meal_id', 'city_code',
                 'region_code', 'center_type', 'category', 'cuisine']
         for eng_cat_feature in eng_cat_features:
             feature_name = eng_cat_feature + '_' + t_var + '_count'
             df_tree = add_merged_feature(df_tree, [eng_cat_feature, t_var], featu
             selectable_features.append([feature_name, eng_cat_feature])

         # global count for each time-step
         df_tree = add_merged_feature(df_tree, [t_var], t_var + '_count', count_co
         feature_name = t_var + '_count'
         selectable_features.append([feature_name])

         feature_name = 'ts_mean'
         grp = df_tree.sort_values(t_var).groupby(['center_id', 'meal_id'])[id_var
         df_tree[feature_name] = grp.transform(lambda x: x.expanding().count())
         df_tree[feature_name] = df_tree[feature_name] / df_tree[t_var]
         selectable_features.append([feature_name])

         # price ratios to mean price grouped by (timestep and categorical feature
         eng_cat_features = ['center_id', 'meal_id', 'city_code', 'region_code', '
         for eng_cat_feature in eng_cat_features:
             eng_cat_features2 = ['base_price', 'checkout_price']
             for eng_cat_feature2 in eng_cat_features2:
                 feature_name = eng_cat_feature + '_' + t_var + '_' + eng_cat_feat
```

```
            df_tree = add_merged_feature(df_tree, [eng_cat_feature, t_var], f
            df_tree[feature_name] = df_tree[eng_cat_feature2] / df_tree[featu
            selectable_features.append([feature_name, eng_cat_feature, eng_ca
        for eng_cat_feature2 in ['emailer_for_promotion','homepage_featured']
            feature_name = eng_cat_feature + '_' + eng_cat_feature2 + '_mean'
            df_tree = add_merged_feature(df_tree, [eng_cat_feature, t_var], f
            selectable_features.append([feature_name, eng_cat_feature, eng_ca
```

In [55]:  `print(f'All possible features:\n {list(df_tree.columns)}')`

```
All possible features:
 ['id', 'week', 'center_id', 'meal_id', 'checkout_price', 'base_price', 'e
mailer_for_promotion', 'homepage_featured', 'city_code', 'region_code', 'c
enter_type', 'op_area', 'category', 'cuisine', 'num_orders', 'base_price_m
ean_ts', 'checkout_price_mean_ts', 'emailer_for_promotion_mean_ts', 'homep
age_featured_mean_ts', 'center_id_week_count', 'meal_id_week_count', 'city
_code_week_count', 'region_code_week_count', 'center_type_week_count', 'ca
tegory_week_count', 'cuisine_week_count', 'week_count', 'ts_mean', 'center
_id_week_base_price_ratio', 'center_id_week_checkout_price_ratio', 'center
_id_emailer_for_promotion_mean', 'center_id_homepage_featured_mean', 'meal
_id_week_base_price_ratio', 'meal_id_week_checkout_price_ratio', 'meal_id_
emailer_for_promotion_mean', 'meal_id_homepage_featured_mean', 'city_code_
week_base_price_ratio', 'city_code_week_checkout_price_ratio', 'city_code_
emailer_for_promotion_mean', 'city_code_homepage_featured_mean', 'region_c
ode_week_base_price_ratio', 'region_code_week_checkout_price_ratio', 'regi
on_code_emailer_for_promotion_mean', 'region_code_homepage_featured_mean',
'center_type_week_base_price_ratio', 'center_type_week_checkout_price_rati
o', 'center_type_emailer_for_promotion_mean', 'center_type_homepage_featur
ed_mean', 'category_week_base_price_ratio', 'category_week_checkout_price_
ratio', 'category_emailer_for_promotion_mean', 'category_homepage_featured
_mean', 'cuisine_week_base_price_ratio', 'cuisine_week_checkout_price_rati
o', 'cuisine_emailer_for_promotion_mean', 'cuisine_homepage_featured_mea
n']
```

The functions below are for loading and saving models/data after various optimization or
selection steps:

In [56]:
```python
######## functions for saving/loading results from each step
def save_model_pickle(filename, model):
    """ use Python pickle to save file to disk for later usage """
    dirname = os.path.dirname(filename)
    if not os.path.exists(dirname):
        os.mkdir(dirname)
    with open(filename, 'wb') as file:
        pickle.dump(model, file)

def load_model_pickle(filename):
    """ use Python pickle to load file from disk """
    with open(filename, 'rb') as file:
        return pickle.load(file)

def get_pickle_file_name(lgb_model_str, do_test, num_step=None, alpha=Non
    if alpha is not None:
        lgb_model_str = lgb_model_str + '_alpha' + str(alpha)
    if do_test:
        lgb_model_str = lgb_model_str + '_' + 'train_stage'
    else:
        lgb_model_str = lgb_model_str + '_' + 'final_stage'
    if num_step is not None:
        lgb_model_str = lgb_model_str + '_' + str(num_step+1)
    return lgb_model_str + '.pkl'

best_features = load_model_pickle(relevant_eng_features_fname)
```

In [57]:
```python
print(best_features)
```

```
['homepage_featured_mean_ts', 'checkout_price_mean_ts', 'checkout_price',
'center_id_week_count', 'ts_mean', 'emailer_for_promotion', 'meal_id', 'ce
nter_id', 'homepage_featured', 'meal_id_week_count']
```

The features above were found to give a good prediction accuracy based on cross-validation from the initial set of features. Interestingly **week** is not one of them which means that the features above can explain the time-dependence better than time (*week*) itself.

Next, *stationary* time-dependence is added through lagged features with window averaging. The final set of lagged features and hyperparameters to create them are loaded from a file previously created.

In [58]:
```python
def make_windows(window_pow, max_lag):
    """ return rolling window average length for each time lag """
    windows = []
    for lag in range(1, max_lag+1):
        window = int((lag) ** window_pow)
        windows.append(window)
    return windows


def make_lagged_series(base_colname, t_cur, unique_cols, window, t_var, d
    """
    return a pandas series of values for base_colname in df_tree
    that is at time variable 't_var', 't_cur' steps into the future and a
    time-series must be identified uniquely by unique_cols
    """
    if base_colname == t_var:  # find the actual time-step
        current_time = df_tree.loc[:, t_var]
    grp = df_tree.groupby(unique_cols)[base_colname]
    t_series = grp.transform(lambda x: x.shift(-t_cur).rolling(window, mi
    if base_colname == t_var:
        t_series = current_time - t_series
    return t_series


def get_lagged_colname(base_colname, t_cur, window):
    """ return str column name for a lagged feature """
    past_str = 'n' if t_cur < 0 else 'p'
    return base_colname + '_' + str(abs(t_cur)) + past_str + str(window)


def get_lagged_features(base_colname, t_var, t_min, t_max, istep, tstep,
    steps, windows = get_lags_windows(t_min, t_max, istep, tstep, window_
    t_colnames = []
    for t_cur, window in zip(steps, windows):
        t_colnames.append(get_lagged_colname(base_colname, t_cur, window)
    if names_only:
        return t_colnames
    else:
        t_df = pd.DataFrame(index=df_tree.index)
        for (t_colname, t_cur, window) in zip(t_colnames, steps, windows)
            t_df[t_colname] = make_lagged_series(base_colname, t_cur, uni
        return t_df, t_colnames

def get_lags_windows(t_min, t_max, istep, tstep, window_pow):
    """
    The point to forecast is at time t = 0
    istep is the time position of the the last 'observed' data: istep <=
    the last 'known' data is at t = tstep + istep >= 0
    we start at istep in order to ensure that averaging windows overlap w
    """
    def get_window(cur_t, window_pow):
        return int((abs(cur_t) + 1) ** window_pow)
    steps = []
    windows = []
    if t_max > tstep + istep:
        raise ValueError(f't_max = {t_max} cannot be greater than {tstep
    if t_min > t_max:
        raise ValueError(f't_min = {t_min} cannot be greater than t_max={
    # get all data before and at istep
    cur_t = istep
    cur_win = get_window(cur_t, window_pow)
    last_t = cur_t
    while cur_t > t_min:
```

