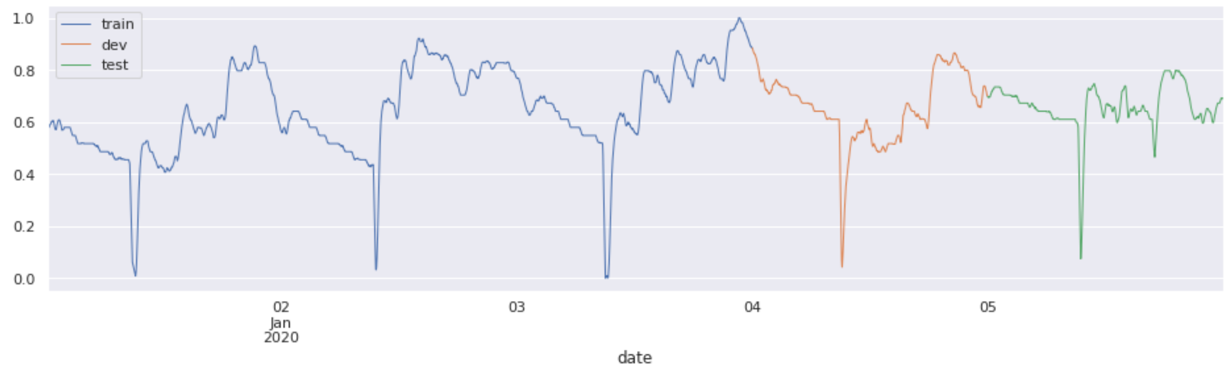
Machine Learning Model

This notebook develops a few machine learning model to forecast the time-series data provided by 'time_series.csv'. Time series are a form of sequential data, which makes recurrent neural networks suitable for the task. Various network architectures are considered, involving Conv1D, LSTM and/or Dense layers.

In [1]:
```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
import tensorflow as tf

from temp_ml_scripts import *
```

Load the time series

In [2]:
```
# Load time series data
time_series = pd.read_csv('../input/temp1-data-preparation/time_series.csv', index_col='date').asf
req('T')['temp']

# Chop series for developing
time_series = time_series.loc['2020-01-01':'2020-01-05'] # 5 days

# Normalize the data (particlularly important for NNs)
min_value = np.min(time_series)
max_value = np.max(time_series)
time_series = (time_series - min_value)/(max_value - min_value)

def un_normalize_series(series):
    original = series * (max_value - min_value) + min_value
    return original

# Size of dev and test sets (in same units as time_series: minutes)
size_dev = 60 * 24 * 1 # one day
size_test = 60 * 24 * 1 # one day

# Split time series into train, dev and test sets
time_series_train, time_series_dev, time_series_test = train_dev_test_split(time_series, size_dev,
size_test)
# for implementation, see temp-utilities.py

# Plot the time series
plot_time_series(time_series_train, time_series_dev, time_series_test)
# for implementation, see temp-utilities.py
```



Train neural network

To train a neural network, it is required to construct a batch of input features `X` and a batch of output labels `y`. For plotting the time-series, it will be convenient to keep track of time in `t` as well.

```
In [3]: # Define the number of time steps fed into the model and the number of subsequent time steps predi
        cted by the model
        n_steps_in = 5      # this number will be varied as a model parameter
        n_steps_out = 10    # this number will be kept constant to match the mathematical analysis in the n
        otebook temp2-mathematical-models.ipynb

        # Construct train, dev and test sets (X, y)
        X_train, y_train, t_train = split_sequence(time_series_train, n_steps_in, n_steps_out)  # for impl
        ementation of split_sequence(), see temp-ml-scripts.py
        X_dev, y_dev, t_dev = split_sequence(time_series_dev, n_steps_in, n_steps_out)
        X_test, y_test, t_test = split_sequence(time_series_test, n_steps_in, n_steps_out)

        print('train shapes (X,y,t) : ', X_train.shape, y_train.shape, t_train.shape)
        print('dev shapes   (X,y,t) : ', X_dev.shape, y_dev.shape, t_dev.shape)
        print('test shapes  (X,y,t) : ', X_test.shape, y_test.shape, t_test.shape)
```

```
train shapes (X,y,t) :  (4292, 5, 1) (4292, 10) (4292, 10)
dev shapes   (X,y,t) :  (1426, 5, 1) (1426, 10) (1426, 10)
test shapes  (X,y,t) :  (1426, 5, 1) (1426, 10) (1426, 10)
```

Define an initial model with two layers:

1. LSTM (Long Short-Term Memory) layer with `n_steps_in` one-dimensional input features and a 20-dimensional hidden state.
2. Dense layer with `n_steps_out` real numbers in its output.

```
In [4]: # Define an initial model
        model = tf.keras.models.Sequential([
            tf.keras.layers.LSTM(20, activation='relu', input_shape=(n_steps_in, 1)),
            tf.keras.layers.Dense(n_steps_out, activation='linear')
        ])

        model.summary()
```

```
Model: "sequential"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
lstm (LSTM)                  (None, 20)                1760
_________________________________________________________________
dense (Dense)                (None, 10)                210
=================================================================
Total params: 1,970
Trainable params: 1,970
Non-trainable params: 0
_________________________________________________________________
```

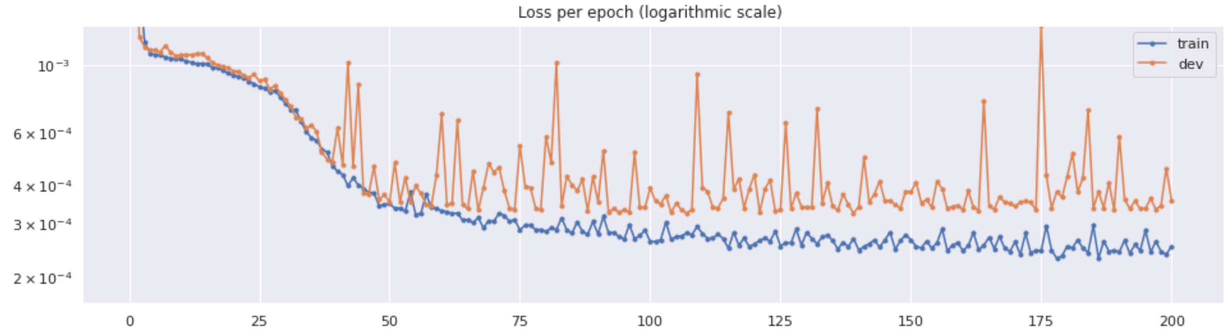
The model contains a very modest number of O(2k) trainable parameters.

Next, the model is compiled to minimize the `'mean-squared-error'` loss function using the efficient adaptive `'adam'` optimizer.

A model checkpoint callback is used to store the version of the model (i.e. state of weights) that achieved the lowest dev loss.

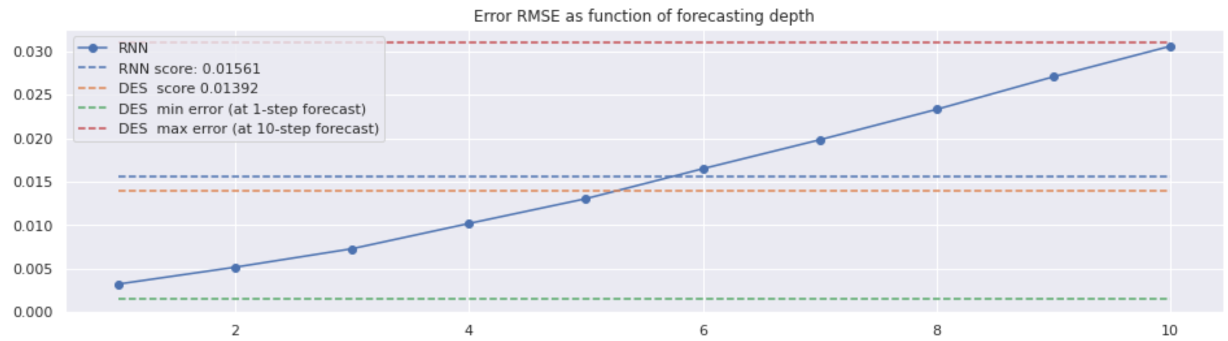
In [5]:
```python
# Compile the model
model.compile(optimizer='adam', loss='mse')

# Callbacks
em = EpochMonitor()
mc = tf.keras.callbacks.ModelCheckpoint('best_model.h5',
                                        monitor='val_loss',
                                        mode='min',
                                        verbose=0,
                                        save_best_only=True)

# Train the model
training_history = model.fit(X_train, y_train,
                             validation_data=(X_dev, y_dev),
                             epochs=200,
                             verbose=0,
                             callbacks=[em, mc])

# Plot the loss during training
# for implementation of plot_training_loss(), see temp-ml-scripts.py
plot_training_loss(training_history, hide_first=2, lin=False)
```

```
Epoch 200
```



The train loss is decreasing with the number of epochs, and starting to level out, so that more training helps increasingly less. The dev loss is larger than the train loss, as would be expected. The gap between the two remains roughly constant, indicating that no overfitting is likely to be taking place yet.

In [6]:
```python
# Load best state of the model
best_model = tf.keras.models.load_model('best_model.h5')

# Forecasting
# for implementation of direct_forecast(), see temp-ml-scripts.py
forecast = direct_forecast(X_dev, y_dev, t_dev, best_model)

# Scoring
# for implementation of evaluate_model_performance(), see temp-ml-scripts.py
errors, score = evaluate_model_performance(forecast)

# Compare score to best model from preceding notebook
# for implementation of compare_score(), see temp-ml-scripts.py
compare_score(errors, score)
```



This simple LSTM model already performs comparably to the best model from the previous notebook `temp2-mathematical-models.ipynb` . The challenge is to improve upon the present model through tuning of the model hyperparameters.

Hyperparameter tuning

The hyperparameter tuning is set up as follows:

- Parameters and their ranges of values are specified in a dictionary `param_values`. These include fixed ('global') parameters `n_steps_out`, `min_n_epochs`, `max_n_epochs`, `patience` as well as variable parameters, such as `model_name`, `n_steps_in`, `hidden_dim`, ...
- A custom function `select_model()` defines models, which are selected with the parameter `model_name`.
- The training and evaluation of each model in the parameter search is carried out by the custom helper function `grid_search()`. Remarks:
  - A `ModelCheckpoint()` callback is used to keep the best performance of each model on the dev set over the whole training.
  - A custom `EarlyStoppingAfter()` callback is used to train each model at least `min_n_epochs` epochs, after which the training is stopped once the dev loss has not lowered its all-time lowest value during the last `patience` epochs, or once `max_n_epochs` epochs have elapsed. This method allows for an efficient and reasonably fair comparison between models of different complexity, which require different amounts of training.

In [7]:

```python
def grid_search(param_values):
    """
    Performs a grid search over the specified parameter ranges, training and evaluating an RNN in each instance

    Input:
    param_values - dictionary with ('parameter name', [list of values]) key-values pairs, dict

    Output:
    table - record of input and output of each run, pandas.DataFrame
    """
    # Create a parameter grid
    param_grid = ParameterGrid(param_values)

    # Separate variable from constant parameters (for printing purpose)
    variable_param = dict()
    constant_param = dict()
    for (key,val) in param_values.items():
        if len(val)>1:
            variable_param[key] = val
        else:
            constant_param[key] = val

    # Initialization
    results = []
    run = 1

    # Grid search
    for param in param_grid:
        time1 = datetime.now()
        # Select model
        model = select_model(param)
        # Compile model
        model.compile(optimizer='adam', loss='mse')
        # Callbacks
        em = EpochMonitor()
        es = EarlyStoppingAfter(monitor='val_loss',
                                mode='min',
                                verbose=0,
                                patience=param['patience'],
                                start_epoch=param['min_n_epochs'])
        mc = tf.keras.callbacks.ModelCheckpoint('best_model.h5',
                                                monitor='val_loss',
                                                mode='min',
                                                verbose=0,
                                                save_best_only=True)
        # Construct train, dev and test sets (X, y)
        X_train, y_train, t_train = split_sequence(time_series_train, param['n_steps_in'], param['n_steps_out'])
        X_dev, y_dev, t_dev = split_sequence(time_series_dev, param['n_steps_in'], param['n_steps_out'])
        # Train model
        train_hist = model.fit(X_train, y_train,
                               validation_data=(X_dev, y_dev),
                               epochs=param['max_n_epochs'],
                               verbose=0,
                               callbacks=[em, es, mc])
        train_hist = train_hist.history
        n_epochs = len(train_hist['loss'])
        # Load best state of the model
        best_model = tf.keras.models.load_model('best_model.h5')
        # Forecast
        # for implementation of direct_forecast(), see temp-ml-scripts.py
        forecast = direct_forecast(X_dev, y_dev, t_dev, best_model)
        # Score
        # for implementation of evaluate_model_performance(), see temp-ml-scripts.py
        errors, score = evaluate_model_performance(forecast)
        # Store result
        col = list(param.keys())
        col = col + ['neurons', 'n_epochs', 'train_hist', 'model', 'forecast', 'errors', 'score']
        res = list(param.values())
        res = res + [model.count_params(), n_epochs, train_hist, best_model, forecast, errors, score]
        results.append(res)
        time2 = datetime.now()
        deltat = time2 - time1
        print('{run:2}/{tot:2}   {time}   {epo:3} epochs {neu:7} neurons   score = {sco:.5}   {par}'.format(
            run=run,
            tot=len(param_grid),
            time=str(deltat).split('.', 2)[0],
```

```
            epo=n_epochs,
            neu=model.count_params(),
            sco=score,
            par={key:param[key] for key in variable_param.keys()}
        ))
        run=run+1

    # Collect result in a table and sort by score
    table = pd.DataFrame(np.array(results), columns=col)
    table = table.sort_values('score')
    return table
```

Search 1: vary number of input steps and hidden dimension

The initial model features two key parameters that can be tuned:

- the number of input time steps `n_steps_in`
- the dimension of the hidden state `hidden_dim`

The initial model uses the values `n_steps_in = 5` and `hidden_dim = 20` without motivation. Here, both parameters are varied in search of a better performing model.

In [8]:
```
# Define models
def select_model(param):
    """
    Selects a model from a list of different neural networks
    """
    # The same model as defined above, but with adjustable parameters:
    if param['model_name'] == 'mod1':
        model = tf.keras.models.Sequential([
            tf.keras.layers.LSTM(param['hidden_dim'], activation='relu', input_shape=(param['n_ste
ps_in'], 1)),
            tf.keras.layers.Dense(param['n_steps_out'], activation='linear')
        ])
    return model

# Define parameter ranges
param_values = {
    # always keep fixed
    'n_steps_out' : [10],
    'min_n_epochs' : [200],
    'max_n_epochs' : [200],
    'patience' : [0],
    # keep fixed
    'model_name' : ['mod1'],
    # vary
    'n_steps_in': [3,5,10,20],
    'hidden_dim' : [20,40,60,80],
}

# Run search
search1 = grid_search(param_values)  # for implementation of grid_search(), see temp-ml-scripts.py
search1.to_csv('search1.csv')
search1[['neurons','n_epochs','n_steps_in','hidden_dim','score']]
```

```
 1/16   0:01:28   200 epochs    1970 neurons    score = 0.019467   {'n_steps_in': 3, 'hidden_dim': 20}
 2/16   0:01:54   200 epochs    1970 neurons    score = 0.015297   {'n_steps_in': 5, 'hidden_dim': 20}
 3/16   0:02:47   200 epochs    1970 neurons    score = 0.016801   {'n_steps_in': 10, 'hidden_dim': 20}
 4/16   0:04:36   200 epochs    1970 neurons    score = 0.014655   {'n_steps_in': 20, 'hidden_dim': 20}
 5/16   0:01:34   200 epochs    7130 neurons    score = 0.013973   {'n_steps_in': 3, 'hidden_dim': 40}
 6/16   0:01:57   200 epochs    7130 neurons    score = 0.016042   {'n_steps_in': 5, 'hidden_dim': 40}
 7/16   0:02:51   200 epochs    7130 neurons    score = 0.015274   {'n_steps_in': 10, 'hidden_dim': 40}
 8/16   0:04:52   200 epochs    7130 neurons    score = 0.013775   {'n_steps_in': 20, 'hidden_dim': 40}
 9/16   0:01:41   200 epochs   15490 neurons    score = 0.014903   {'n_steps_in': 3, 'hidden_dim': 60}
10/16   0:02:04   200 epochs   15490 neurons    score = 0.015454   {'n_steps_in': 5, 'hidden_dim': 60}
11/16   0:03:09   200 epochs   15490 neurons    score = 0.014439   {'n_steps_in': 10, 'hidden_dim': 60}
12/16   0:05:20   200 epochs   15490 neurons    score = 0.013208   {'n_steps_in': 20, 'hidden_dim': 60}
13/16   0:01:50   200 epochs   27050 neurons    score = 0.013995   {'n_steps_in': 3, 'hidden_dim': 80}
14/16   0:02:24   200 epochs   27050 neurons    score = 0.015762   {'n_steps_in': 5, 'hidden_dim': 80}
15/16   0:03:51   200 epochs   27050 neurons    score = 0.013046   {'n_steps_in': 10, 'hidden_dim': 80}
16/16   0:06:20   200 epochs   27050 neurons    score = 0.013258   {'n_steps_in': 20, 'hidden_dim': 80}
```