```python
            if cur_t == last_t:
                cur_win = get_window(cur_t, window_pow)
                if cur_t >= t_min and cur_t <= t_max and cur_t != 0:
                    steps.insert(0, cur_t)
                    windows.insert(0, cur_win)
                last_t = cur_t - cur_win
            cur_t -= 1
        # get all data after istep (operation is only valid for 'known' input
        cur_t = istep
        cur_win = get_window(cur_t + 1, window_pow)
        last_t = cur_t + cur_win
        while cur_t <= t_max:
            if cur_t == last_t:
                if cur_t >= t_min and cur_t <= t_max and cur_t != 0:
                    steps.append(cur_t)
                    windows.append(cur_win)
                cur_win = get_window(cur_t + 1, window_pow)
                last_t = cur_t + cur_win
            cur_t += 1
        return steps, windows

def modify_tree_recurrent(df_tree, observed_cols, known_cols, observed_co
        t_var, t_min, t_max, istep, tstep, window_pow, best_features):
    df_tree_t = df_tree.copy()
    df_tree_t_columns = best_features.copy()
    for observed_col in observed_cols:
        t_df, t_colnames = get_lagged_features(observed_col, t_var, t_min
                unique_cols, df_tree)
        df_tree_t = pd.concat((df_tree_t, t_df), axis=1)
        df_tree_t_columns.extend(t_colnames)
    for known_col in known_cols:
        t_df, t_colnames = get_lagged_features(known_col, t_var, t_min, t
                unique_cols, df_tree)
        df_tree_t = pd.concat((df_tree_t, t_df), axis=1)
        df_tree_t_columns.extend(t_colnames)
    for observed_col_stat in observed_cols_stats:
        t_df, t_colnames = get_lagged_features(observed_col_stat, t_var,
                unique_cols, df_tree)
        df_tree_t = pd.concat((df_tree_t, t_df), axis=1)
        df_tree_t_columns.extend(t_colnames)
    return df_tree_t, df_tree_t_columns

fname_recurrent_params = f"{lgb_model_str}_steps_features_params.pkl"
best_features_steps, params_recurrent, best_features = load_model_pickle(
print(params_recurrent)
```

```
[[-1, -16, 0, 0.4596953866951567, ['num_orders'], ['checkout_price', 'home
page_featured', 'center_id_week_count', 'week'], []], [-2, -19, 3, 0.67036
94841647946, ['num_orders'], ['checkout_price', 'homepage_featured', 'meal
_id_week_count'], []], [-3, -18, 1, 0.1679195064893821, ['num_orders'],
['checkout_price', 'homepage_featured', 'meal_id_week_count', 'week'],
[]], [-4, -18, 1, 0.1679195064893821, ['num_orders'], ['checkout_price', '
homepage_featured', 'meal_id_week_count'], []], [-5, -12, 1, 0.39183863327
402246, ['num_orders'], ['checkout_price', 'homepage_featured', 'center_id
_week_count', 'meal_id_week_count'], []], [-6, -12, 1, 0.39183863327402246
, ['num_orders'], ['checkout_price', 'homepage_featured', 'meal_id_week_co
unt'], []], [-7, -12, 1, 0.39183863327402246, ['num_orders'], ['checkout_p
rice', 'homepage_featured'], []], [-8, -15, -3, 0.22309911406452448, ['num
_orders'], ['checkout_price', 'homepage_featured', 'meal_id_week_count'],
[]], [-9, -19, 1, 0.10089407620493536, ['num_orders'], ['checkout_price',
```

```
          'homepage_featured', 'meal_id_week_count', 'week'], []], [-10, -20, 0, 0.7
          375200627830971, ['num_orders'], ['checkout_price', 'homepage_featured',
          'meal_id_week_count'], []]]
```

Load the final generated forecasts (csv file) which was created using the above lagged
feature parameters.

In [59]:
```python
alphas = [None]
if quantile_alphas is not None:
    alphas.extend(quantile_alphas)
test_preds_gbm = []
final_preds_gbm = []
for ind, alpha in enumerate(alphas):
    fname_pred = lgb_model_str + '_test_alpha'+ str(alpha if alpha is not
    fname_final = lgb_model_str + '_alpha'+str(alpha if alpha is not None
    test_preds_gbm.append(pd.read_csv(fname_pred))
    final_preds_gbm.append(pd.read_csv(fname_final))
```

The coefficient of determination $R^2$ is dimensionless and inversely related to the L2
loss. It is used to evaluate the forecasting predictions and confidence (quantile)
estimates.

In [60]:
```python
def get_R2_score(predictions, target_values, weights=None):
    """
    Calculate final score (R**2 value)
    Note that sklearn.metrics.r2_score gives weird results when input arr

    :param predictions: [np.array] predicted values
    :param target_values: [np.array] corresponding target values
    :param weights: [np.array] inverse variance estimates

    :Return float
    """
    predictions_f = predictions.astype('f8')
    target_values_f = target_values.astype('f8')
    if weights is None:
        weights_f = np.ones_like(predictions_f)
    else:
        weights_f = weights.astype('f8')
    unexplained_var = np.mean(weights_f * (target_values_f - predictions_
    mean_target_value = np.sum(target_values_f * weights_f) / np.sum(weig
    explained_var = np.mean(weights_f * (target_values_f - mean_target_va
    return 1. - unexplained_var / explained_var

def get_lgb_scores(df, preds_gbm, id_var, target_feature, alphas):
    df_tree_scores = []
    for ind, alpha in enumerate(alphas):
        preds_gbm_ = preds_gbm[ind]
        mask_gbm = df[id_var].isin(preds_gbm_[id_var])
        lgb_targets = df[mask_gbm].sort_values(id_var)[target_feature].va
        lgb_preds = preds_gbm_.sort_values(id_var)[target_feature].values
        df_tree_scores.append(get_R2_score(lgb_preds, lgb_targets))
        print(f'alpha: {alpha}, score: {df_tree_scores[-1]}')
    return df_tree_scores

print('test scores: ')
df_tree_test_scores =  get_lgb_scores(df_tree, test_preds_gbm, id_var, ta
if run_mode == 2:
    print('final scores:' )
    df_tree_final_scores = get_lgb_scores(df_sample, final_preds_gbm, id_
```

```
test scores:
alpha: None, score: 0.8571233099910697
alpha: 0.05, score: 0.39415371574864855
alpha: 0.5, score: 0.8558968843164776
alpha: 0.95, score: 0.5731749740670733
```

Define features to plot vs time and plot averaged time series.

In [61]:
```python
plot_cols = ['checkout_price', 'emailer_for_promotion', 'homepage_feature
num_pars = len(plot_cols) # number of features
default_alg_index = algorithms.index(default_algorithm)

# populate known data for plotting/visualization of time series
if run_mode == 2:
    for row in df_sample.iterrows():
        df.loc[df[id_var] == row[1][id_var], target_feature] = row[1][tar

# By plotting averaged quantities vs time we see that target_feature is c
ml_vis_eda.df_plot_ts(df_copy, t_var, f'time ({t_var})', ycols=plot_cols,
```

```
Averaging repeated points for []:[0]
```
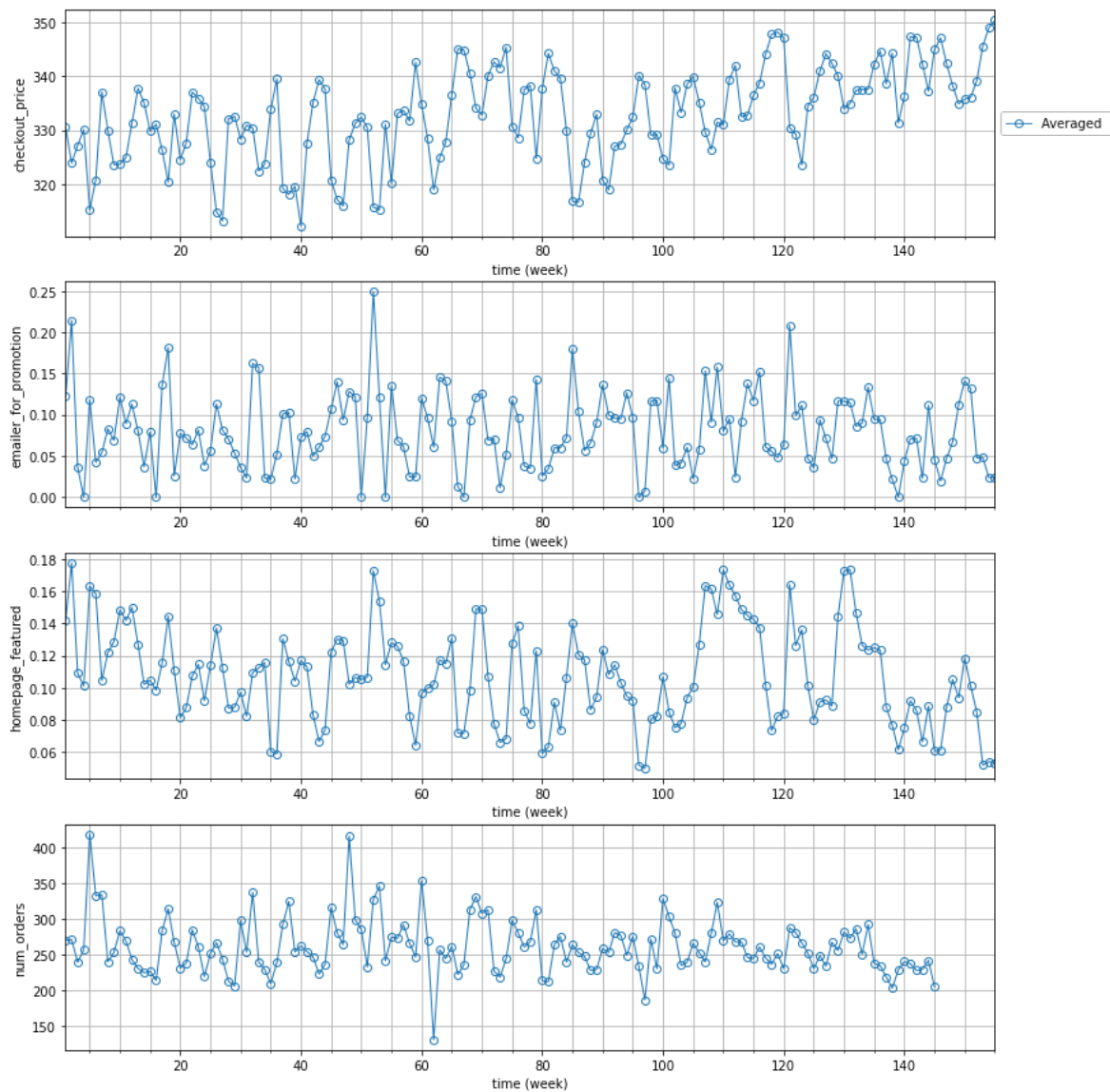
```
Showing plots 0 to 1 from a total of 1 categories
```

Out[61]: (0, 1, 1)

The plots of time-averaged time series show that **checkout_price** has evidence that it increases slowly with time. Below are the averaged features grouped by region code.

In [62]: ```
ml_vis_eda.df_plot_ts(df, t_var, f'time ({t_var})', plot_cols, plot_cols,
```

```
Averaging repeated points for ['region_code']:[23]
Averaging repeated points for ['region_code']:[34]
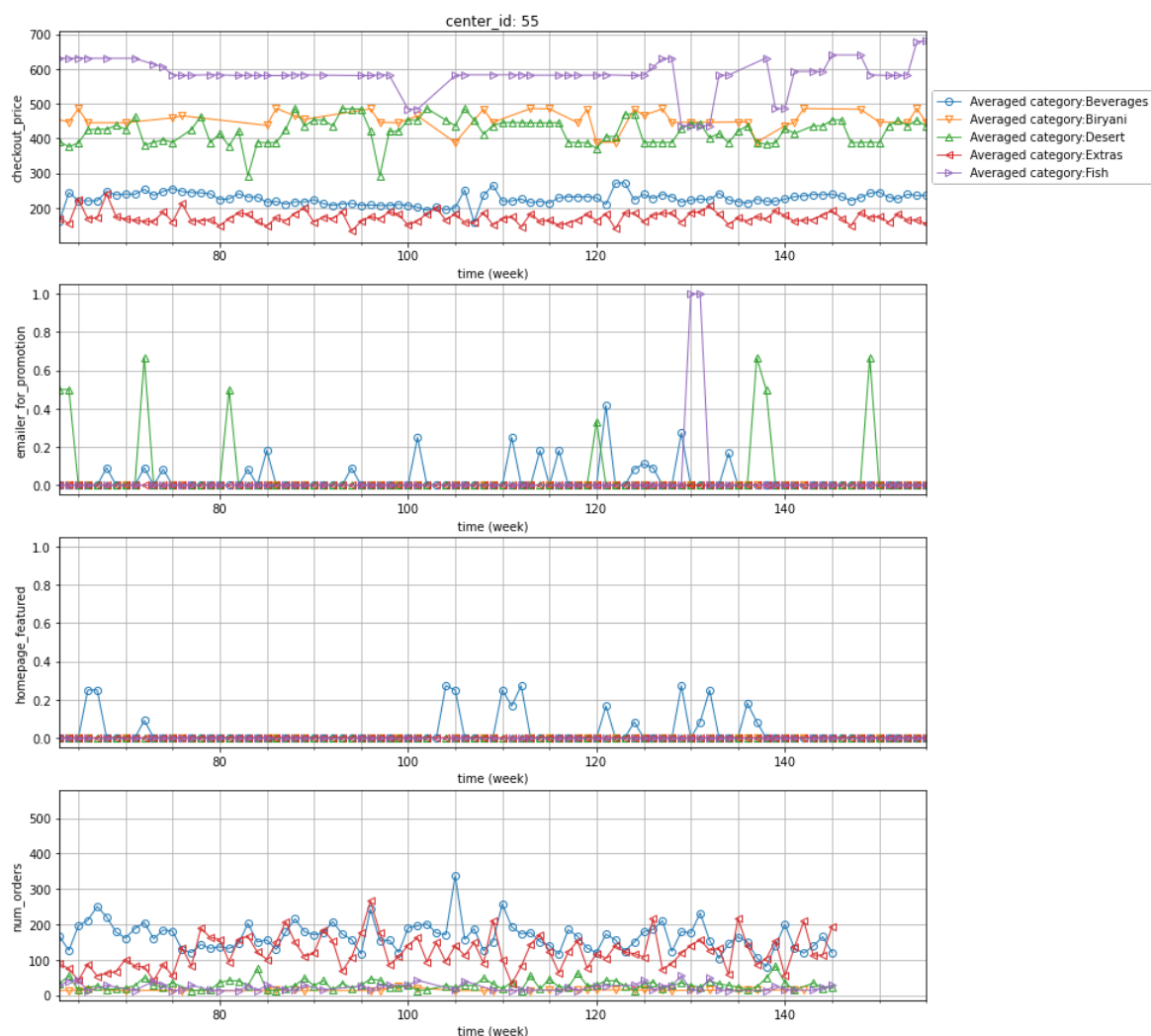Averaging repeated points for ['region_code']:[35]
Averaging repeated points for ['region_code']:[56]
Averaging repeated points for ['region_code']:[71]
Averaging repeated points for ['region_code']:[77]
Averaging repeated points for ['region_code']:[85]
Averaging repeated points for ['region_code']:[93]
```