Out[8]:

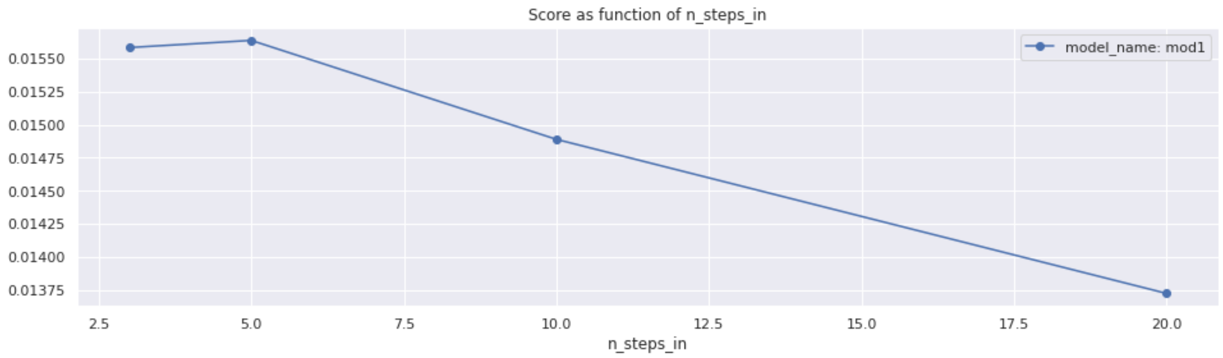
	neurons	n_epochs	n_steps_in	hidden_dim	score
14	27050	200	10	80	0.0130463
11	15490	200	20	60	0.0132082
15	27050	200	20	80	0.0132585
7	7130	200	20	40	0.0137749
4	7130	200	3	40	0.0139732
12	27050	200	3	80	0.0139952
10	15490	200	10	60	0.0144391
3	1970	200	20	20	0.014655
8	15490	200	3	60	0.0149026
6	7130	200	10	40	0.0152741
1	1970	200	5	20	0.015297
9	15490	200	5	60	0.0154536
13	27050	200	5	80	0.0157617
5	7130	200	5	40	0.0160418
2	1970	200	10	20	0.016801
0	1970	200	3	20	0.0194674

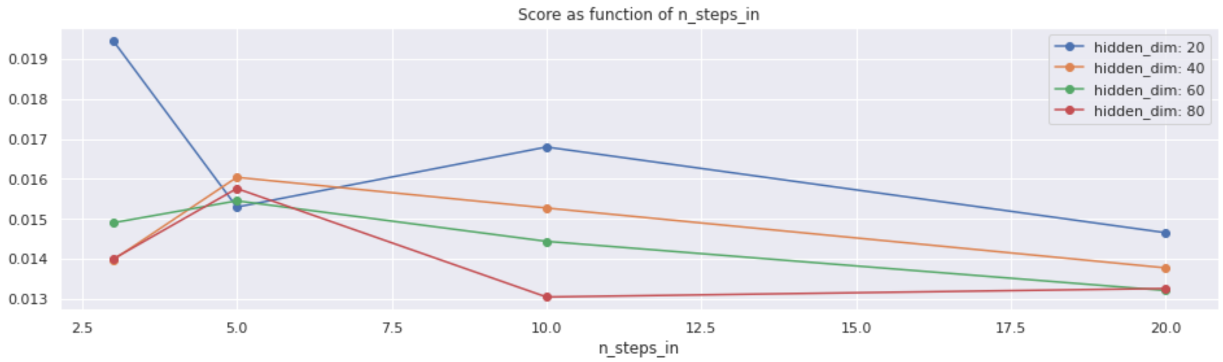
- Plot the results of each run
- Plot the training history of each run
- Plot the best score in comparison to the mathematical model

In [9]:

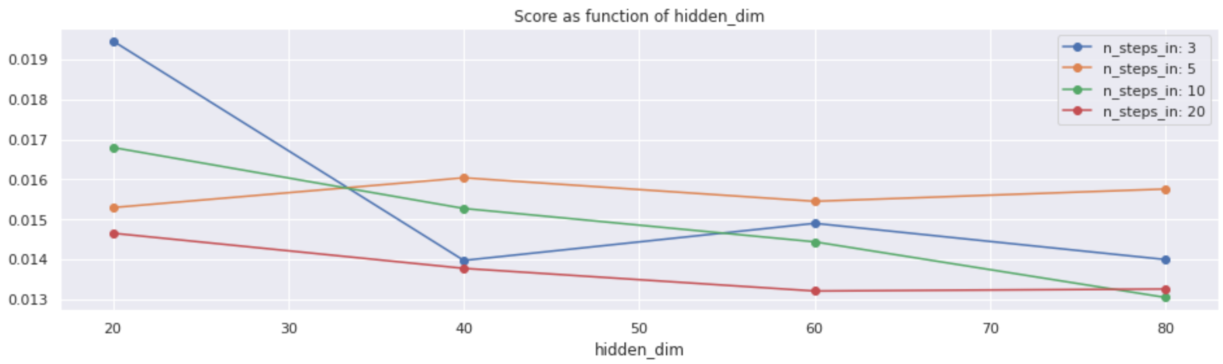
```
# Set data to plot
data = search1
best = data.iloc[0]
```

```
In [10]: # Plot score vs n_steps_in
plot_score(data, variable='n_steps_in', category='model_name') # averaged over hidden_dim
plot_score(data, variable='n_steps_in', category='hidden_dim')
```