Showing plots 0 to 8 from a total of 8 categories

Out[62]:  (0, 8, 8)

The time series averaged by category for center_id=55 are shown below:

```
In [63]: ml_vis_eda.df_plot_ts(df, t_var, f'time ({t_var})', ycols=plot_cols, ylab
                   cat_cols=['category'])
```

```
Averaging repeated points for ['category']:['Beverages']
Averaging repeated points for ['category']:['Biryani']
Averaging repeated points for ['category']:['Desert']
Averaging repeated points for ['category']:['Extras']
Averaging repeated points for ['category']:['Fish']
```

```
Showing plots 0 to 5 from a total of 13 categories
```

Out[63]:  (0, 5, 13)

Randomly-selected time-series identified uniquely by **center_id** and **meal_id** are plotted below. There is a validation (test) prediction (weeks 136-145) plot followed by the forecasting (weeks 146-155) plot for each time series identifier. The target (**num_orders**) 90% confidence interval (*quantile*), *median* (50% quantile), and the *RMSE* estimates, as well as the *mean* of previous training data are shown for comparisons.

```
In [64]: np.random.seed(1)  # for reproducible plots
         if plot_ts > 0:
             for ind_ts in np.random.choice(num_ts, plot_ts, replace=False):
                 for do_test in [True, False]:
                     if do_test:
                         preds_gbm = test_preds_gbm
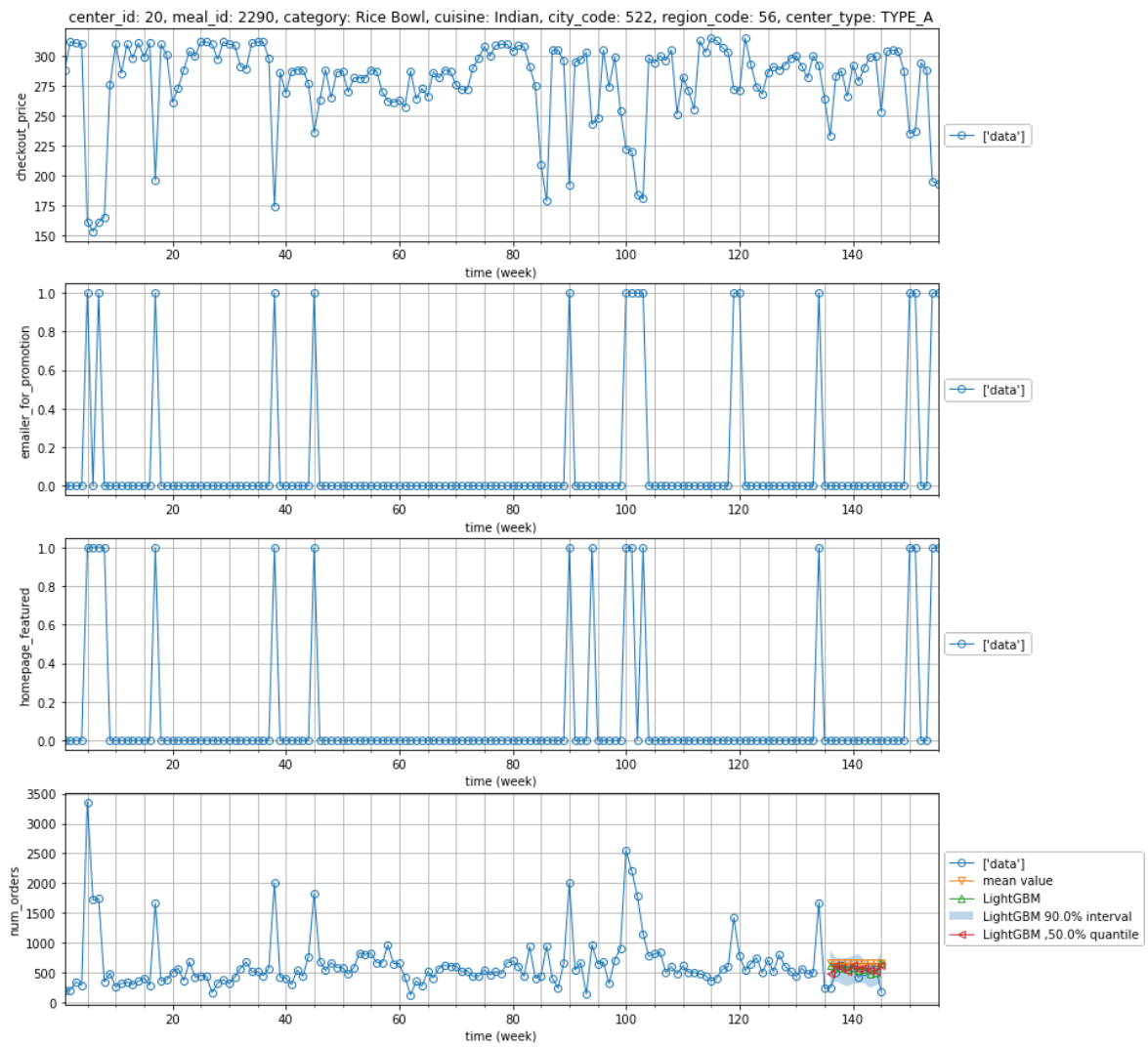                         ts_inds_pred = [1, 2]
                     else:
                         preds_gbm = final_preds_gbm
                         ts_inds_pred = [2, 3]

                     # row indices of dataframe for the time series
                     df_row_inds_train = np.arange(ts_inds[ind_ts, 0], ts_inds[ind
                     df_row_inds_pred = np.arange(ts_inds[ind_ts, ts_inds_pred[0]]