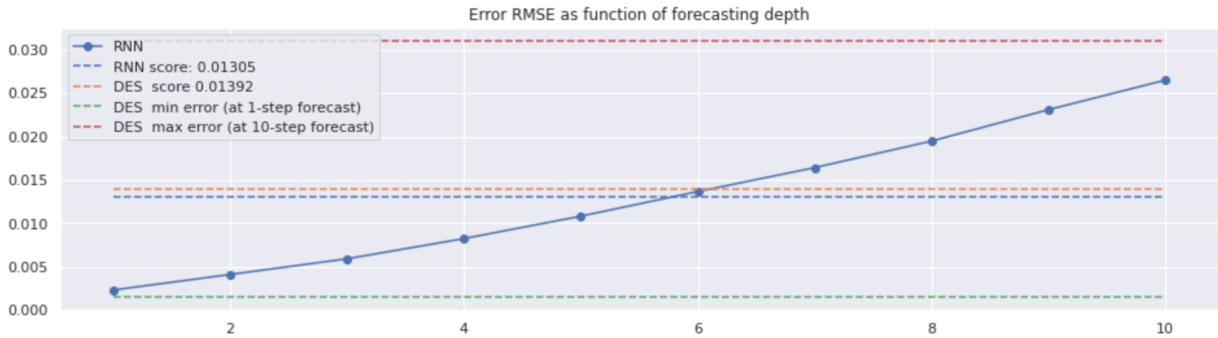



```
In [11]: # Plot score vs hidden_dim
plot_score(data, variable='hidden_dim', category='model_name') # averaged over n_steps_in
plot_score(data, variable='hidden_dim', category='n_steps_in')
```




```
In [ ]: # # Plot training histories
# labels = ['n_steps_in','hidden_dim']
# for i in range(len(data)):
#     title = ' run '+str(i+1)
#     for lab in labels: title=title+'   '+lab+': '+str(data[lab].loc[i])
#     plot_training_loss(data['train_hist'].loc[i], hide_first=2, title=title, lin=False)
```

In [13]:
```
# Construct train and dev sets
X_train, y_train, t_train = split_sequence(time_series_train, best['n_steps_in'], best['n_steps_ou
t'])
X_dev, y_dev, t_dev = split_sequence(time_series_dev, best['n_steps_in'], best['n_steps_out'])
# Forecasting and scoring
forecast = direct_forecast(X_dev, y_dev, t_dev, best['model'])  # for implementation of direct_for
ecast(), see temp-ml-scripts.py
errors, score = evaluate_model_performance(forecast)           # for implementation of evaluate_m
odel_performance(), see temp-ml-scripts.py
compare_score(errors, score)                                    # for implementation of compare_sc
ore(), see temp-ml-scripts.py
```



In [14]:
```
# Best score (lowest) in current search
print('best score: ',best['score'])
print('n_steps_in: ',best['n_steps_in'])
print('hidden_dim: ',best['hidden_dim'])
```

```
best score:  0.013046260658448596
n_steps_in:  10
hidden_dim:  80
```

For the estimated best combination of `n_steps_out` and `hidden_dim` , this RNN model outperforms the mathematical DES model.

Search 2: Vary architectures and number of input steps

Looking for better performance, a next step would be to change the neural network architecture itself. In this search, three different architectures are considered, schematically:

- LSTM + Dense
- LSTM + LSTM + Dense
- Conv1D + LSTM + Dense

and each are considered with a few values of `n_steps_in` .

In [15]:

```
# Define models
def select_model(param):
    """
    Selects a model from a list of different neural networks
    """
    # Three different recurrent neural network architectures with a comparable number of neurons ~
O(30k-40k)
    # Same network architecture as above
    if param['model_name'] == 'mod1':
        model = tf.keras.models.Sequential([
            tf.keras.layers.LSTM(100, activation='relu', input_shape=(param['n_steps_in'], 1)),
            tf.keras.layers.Dense(param['n_steps_out'], activation='linear')
        ])
    # Deeper network: stack of two LSTM layers
    if param['model_name'] == 'mod2':
        model = tf.keras.models.Sequential([
            tf.keras.layers.LSTM(60, activation='relu', return_sequences=True, input_shape=(param[
'n_steps_in'], 1)),
            tf.keras.layers.LSTM(50, activation='relu'),
            tf.keras.layers.Dense(param['n_steps_out'], activation='linear')
        ])
    # Deeper network: preprocess input with Conv1D, before feeding into LSTM
    if param['model_name'] == 'mod3':
        model = tf.keras.models.Sequential([
            tf.keras.layers.Conv1D(filters=128, kernel_size=5, strides=1, padding='causal', activa
tion='relu', input_shape=(param['n_steps_in'], 1)),
            tf.keras.layers.LSTM(50, activation='relu'),
            tf.keras.layers.Dense(param['n_steps_out'], activation='linear')
        ])
    return model

for name in ['mod1','mod2','mod3']:
    print(name,select_model({'model_name':name,'n_steps_in':20,'n_steps_out':10}).count_params())
```

```
mod1 41810
mod2 37590
mod3 37078
```

In [16]:

```
# Define parameter ranges
param_values = {
    # always keep fixed
    'n_steps_out' : [10],
    'min_n_epochs' : [200],
    'max_n_epochs' : [200],
    'patience' : [0],
    # vary
    'model_name' : ['mod1','mod2','mod3'],
    'n_steps_in': [5,10,20]
}

# Run grid search
search2 = grid_search(param_values)
search2.to_csv('search2.csv')
search2[['neurons','n_epochs','model_name','n_steps_in','score']]
```

```
 1/ 9   0:02:41   200 epochs   41810 neurons   score = 0.015034   {'model_name': 'mod1', 'n_steps
_in': 5}
 2/ 9   0:04:20   200 epochs   41810 neurons   score = 0.013529   {'model_name': 'mod1', 'n_steps
_in': 10}
 3/ 9   0:07:33   200 epochs   41810 neurons   score = 0.012665   {'model_name': 'mod1', 'n_steps
_in': 20}
 4/ 9   0:03:34   200 epochs   37590 neurons   score = 0.014552   {'model_name': 'mod2', 'n_steps
_in': 5}
 5/ 9   0:05:39   200 epochs   37590 neurons   score = 0.012213   {'model_name': 'mod2', 'n_steps
_in': 10}
 6/ 9   0:10:03   200 epochs   37590 neurons   score = 0.011758   {'model_name': 'mod2', 'n_steps
_in': 20}
 7/ 9   0:02:23   200 epochs   37078 neurons   score = 0.013453   {'model_name': 'mod3', 'n_steps
_in': 5}
 8/ 9   0:03:32   200 epochs   37078 neurons   score = 0.011682   {'model_name': 'mod3', 'n_steps
_in': 10}
 9/ 9   0:05:51   200 epochs   37078 neurons   score = 0.011858   {'model_name': 'mod3', 'n_steps
_in': 20}
```

Out[16]:

	neurons	n_epochs	model_name	n_steps_in	score
7	37078	200	mod3	10	0.0116822
5	37590	200	mod2	20	0.0117579
8	37078	200	mod3	20	0.0118578
4	37590	200	mod2	10	0.0122131
2	41810	200	mod1	20	0.0126651
6	37078	200	mod3	5	0.0134535
1	41810	200	mod1	10	0.013529
3	37590	200	mod2	5	0.0145517
0	41810	200	mod1	5	0.0150335

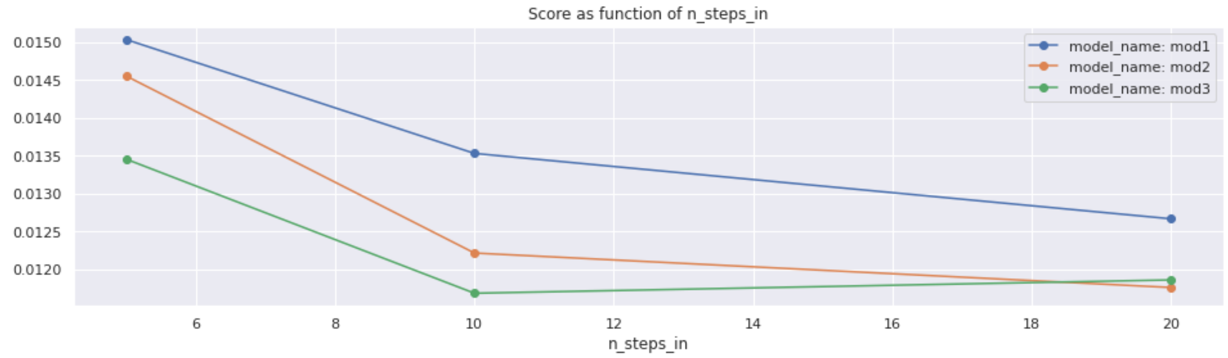
- Plot the results of each run
- Plot the training history of each run
- Plot the best score in comparison to the mathematical model

In [17]:

```
# Set data to plot
data = search2
best = data.iloc[0]
```

In [18]:

```
# Plot score vs model_name
plot_score(data, variable='n_steps_in', category='model_name')
```

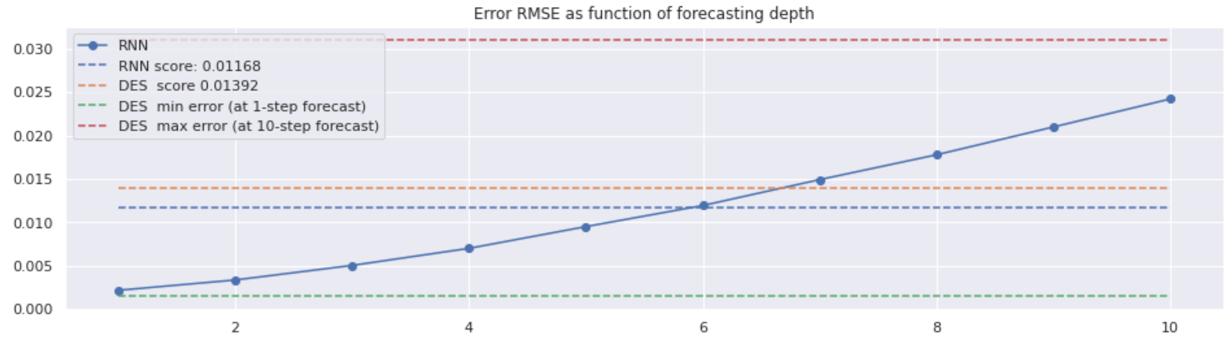


In [ ]:

```
# # Plot training histories
# labels = ['model_name', 'n_steps_in']
# for i in range(len(data)):
#     title = ' run '+str(i+1)
#     for lab in labels: title=title+'   '+lab+': '+str(data[lab].loc[i])
#     plot_training_loss(data['train_hist'].loc[i], hide_first=2, title=title, lin=False)
```

In [20]:

```
# Construct train and dev sets
X_train, y_train, t_train = split_sequence(time_series_train, best['n_steps_in'], best['n_steps_out'])
X_dev, y_dev, t_dev = split_sequence(time_series_dev, best['n_steps_in'], best['n_steps_out'])
# Forecasting and scoring
forecast = direct_forecast(X_dev, y_dev, t_dev, best['model'])  # for implementation of direct_forecast(), see temp-ml-scripts.py
errors, score = evaluate_model_performance(forecast)            # for implementation of evaluate_model_performance(), see temp-ml-scripts.py
compare_score(errors, score)                                    # for implementation of compare_score(), see temp-ml-scripts.py
```



In [21]:

```
# Best score (lowest) in current search
print('best score: ',best['score'])
print('model_name: ',best['model_name'])
print('n_steps_in: ',best['n_steps_in'])
```

```
best score:  0.011682168575362629
model_name:  mod3
n_steps_in:  10
```

The third model, Conv1D + LSTM + Dense, has shown significant performance improvement.

Search 3: vary Conv1D model parameters: filters, input steps, kernel

This search focusses on the third model and attempts to optimize the parameters of the Conv1D layer

- filters
- input steps
- kernel size

In [22]:
```
# Define models
def select_model(param):
    """
    Selects a model from a list of different neural networks
    """
    # Conv1D + LSTM + Dense
    if param['model_name'] == 'mod3':
        model = tf.keras.models.Sequential([
            tf.keras.layers.Conv1D(filters=param['filters'], kernel_size=param['kernel'], strides=
1, padding='causal', activation='relu', input_shape=(param['n_steps_in'], 1)),
            tf.keras.layers.LSTM(param['hidden_dim'], activation='relu'),
            tf.keras.layers.Dense(param['n_steps_out'], activation='linear')
        ])
    return model
```

In [23]:
```
# Define parameter ranges
param_values = {
    # always keep fixed
    'n_steps_out' : [10],
    'min_n_epochs' : [200],
    'max_n_epochs' : [400],
    'patience' : [50],
    # keep fixed
    'model_name' : ['mod3'],
    'hidden_dim' : [20],
    # vary
    'filters' : [32,64,128],
    'n_steps_in': [5,10,20],
    'kernel' : [3,5,10]
}

# Run grid search
search3 = grid_search(param_values)
search3.to_csv('search3.csv')
search3[['neurons','n_epochs','filters','n_steps_in','kernel','score']]
```

```
 1/27   0:03:59   400 epochs    4578 neurons   score = 0.012606   {'filters': 32, 'n_steps_in':
5, 'kernel': 3}
 2/27   0:04:58   332 epochs    4578 neurons   score = 0.011662   {'filters': 32, 'n_steps_in': 1
0, 'kernel': 3}
 3/27   0:09:46   400 epochs    4578 neurons   score = 0.011982   {'filters': 32, 'n_steps_in': 2
0, 'kernel': 3}
 4/27   0:03:53   400 epochs    4642 neurons   score = 0.013564   {'filters': 32, 'n_steps_in':
5, 'kernel': 5}
 5/27   0:05:55   400 epochs    4642 neurons   score = 0.011797   {'filters': 32, 'n_steps_in': 1
0, 'kernel': 5}
 6/27   0:07:06   284 epochs    4642 neurons   score = 0.012197   {'filters': 32, 'n_steps_in': 2
0, 'kernel': 5}
 7/27   0:03:53   400 epochs    4802 neurons   score = 0.013823   {'filters': 32, 'n_steps_in':
5, 'kernel': 10}
 8/27   0:05:22   353 epochs    4802 neurons   score = 0.012422   {'filters': 32, 'n_steps_in': 1
0, 'kernel': 10}
 9/27   0:08:10   326 epochs    4802 neurons   score = 0.012344   {'filters': 32, 'n_steps_in': 2
0, 'kernel': 10}
10/27   0:03:57   400 epochs    7266 neurons   score = 0.012675   {'filters': 64, 'n_steps_in':
5, 'kernel': 3}
11/27   0:05:22   342 epochs    7266 neurons   score = 0.011739   {'filters': 64, 'n_steps_in': 1
0, 'kernel': 3}
12/27   0:06:54   257 epochs    7266 neurons   score = 0.011618   {'filters': 64, 'n_steps_in': 2
0, 'kernel': 3}
13/27   0:03:35   329 epochs    7394 neurons   score = 0.013882   {'filters': 64, 'n_steps_in':
5, 'kernel': 5}
14/27   0:05:18   340 epochs    7394 neurons   score = 0.012022   {'filters': 64, 'n_steps_in': 1
0, 'kernel': 5}
15/27   0:09:31   373 epochs    7394 neurons   score = 0.011919   {'filters': 64, 'n_steps_in': 2
0, 'kernel': 5}
16/27   0:04:10   400 epochs    7714 neurons   score = 0.013433   {'filters': 64, 'n_steps_in':
5, 'kernel': 10}
17/27   0:05:33   345 epochs    7714 neurons   score = 0.012373   {'filters': 64, 'n_steps_in': 1
0, 'kernel': 10}
18/27   0:07:49   299 epochs    7714 neurons   score = 0.012636   {'filters': 64, 'n_steps_in': 2
0, 'kernel': 10}
19/27   0:04:17   400 epochs   12642 neurons   score = 0.011877   {'filters': 128, 'n_steps_in':
5, 'kernel': 3}
20/27   0:05:26   342 epochs   12642 neurons   score = 0.01175   {'filters': 128, 'n_steps_in': 1
0, 'kernel': 3}
21/27   0:09:48   373 epochs   12642 neurons   score = 0.012328   {'filters': 128, 'n_steps_in':
20, 'kernel': 3}
22/27   0:02:51   263 epochs   12898 neurons   score = 0.012719   {'filters': 128, 'n_steps_in':
5, 'kernel': 5}
23/27   0:04:43   290 epochs   12898 neurons   score = 0.011943   {'filters': 128, 'n_steps_in':
10, 'kernel': 5}
24/27   0:07:45   281 epochs   12898 neurons   score = 0.011558   {'filters': 128, 'n_steps_in':
20, 'kernel': 5}
25/27   0:04:28   400 epochs   13538 neurons   score = 0.012563   {'filters': 128, 'n_steps_in':
5, 'kernel': 10}
26/27   0:06:50   400 epochs   13538 neurons   score = 0.011382   {'filters': 128, 'n_steps_in':
10, 'kernel': 10}
27/27   0:08:43   320 epochs   13538 neurons   score = 0.011974   {'filters': 128, 'n_steps_in':
20, 'kernel': 10}
```

Out[23]:

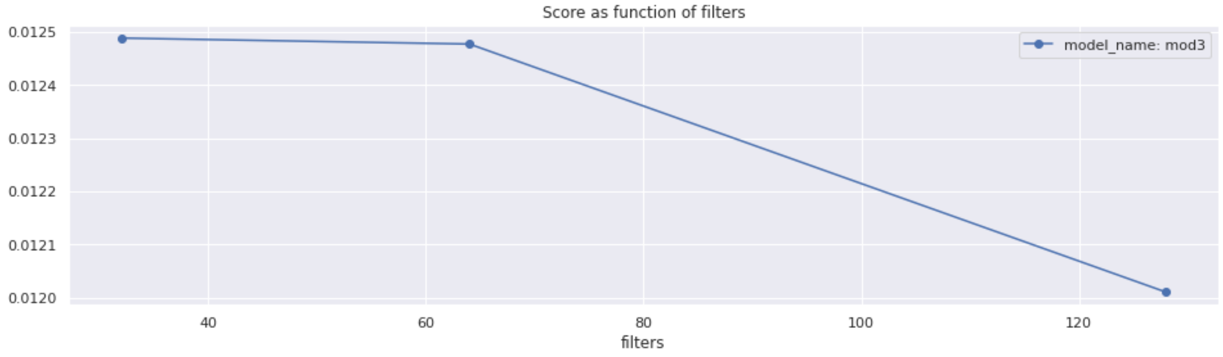
	neurons	n_epochs	filters	n_steps_in	kernel	score
25	13538	400	128	10	10	0.0113822
23	12898	281	128	20	5	0.011558
11	7266	257	64	20	3	0.0116181
1	4578	332	32	10	3	0.0116621
10	7266	342	64	10	3	0.0117389
19	12642	342	128	10	3	0.0117503
4	4642	400	32	10	5	0.011797
18	12642	400	128	5	3	0.011877
14	7394	373	64	20	5	0.0119194
22	12898	290	128	10	5	0.011943
26	13538	320	128	20	10	0.0119741
2	4578	400	32	20	3	0.0119817
13	7394	340	64	10	5	0.0120216
5	4642	284	32	20	5	0.012197
20	12642	373	128	20	3	0.0123278
8	4802	326	32	20	10	0.0123439
16	7714	345	64	10	10	0.0123727
7	4802	353	32	10	10	0.0124217
24	13538	400	128	5	10	0.0125631
0	4578	400	32	5	3	0.0126055
17	7714	299	64	20	10	0.0126355
9	7266	400	64	5	3	0.012675
21	12898	263	128	5	5	0.0127193
15	7714	400	64	5	10	0.0134331
3	4642	400	32	5	5	0.0135644
6	4802	400	32	5	10	0.0138235
12	7394	329	64	5	5	0.0138816

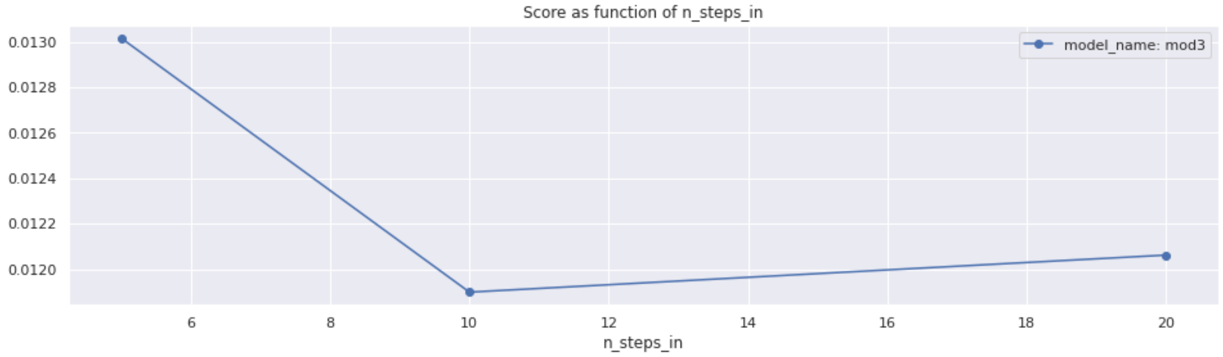
- Plot the results of each run
- Plot the training history of each run
- Plot the best score in comparison to the mathematical model

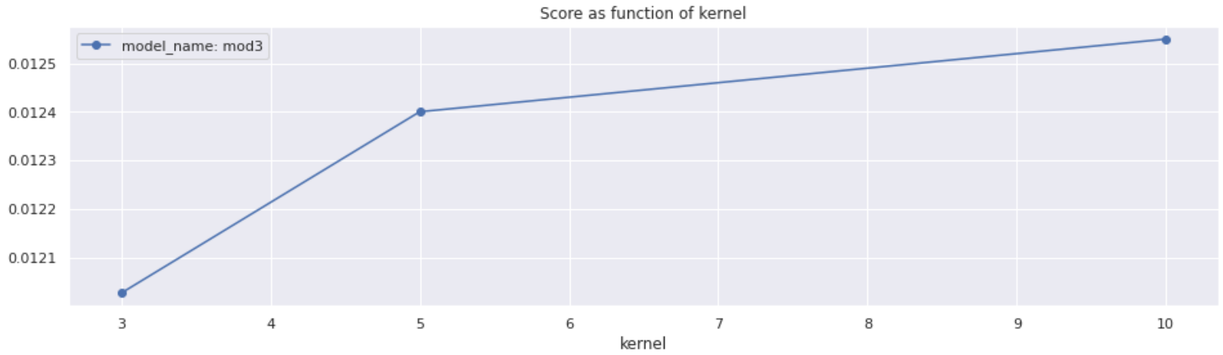
In [24]:

```
# Set data to plot
data = search3
best = data.iloc[0]
```

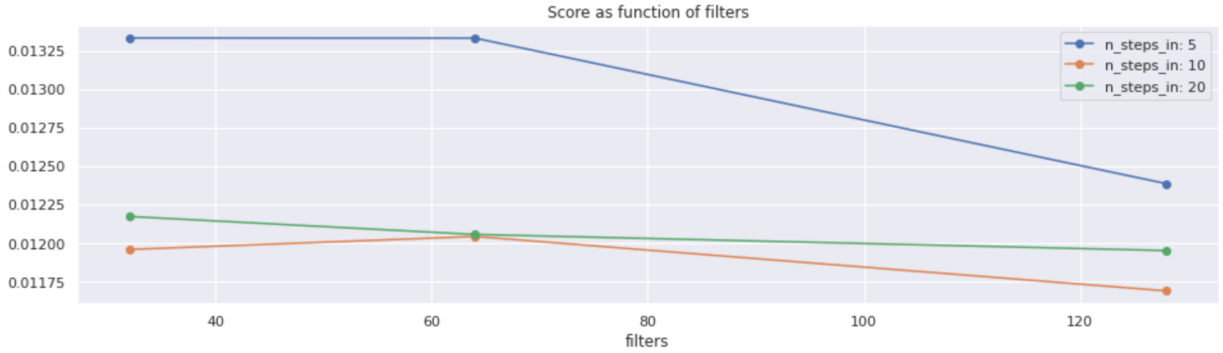
In [25]:
```
# Plot score
plot_score(data, variable='filters', category='model_name') # averaged over n_steps_in and kernel
plot_score(data, variable='n_steps_in', category='model_name') # averaged over filters and kernel
plot_score(data, variable='kernel', category='model_name') # averaged over filters and n_steps_in
```

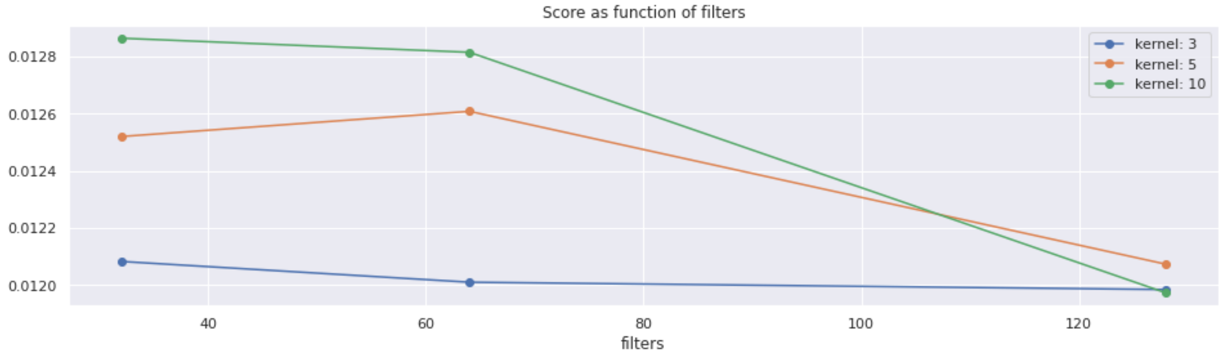




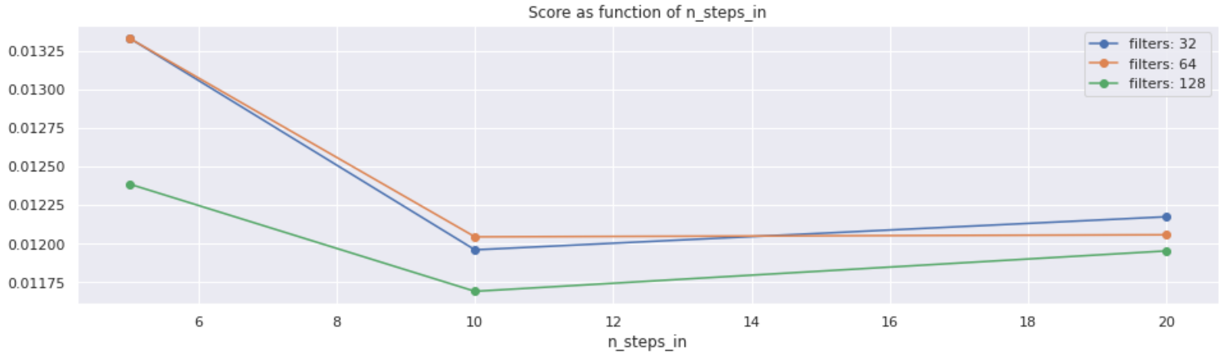


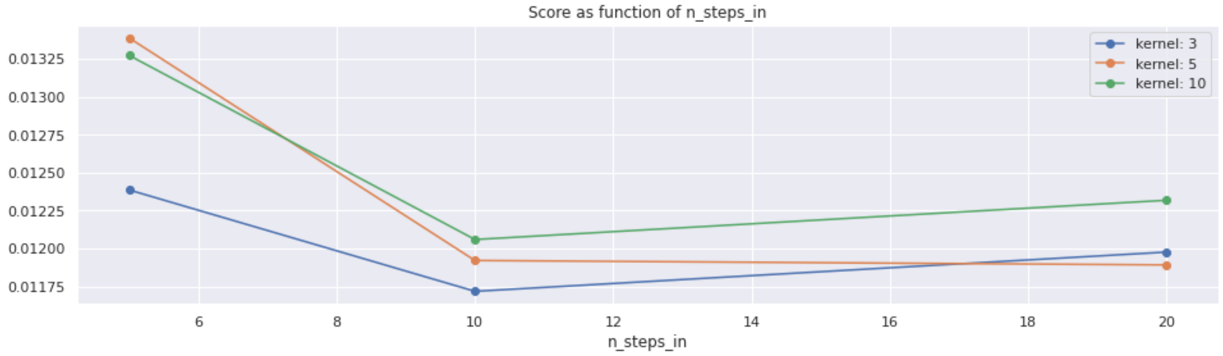
In [26]:
```
# More precise plots
plot_score(data, variable='filters', category='n_steps_in') # averaged over kernel
plot_score(data, variable='filters', category='kernel') # averaged over n_steps_in
```



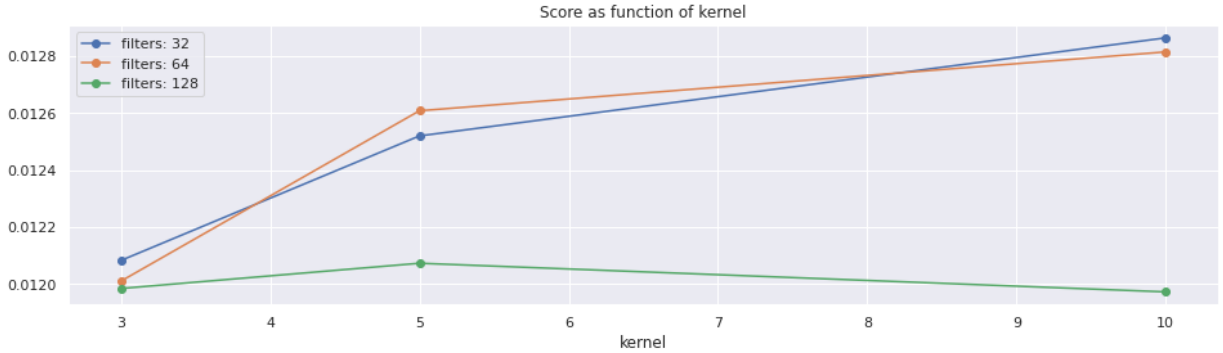


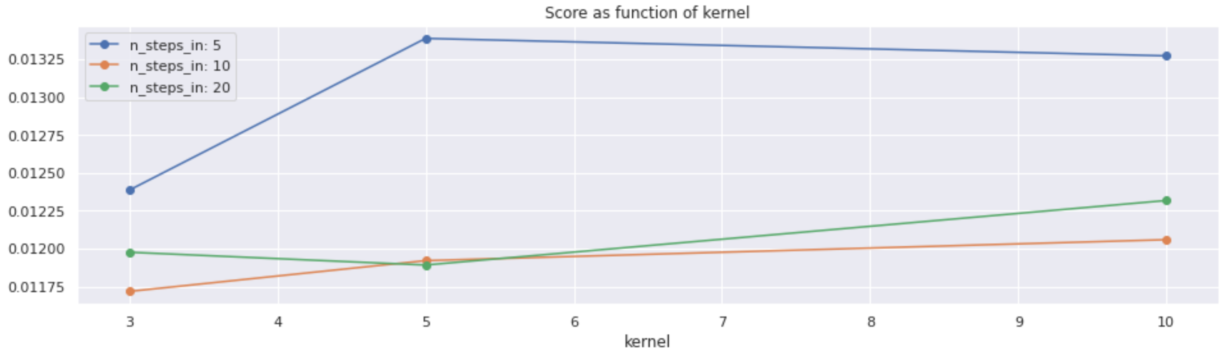
In [27]:
```
# More precise plots
plot_score(data, variable='n_steps_in', category='filters') # averaged over kernel
plot_score(data, variable='n_steps_in', category='kernel') # averaged over filters
```





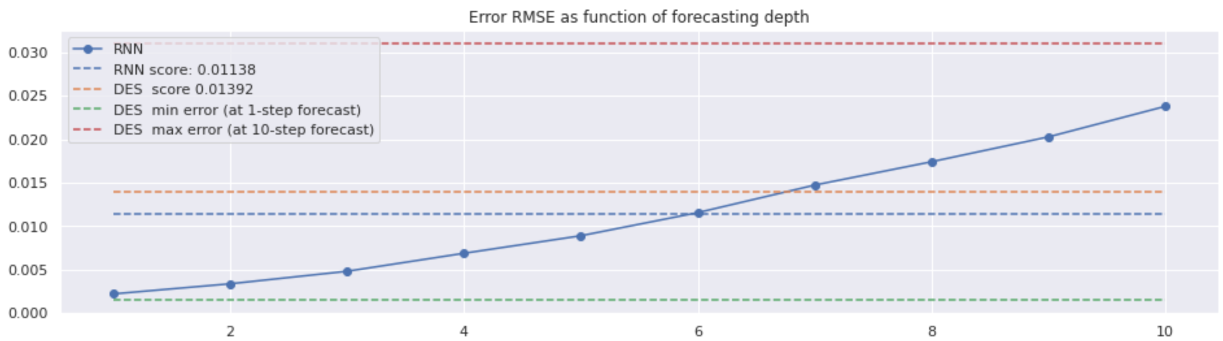
In [28]:
```python
# More precise plots
plot_score(data, variable='kernel', category='filters') # averaged over n_steps_in
plot_score(data, variable='kernel', category='n_steps_in') # averaged over filters
```





In [29]:
```python
# # Plot training histories
# labels = ['filters', 'n_steps_in', 'kernel']
# for i in range(len(data)):
#     title = ' run '+str(i+1)
#     for lab in labels: title=title+'   '+lab+': '+str(data[lab].loc[i])
#     plot_training_loss(data['train_hist'].loc[i], hide_first=2, title=title, lin=False)
```

In [30]:
```python
# Construct train and dev sets
X_train, y_train, t_train = split_sequence(time_series_train, best['n_steps_in'], best['n_steps_out'])
X_dev, y_dev, t_dev = split_sequence(time_series_dev, best['n_steps_in'], best['n_steps_out'])
# Forecasting and scoring
forecast = direct_forecast(X_dev, y_dev, t_dev, best['model'])  # for implementation of direct_forecast(), see temp-ml-scripts.py
errors, score = evaluate_model_performance(forecast)            # for implementation of evaluate_model_performance(), see temp-ml-scripts.py
compare_score(errors, score)                                    # for implementation of compare_score(), see temp-ml-scripts.py
```



In [31]:
```python
# Best score (lowest) in current search
print('best score: ',best['score'])
print('model_name: ',best['model_name'])
print('filters: ',best['filters'])
print('n_steps_in: ',best['n_steps_in'])
print('kernel: ',best['kernel'])
```

```
best score:  0.011382175017157109
model_name:  mod3
filters:  128
n_steps_in:  10
kernel:  10
```

After this parameter search, it is time to select the best model and demonstrate its performance.

Demonstration of best model

Load the best model from all runs in all searches

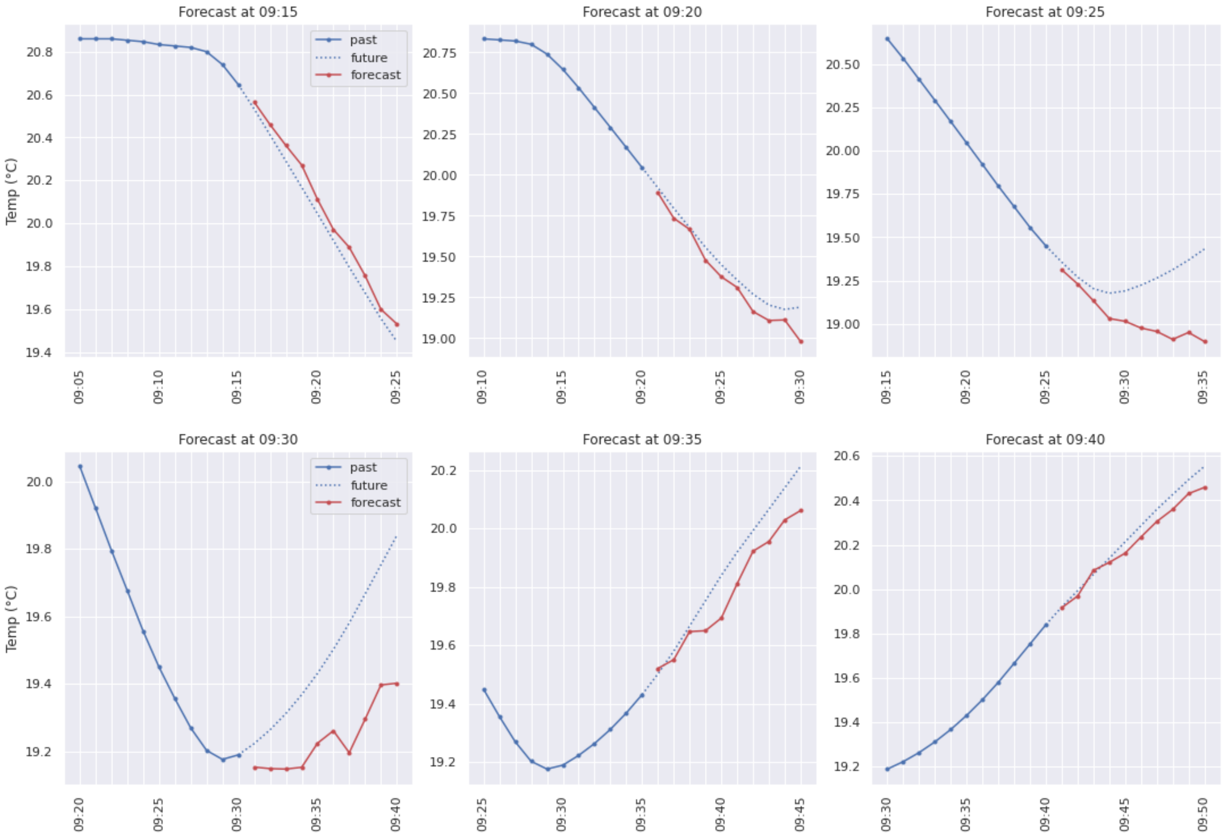
In [32]:
```
searches = [search1, search2, search3]
best_score = 999
for search in searches:
    cand = search.iloc[0]
    print('>',cand['score'])
    if cand['score'] < best_score:
        best_score = cand['score']
        best = cand

print('\nBest score: ',best_score)
print('\nModel details:\n'+str(best.iloc[:-5]))
```

```
> 0.013046260658448596
> 0.011682168575362629
> 0.011382175017157109

Best score:  0.011382175017157109

Model details:
filters            128
hidden_dim          20
kernel              10
max_n_epochs       400
min_n_epochs       200
model_name        mod3
n_steps_in          10
n_steps_out         10
patience            50
neurons          13538
n_epochs           400
Name: 25, dtype: object
```

In [33]:
```
best_model = best['model']
n_steps_in = best['n_steps_in']
n_steps_out = best['n_steps_out']

best_model.save('selected_best_model.h5')

# Construct dev and test sets
X_dev, y_dev, t_dev = split_sequence(time_series_dev, n_steps_in, n_steps_out)
X_test, y_test, t_test = split_sequence(time_series_test, n_steps_in, n_steps_out)

# Demonstrate model on test set
past = time_series_dev.iloc[-n_steps_out:]                    # past = last steps of dev...
past = past.append(time_series_test.iloc[:n_steps_out])       # ... and first steps of test
past = un_normalize_series(past)                              # un-normalize to degree Centigrad
e

# Forecasting
forecast = direct_forecast(X_test, y_test, t_test, best_model)  # for implementation of direct_for
ecast(), see temp-ml-scripts.py
forecast = un_normalize_series(forecast)                      # un-normalize to degree Centigrad
e
```

In [34]:

```
# Forecasting in a valley
Demonstration(past, forecast, cols=3, rows=2, start=557-10, step=5)
```



In [35]:

```
# Forecasting on a bumpy downhill slope
Demonstration(past, forecast, cols=3, rows=2, start=662-10, step=5)
```