                     time_values_pred = list(df.iloc[df_row_inds_pred][t_var])  #

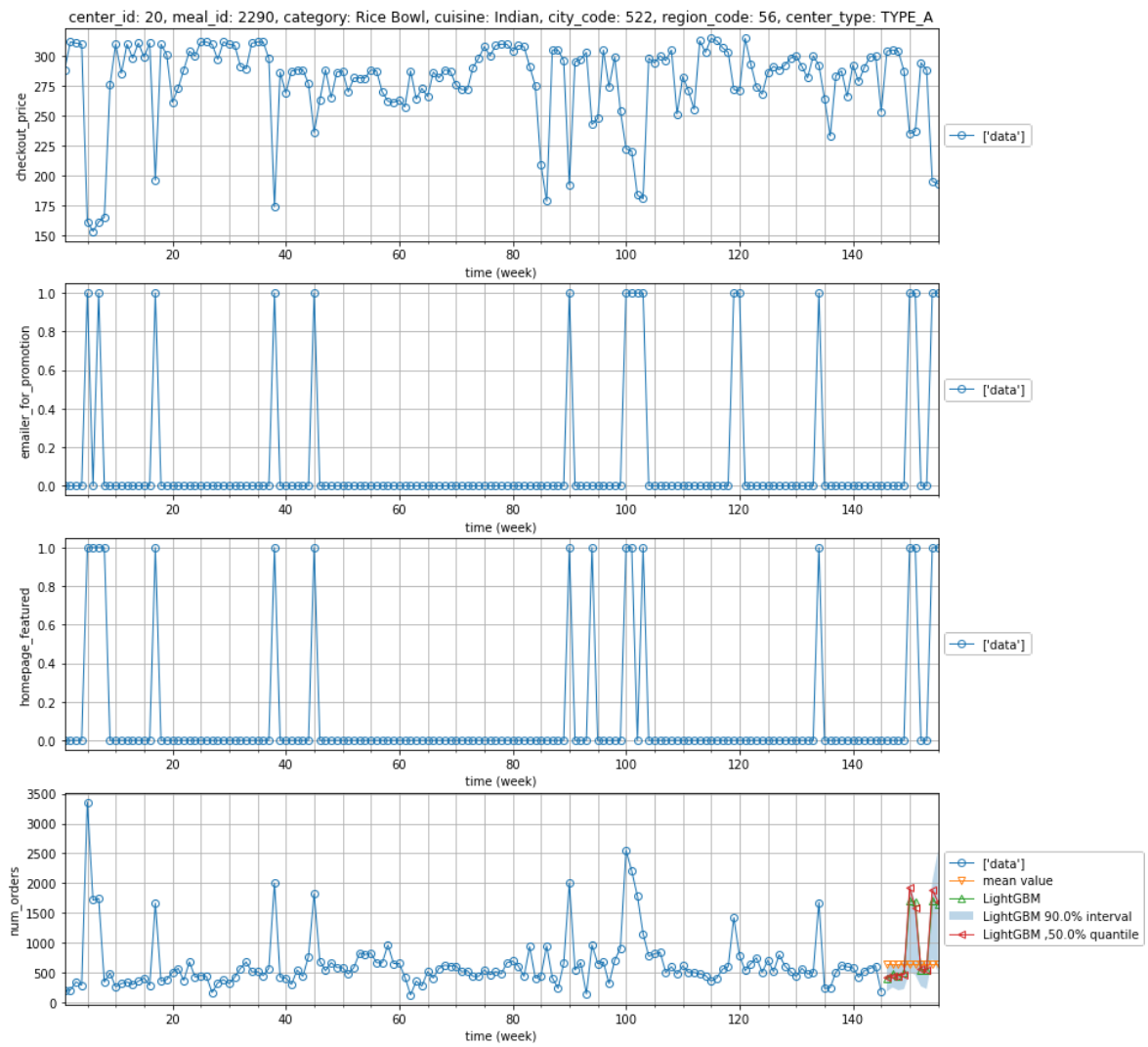                     # mean value of the target for comparison
                     target_values_train = df.iloc[df_row_inds_train][target_featu
                     test_pred1 = np.full([len(df_row_inds_pred)], target_values_t

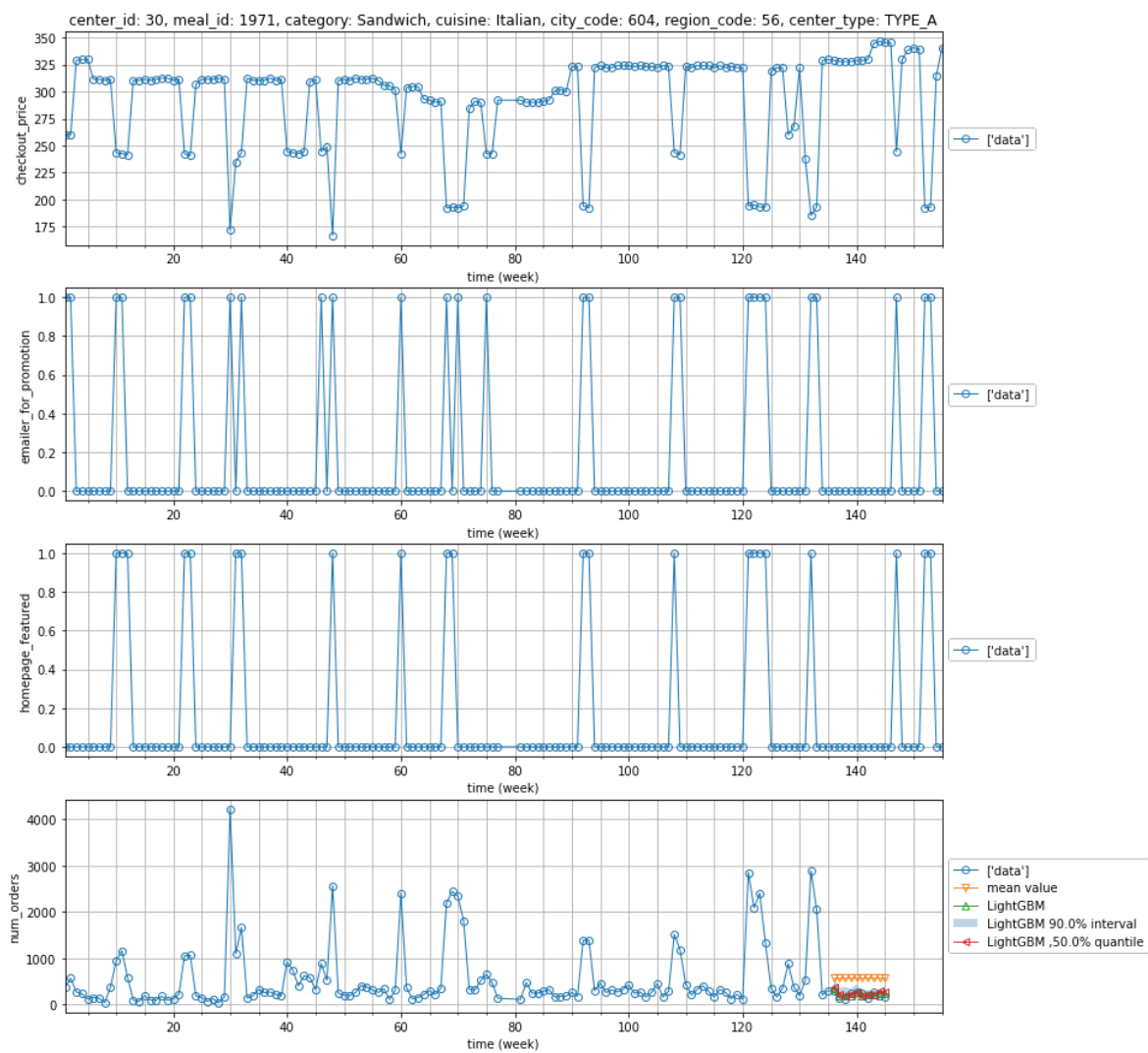                     # predictions and corresponding confidence (quantile) estimat
                     test_pred2 = []
                     for ind, alpha in enumerate(alphas):
                         target_values_pred_ids = df.iloc[df_row_inds_pred][id_var
                         mask_gbm = preds_gbm[ind][id_var].isin(target_values_pred
                         test_pred2.append(preds_gbm[ind].loc[mask_gbm, target_fea
                         if alpha is None:
                             ind_use = ind

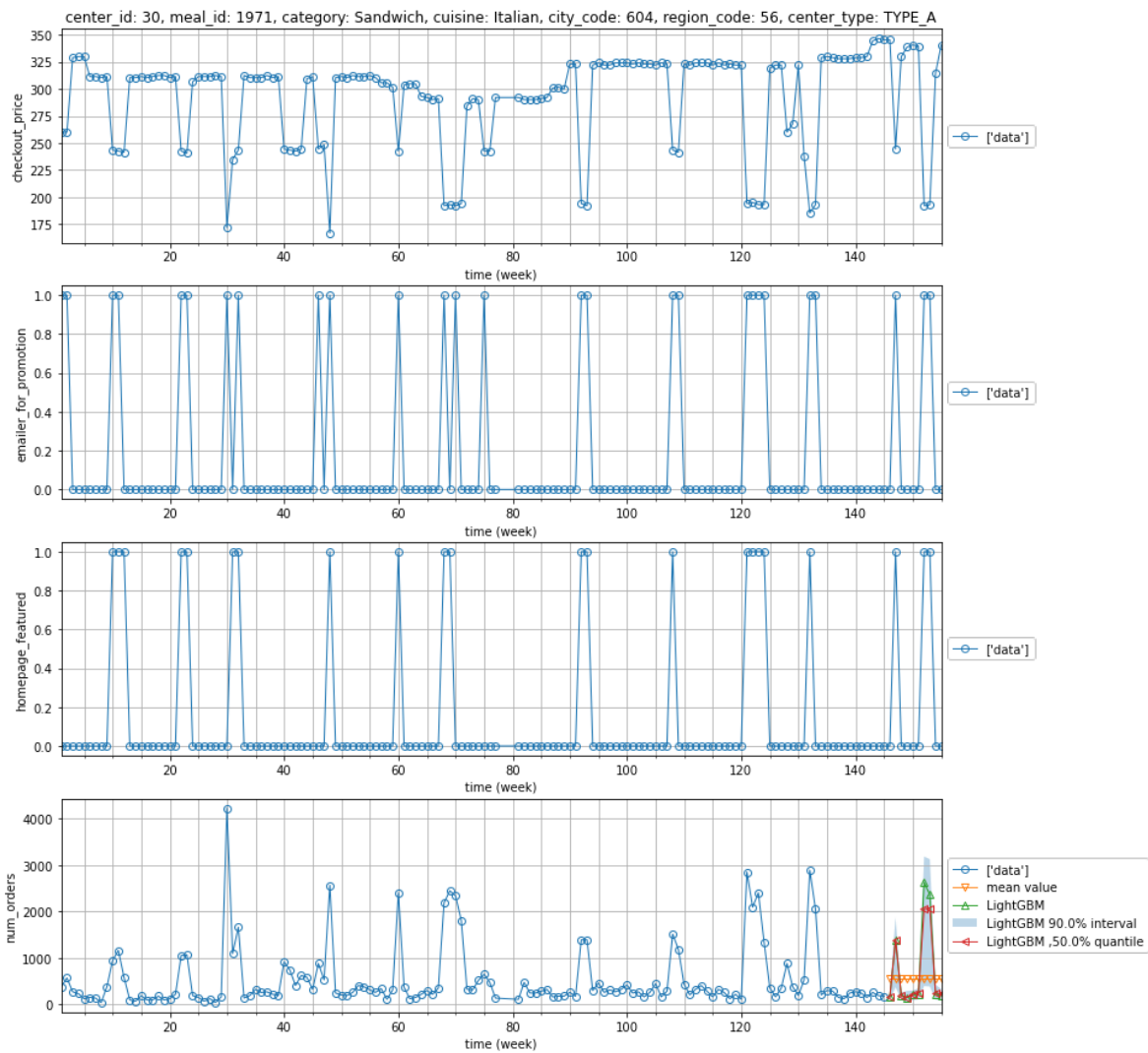                     # plot the data using the plotter object
                     category_title_vals = list(df.iloc[df_row_inds_pred[0]][categ
                     col_keyvals = {k:v for k,v in zip(categorical_features, categ
                     plotter = ml_vis_eda.TimeSeriesPlotter(df)
                     plotter.filter_data(col_keyvals)
                     test_preds = np.array([test_pred1, test_pred2[ind_use]])
                     plotter.plot_single_time_series(t_var, plot_cols, plot_cols,
                     test_preds, algorithms, \
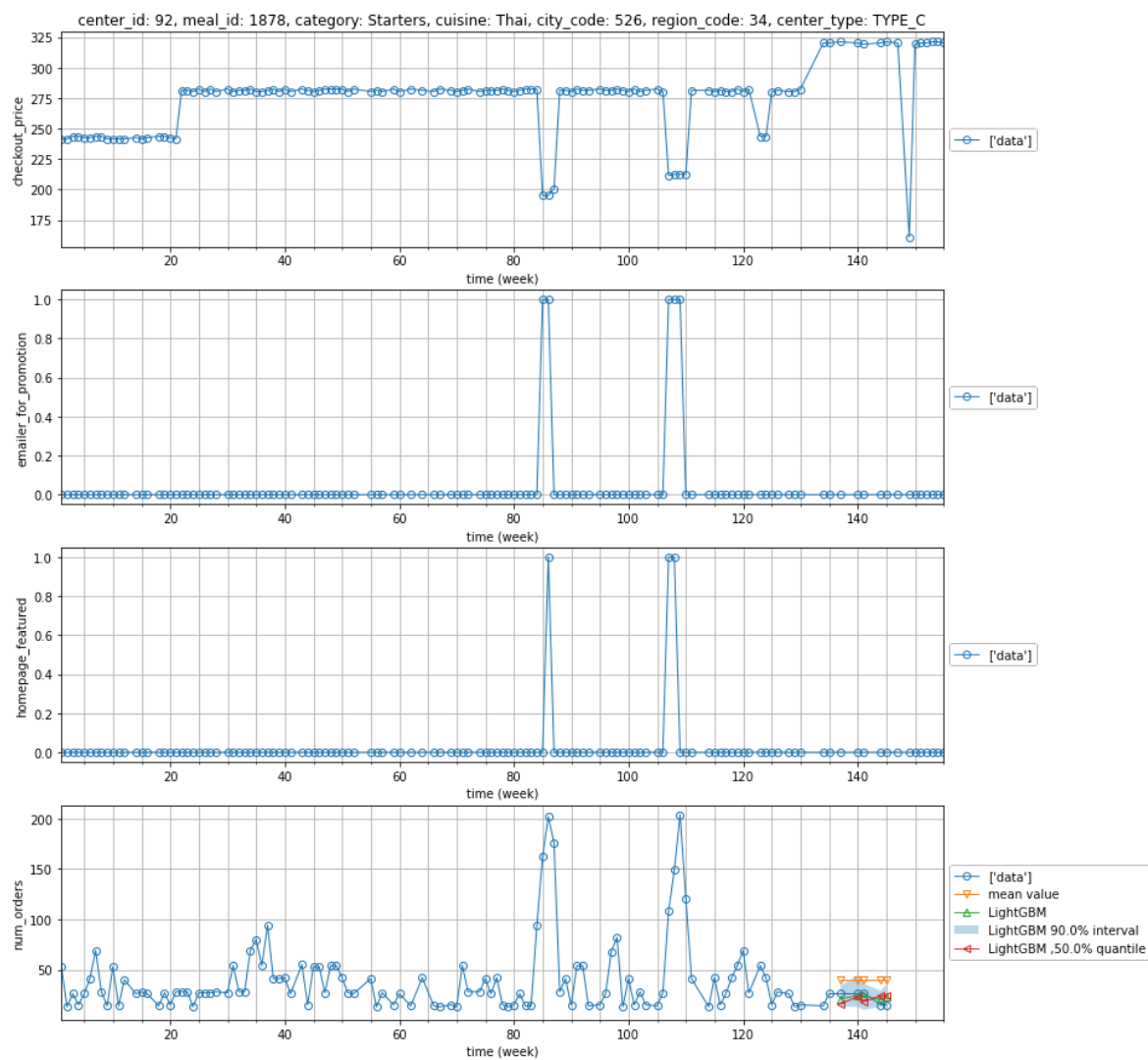                     [time_values_pred]*len(algorithms), test_pred2[1:], alphas[1:
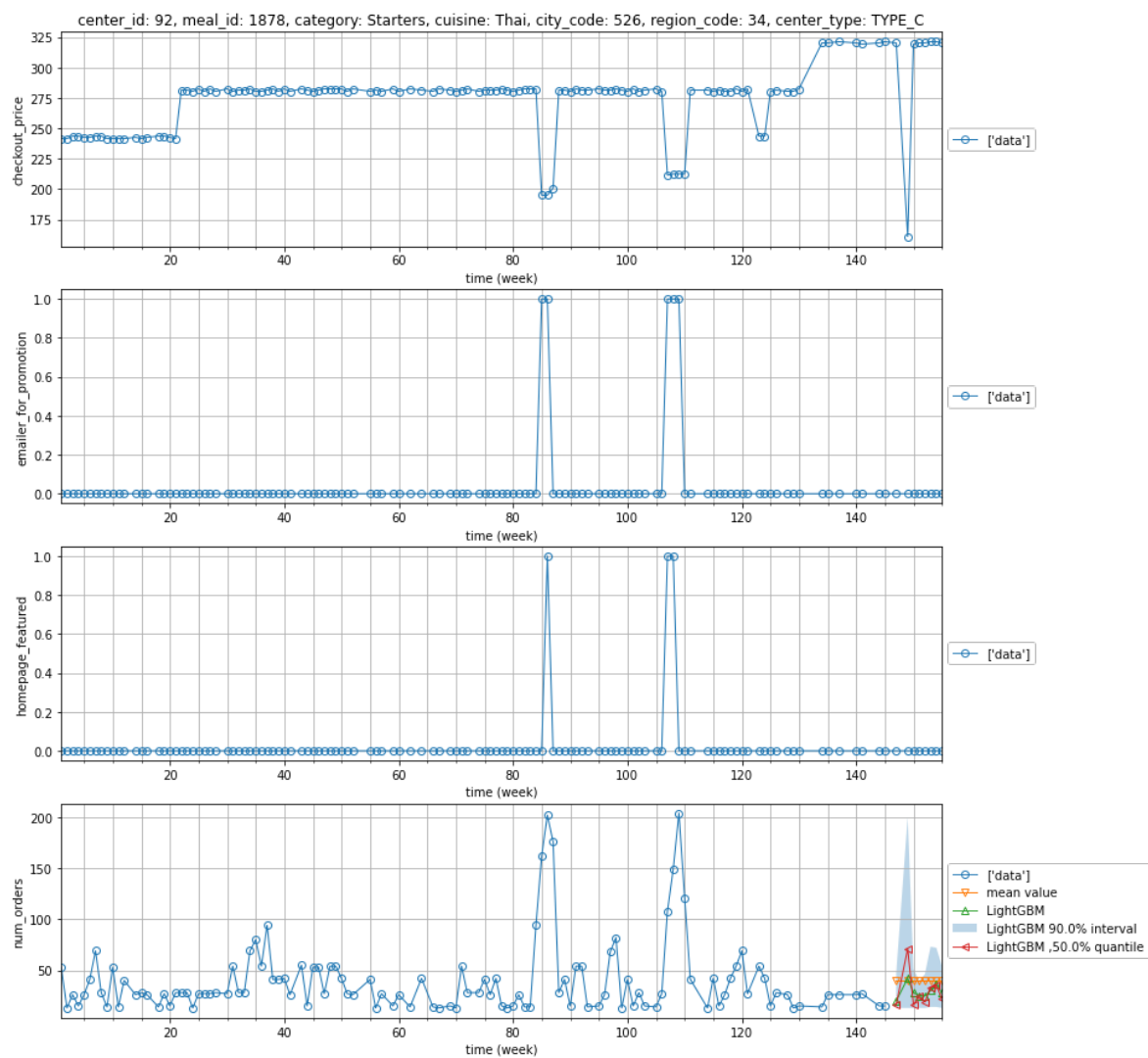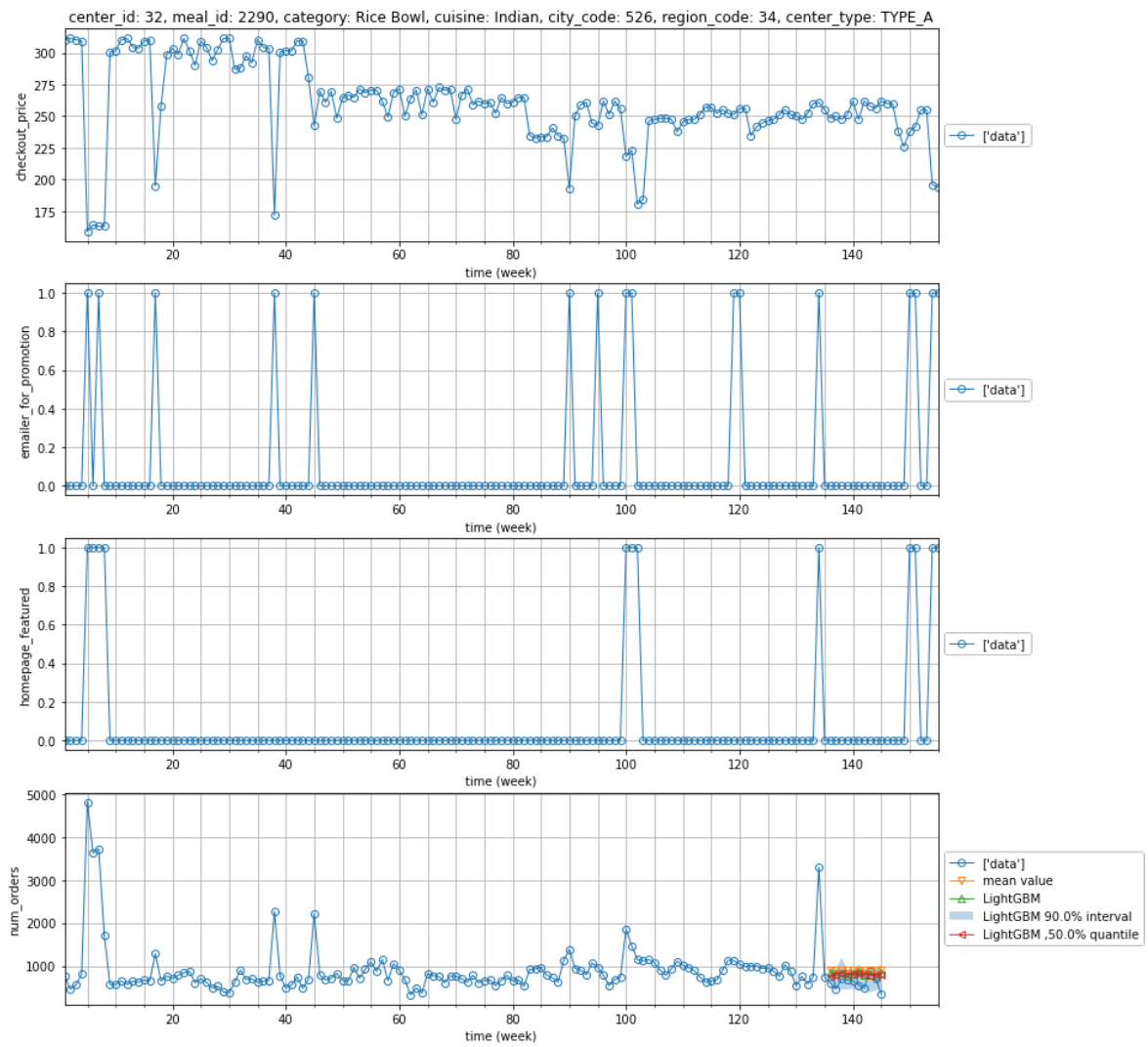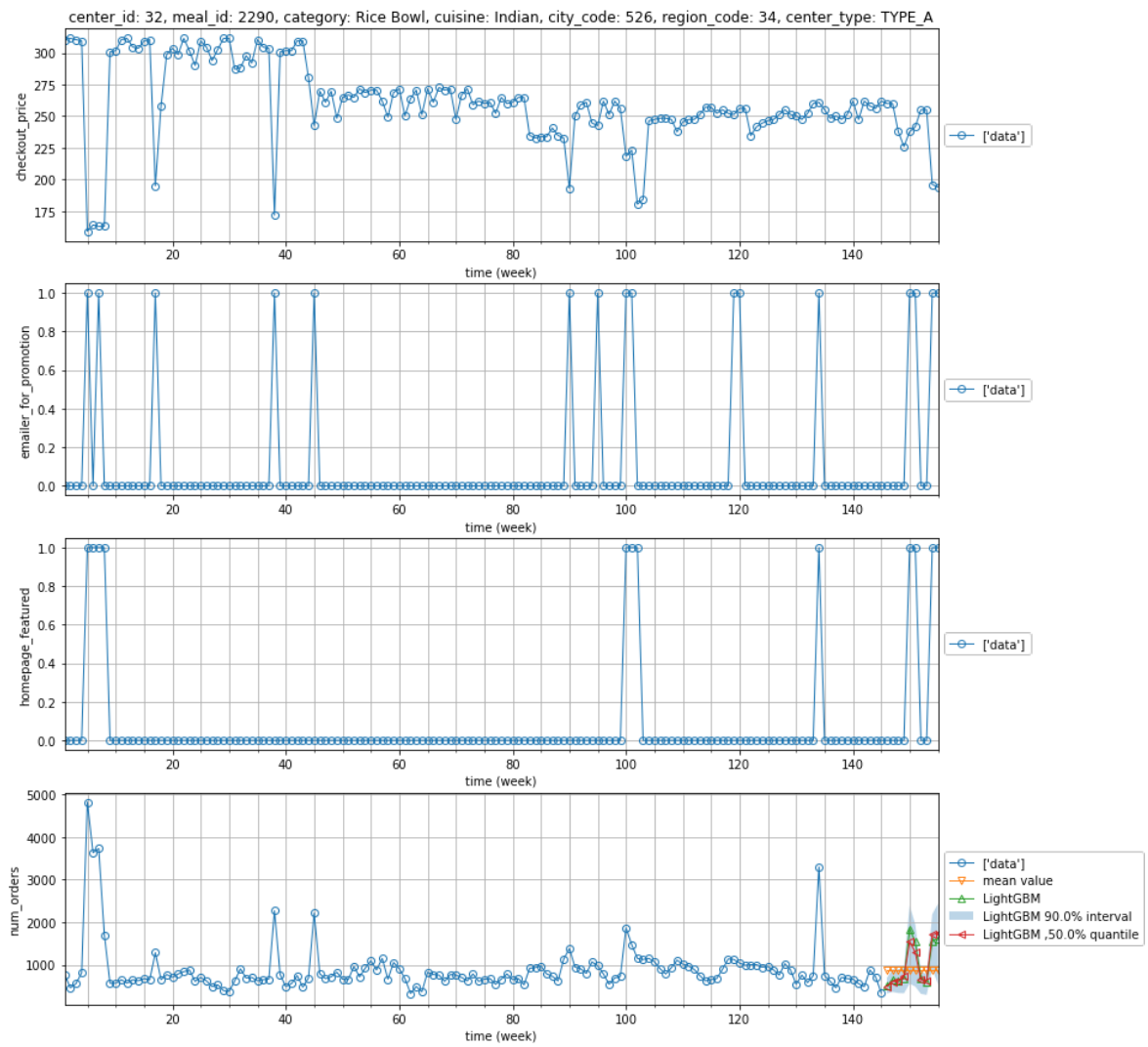         plt.show()
```

center_id: 20, meal_id: 2290, category: Rice Bowl, cuisine: Indian, city_code: 522, region_code: 56, center_type: TYPE_A

center_id: 20, meal_id: 2290, category: Rice Bowl, cuisine: Indian, city_code: 522, region_code: 56, center_type: TYPE_A

center_id: 30, meal_id: 1971, category: Sandwich, cuisine: Italian, city_code: 604, region_code: 56, center_type: TYPE_A

center_id: 92, meal_id: 1878, category: Starters, cuisine: Thai, city_code: 526, region_code: 34, center_type: TYPE_C

center_id: 92, meal_id: 1878, category: Starters, cuisine: Thai, city_code: 526, region_code: 34, center_type: TYPE_C

center_id: 32, meal_id: 2290, category: Rice Bowl, cuisine: Indian, city_code: 526, region_code: 34, center_type: TYPE_A

center_id: 32, meal_id: 2290, category: Rice Bowl, cuisine: Indian, city_code: 526, region_code: 34, center_type: TYPE_A

center_id: 113, meal_id: 2126, category: Pasta, cuisine: Italian, city_code: 680, region_code: 77, center_type: TYPE_C

## Conclusions

A time series forecasting model was developed using gradient boosting algorithm
(LightGBM) with lags of up to 20 weeks to forecast order demand and achieved a
reasonable accuracy ($R^2$ = 85.7%) on the test data (weeks 136 to 145 for 3600 time
series). The model can forecast RMSE predictions and confidence (quantile) estimates,
and was optimized using feature engineering, feature selection and hyperparameter
tuning in a semi-automated fashion. Slow (subtle) time-dependence of the features over
the course of the data (155 weeks) was observed and its modeling can be investigated
further (e.g. capturing effects of inflation with slow price increases).

In [ ]: