# prior_montecarlo

May 11, 2019

## 1 Run and process the prior monte carlo and pick a "truth" realization

A great advantage of exploring a synthetic model is that we can enforce a "truth" and then evaluate how our various attempts to estimate it perform. One way to do this is to run a monte carlo ensemble of multiple parameter realizations and then choose one of them to represent the "truth". That will be accomplished in this notebook.

In [1]:
```
import os
import shutil
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import matplotlib as mpl
plt.rcParams['font.size']=12
import flopy
import pyemu
```

```
flopy is installed in /Users/jeremyw/Dev/gw1876/activities_2day_mfm/notebooks/flopy
```

#### 1.0.1 set the `t_d` or "template directory" variable to point at the template folder and read in the PEST control file

In [2]:
```
t_d = "template"
pst = pyemu.Pst(os.path.join(t_d,"freyberg.pst"))
```

#### 1.0.2 Decide what pars are uncertain in the truth

We need to decide what our truth looks like - should the pilot points or the grid-scale pars be the source of spatial variability? or both?

In [3]:
```
par = pst.parameter_data
# grid pars
#should_fix = par.loc[par.pargp.apply(lambda x: "gr" in x),"parnme"]
# pp pars
#should_fix = par.loc[par.pargp.apply(lambda x: "pp" in x),"parnme"]
#pst.npar - should_fix.shape[0]
```

```
In [4]: pe = pyemu.ParameterEnsemble.from_binary(pst=pst,filename=os.path.join(t_d,"prior.jcb"
        #pe.loc[:,should_fix] = 1.0
        pe.to_csv(os.path.join(t_d,"sweep_in.csv"))
```

```
new binary format detected...
```

### 1.0.3 run the prior ensemble in parallel locally

This takes advantage of the program `pestpp-swp` which runs a parameter sweep through a set of parameters. By default, `pestpp-swp` reads in the ensemble from a file called `sweep_in.csv` which in this case we made just above.

```
In [5]: m_d = "master_prior_sweep"
        pyemu.os_utils.start_slaves(t_d,"pestpp-swp","freyberg.pst",num_slaves=20,slave_root="
```

### 1.0.4 Load the output ensemble and plot a few things

```
In [6]: obs_df = pd.read_csv(os.path.join(m_d,"sweep_out.csv"),index_col=0)
        print('number of realization in the ensemble before dropping: ' + str(obs_df.shape[0])
```

```
number of realization in the ensemble before dropping: 200
```

drop any failed runs

```
In [7]: obs_df = obs_df.loc[obs_df.failed_flag==0,:]
        print('number of realization in the ensemble **after** dropping: ' + str(obs_df.shape[
```

```
number of realization in the ensemble **after** dropping: 200
```

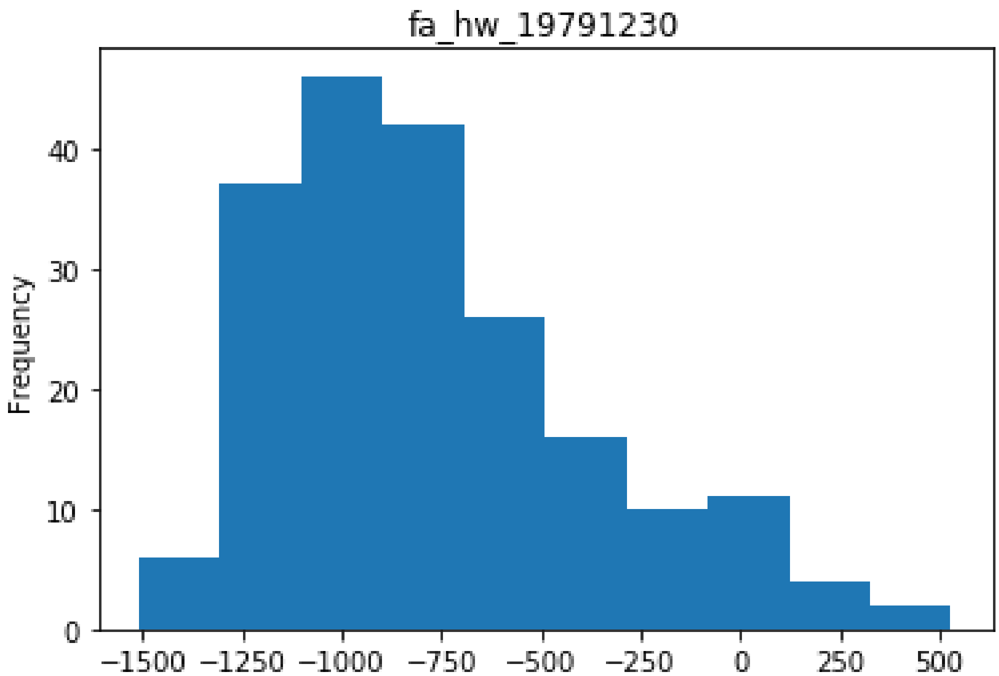
### 1.0.5 confirm which quantities were identified as forecasts

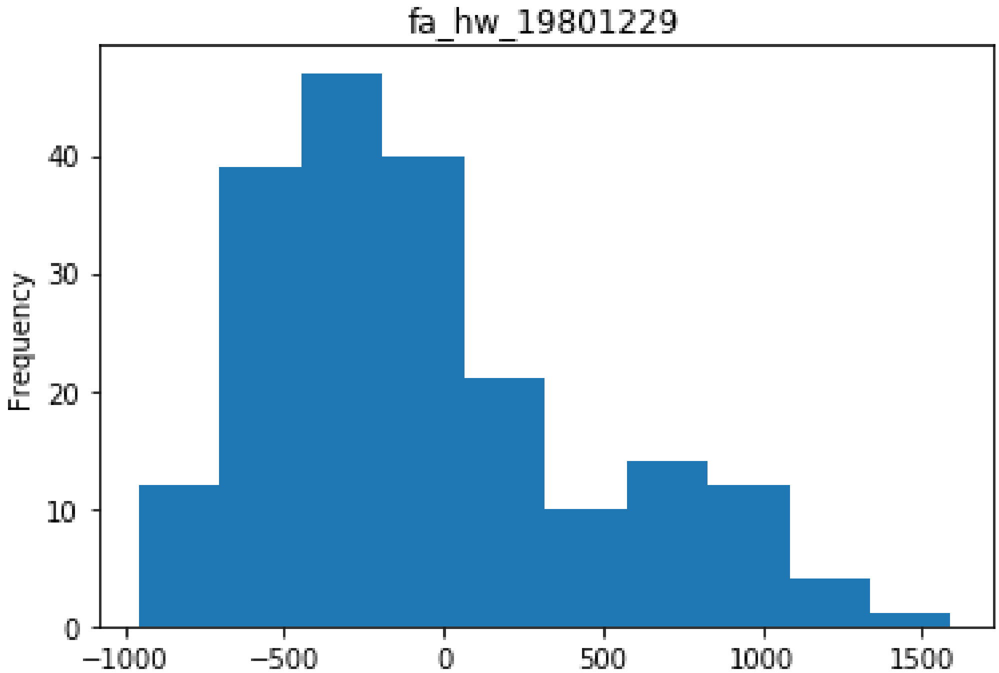
```
In [8]: fnames = pst.pestpp_options["forecasts"].split(',')
        fnames
```

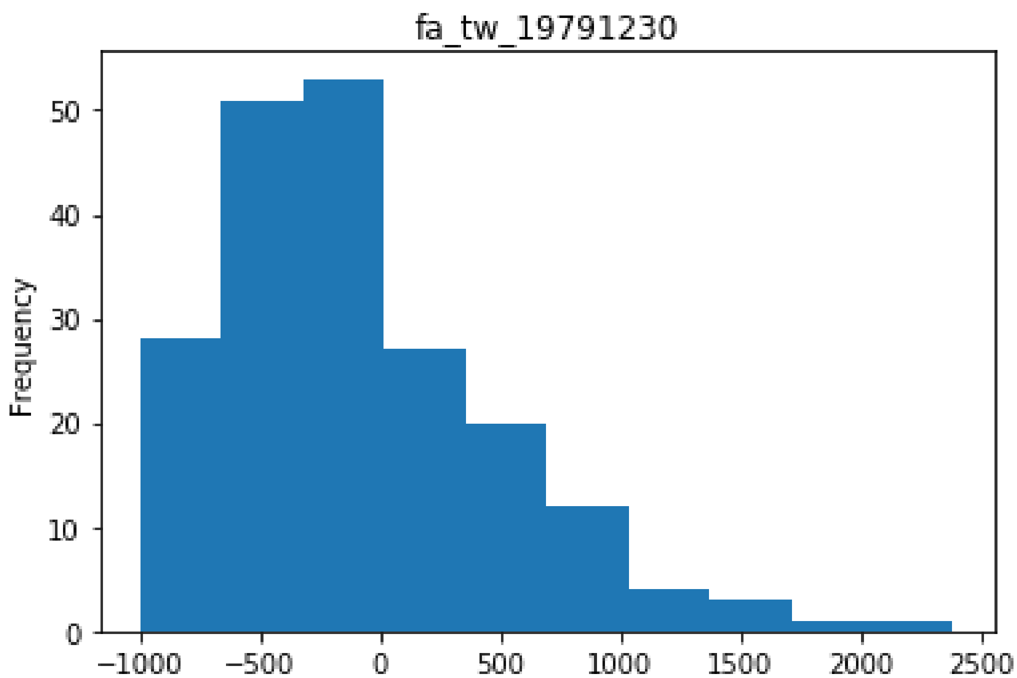
```
Out[8]: ['fa_hw_19791230',
         'fa_hw_19801229',
         'fa_tw_19791230',
         'fa_tw_19801229',
         'hds_00_013_002_000',
         'hds_00_013_002_001',
         'part_time',
         'part_status']
```

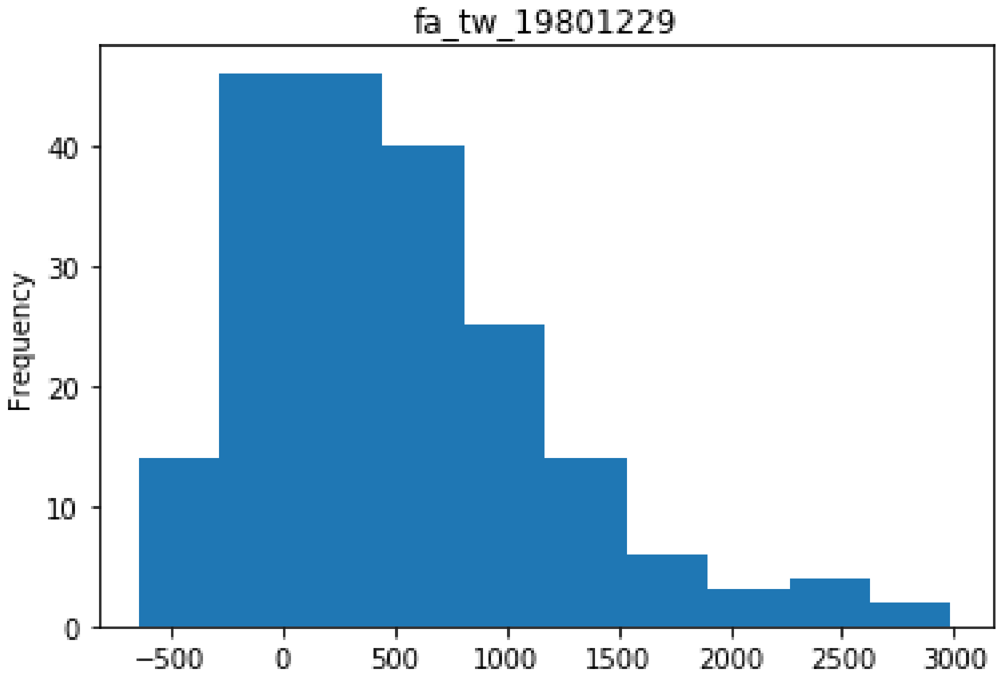
### 1.0.6 now we can plot the distributions of each forecast

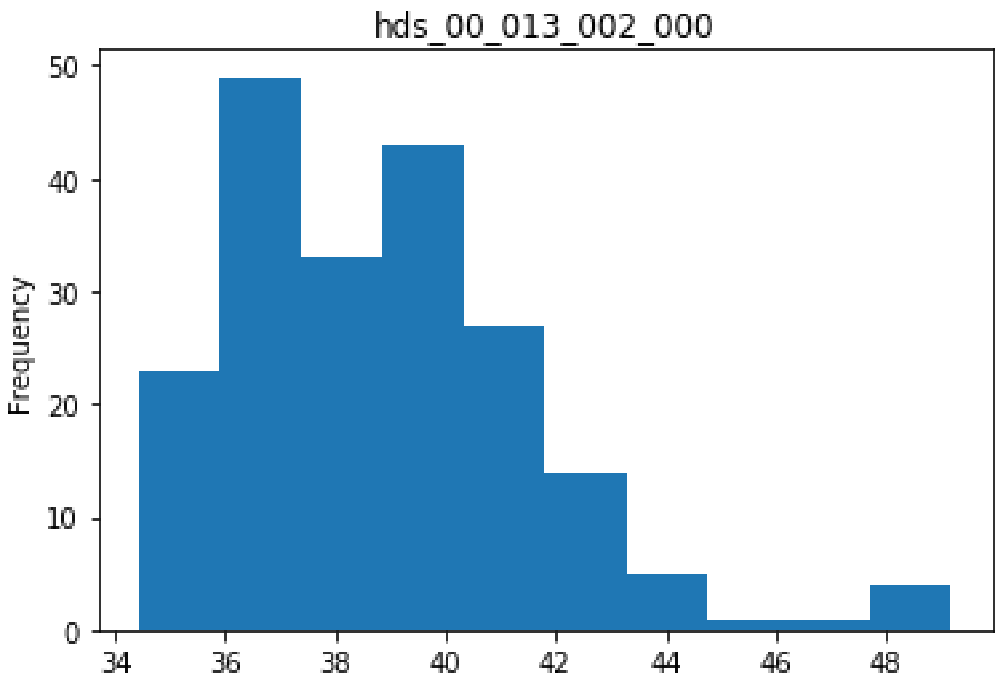
```
In [9]: for forecast in fnames:
            plt.figure()
            ax = obs_df.loc[:,forecast].plot(kind="hist")
            ax.set_title(forecast)
        plt.show()
```

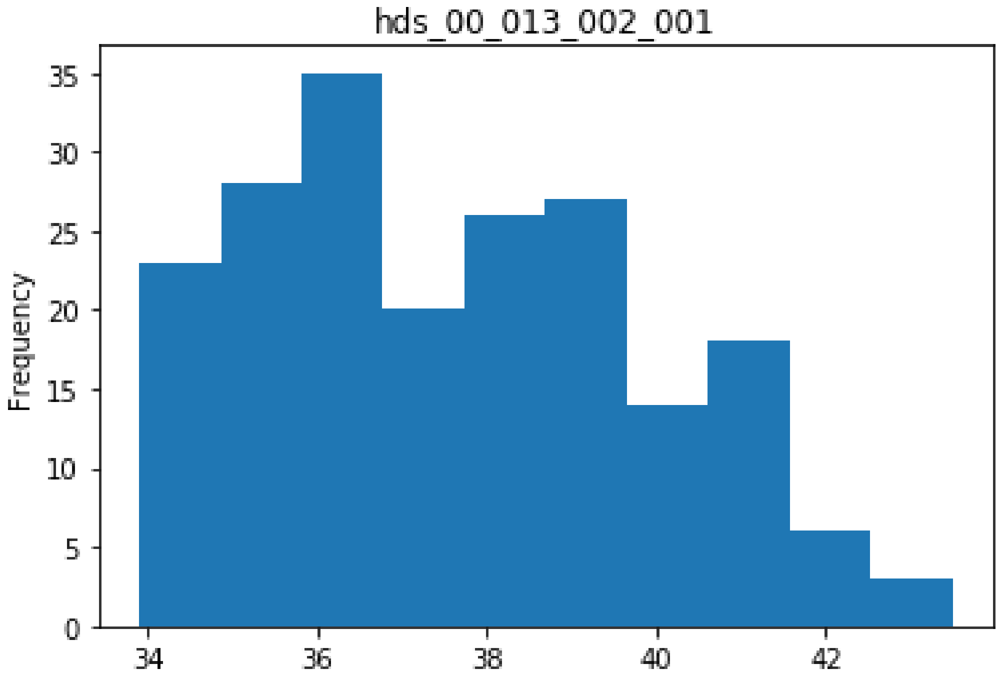


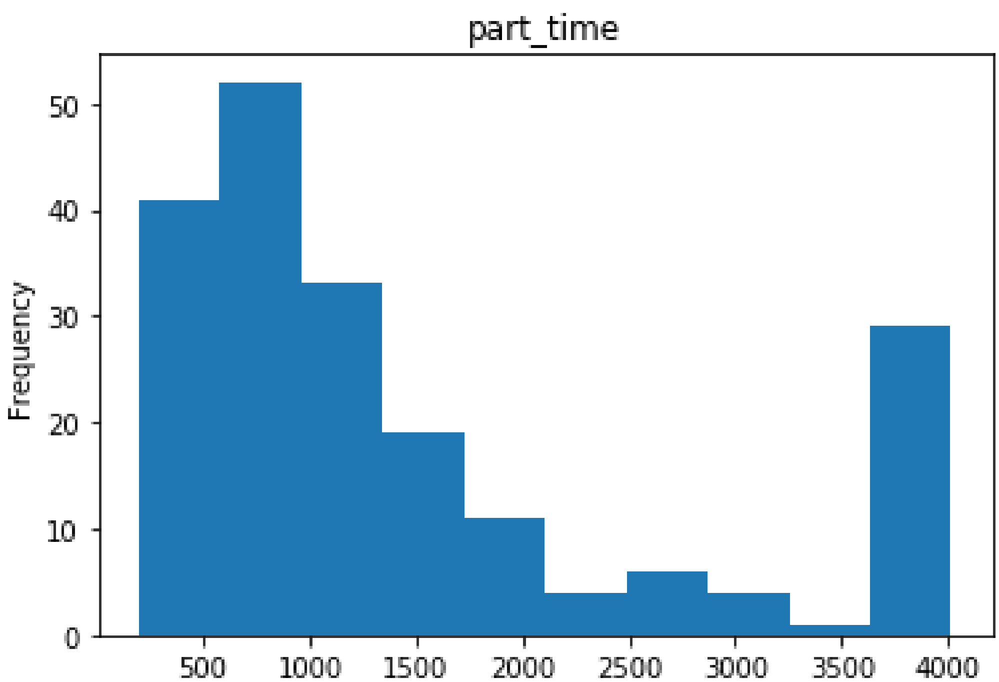

fa_hw_19801229
Frequency
0
10
20
30
40
−1000
−500
0
500
1000
1500

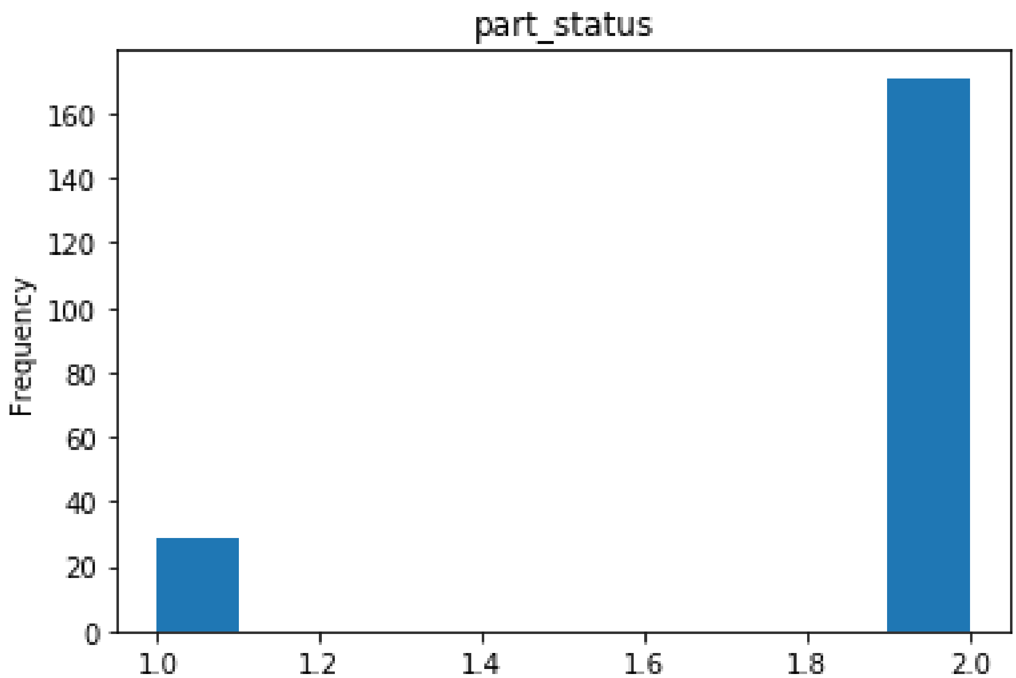

fa_tw_19791230
Frequency
0
10
20
30
40
50
−1000
−500
0
500
1000
1500
2000
2500


fa_tw_19801229
Frequency
0
10
20
30
40
−500
0
500
1000
1500
2000
2500
3000


hds_00_013_002_000
Frequency
0
10
20
30
40
50
34
36
38
40
42
44
46
48

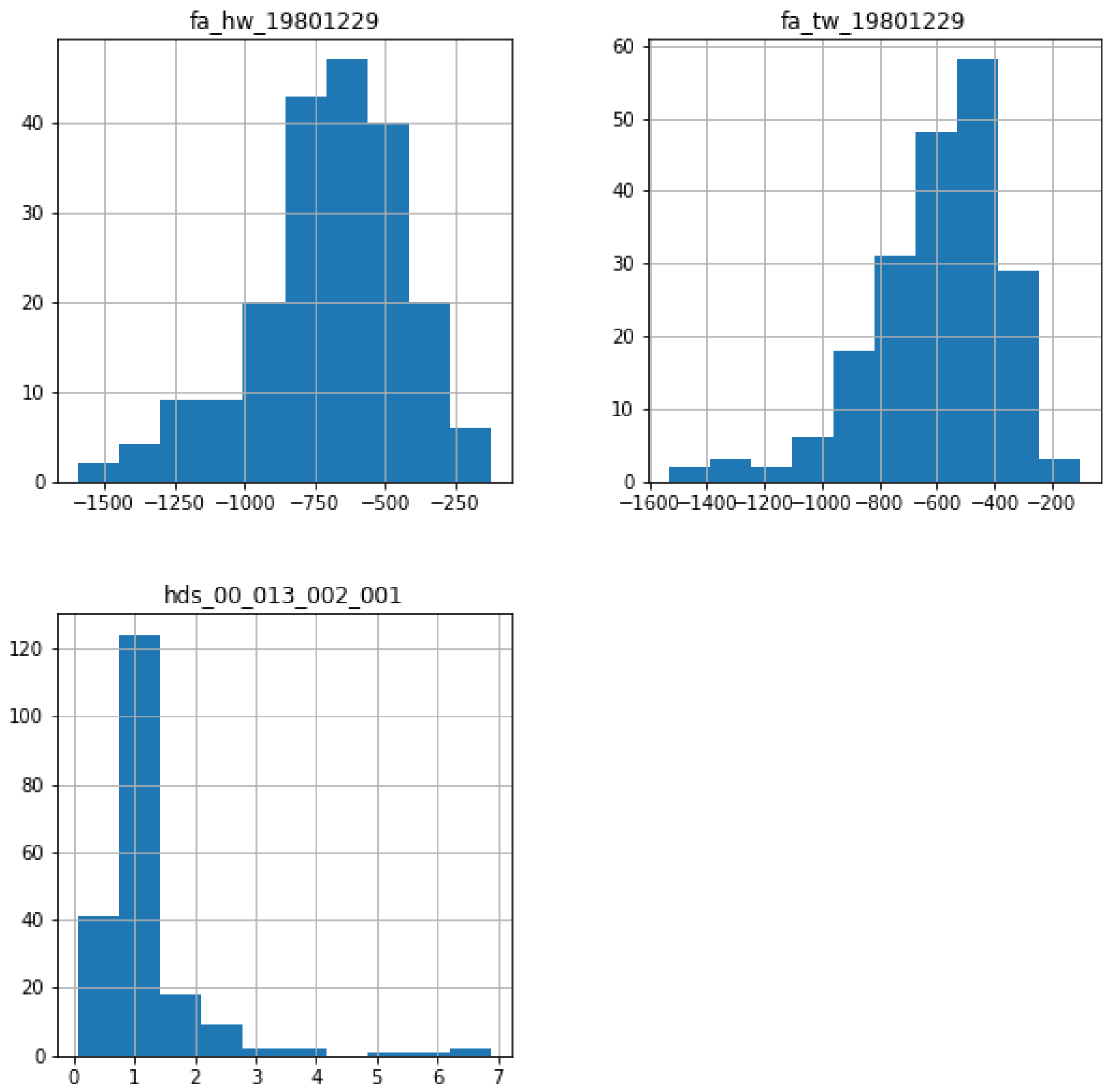

hds_00_013_002_001
Frequency
35
30
25
20
15
10
5
0
34
36
38
40
42


part_time
Frequency
50
40
30
20
10
0
500
1000
1500
2000
2500
3000
3500
4000




We see that under scenario conditions, many more realizations for the flow to the aquifer in the headwaters are postive (as expected). Lets difference these two:

```
In [10]: sfnames = [f for f in fnames if "1980" in f or "_001" in f]
         hfnames = [f for f in fnames if "1979" in f or "_000" in f]
         diff = obs_df.loc[:,hfnames].values - obs_df.loc[:,sfnames].values
         diff = pd.DataFrame(diff,columns=sfnames)
         diff.hist(figsize=(10,10))
         plt.show()
```




We now see that the most extreme scenario yields a large decrease in flow from the aquifer to the headwaters (the most negative value)

#### 1.0.7 setting the "truth"

We just need to replace the observed values (`obsval`) in the control file with the outputs for one of the realizations on `obs_df`. In this way, we now have the nonzero values for history matching, but also the `truth` values for comparing how we are doing with other unobserved quantities. I'm going to pick a realization that yields an "average" variability of the observed gw levels:

```
In [11]: # choose the realization with a low historic gw to sw headwater flux
         #hist_swgw = obs_df.loc[:,"fa_hw_19791230"].sort_values()
         hist_swgw = obs_df.loc[:,"part_time"].sort_values()
         idx = hist_swgw.index[20]
```

```
         idx
         hist_swgw

Out[11]: run_id
         149     198.1387
         41      265.3273
         165     276.1939
         120     293.1571
         37      313.4481
         96      325.5403
         0       342.4888
         173     358.4053
         77      361.9629
         64      372.9315
         73      374.5064
         145     380.7252
         16      394.1340
         40      395.1985
         35      405.8629
         128     424.2145
         78      427.1186
         51      447.5162
         21      451.1969
         117     451.4228
         194     458.4655
         131     463.7558
         27      464.6402
         184     476.3412
         57      484.2876
         19      501.6304
         162     520.8668
         182     524.6132
         107     525.4871
         141     529.1481
                    ...
         192    3467.2040
         101    4015.0000
         17     4015.0000
         187    4015.0000
         191    4015.0000
         118    4015.0000
         20     4015.0000
         193    4015.0000
         6      4015.0000
         3      4015.0000
         12     4015.0000
         183    4015.0000
         138    4015.0000
```

```
100    4015.0000
157    4015.0000
61     4015.0000
47     4015.0000
166    4015.0000
46     4015.0000
153    4015.0000
24     4015.0000
75     4015.0000
82     4015.0000
88     4015.0000
175    4015.0000
176    4015.0000
159    4015.0000
29     4015.0000
76     4015.0000
130    4015.0000
Name: part_time, Length: 200, dtype: float64
```

In [12]:
```
obs_df.loc[idx,pst.nnz_obs_names]
```

Out[12]:
```
fo_39_19791230          11302.000000
hds_00_002_009_000         36.058125
hds_00_002_015_000         35.212799
hds_00_003_008_000         36.083511
hds_00_009_001_000         37.389400
hds_00_013_010_000         35.048706
hds_00_015_016_000         34.838463
hds_00_021_010_000         34.814125
hds_00_022_015_000         34.552216
hds_00_024_004_000         35.209511
hds_00_026_006_000         34.681568
hds_00_029_015_000         34.122902
hds_00_033_007_000         33.345665
hds_00_034_010_000         33.317856
Name: 194, dtype: float64
```

Lets see how our selected truth does with the sw/gw forecasts:

In [13]:
```
obs_df.loc[idx,fnames]
```

Out[13]:
```
fa_hw_19791230        -826.113600
fa_hw_19801229        -412.139600
fa_tw_19791230         341.545050
fa_tw_19801229         704.034190
hds_00_013_002_000      36.989079
hds_00_013_002_001      36.173130
part_time              458.465500
part_status              2.000000
Name: 194, dtype: float64
```

Assign some initial weights. Now, it is custom to add noise to the observed values. . . we will use the classic Gaussian noise. . . zero mean and standard deviation of 1 over the weight

```
In [14]: pst = pyemu.Pst(os.path.join(t_d,"freyberg.pst"))
         obs = pst.observation_data
         obs.loc[:,"obsval"] = obs_df.loc[idx,pst.obs_names]
         obs.loc[obs.obgnme=="calhead","weight"] = 10.0
         obs.loc[obs.obgnme=="calflux","weight"] = 1.0
```

here we just get a sample from a random normal distribution with mean=0 and std=1. The argument indicates how many samples we want - and we choose `pst.nnz_obs` which is the the number of nonzero-weighted observations in the PST file

```
In [15]: np.random.seed(seed=0)
         snd = np.random.randn(pst.nnz_obs)
         noise = snd * 1./obs.loc[pst.nnz_obs_names,"weight"]
         pst.observation_data.loc[noise.index,"obsval"] += noise
         noise
```

```
Out[15]: obsnme
         fo_39_19791230        1.764052
         hds_00_002_009_000    0.040016
         hds_00_002_015_000    0.097874
         hds_00_003_008_000    0.224089
         hds_00_009_001_000    0.186756
         hds_00_013_010_000   -0.097728
         hds_00_015_016_000    0.095009
         hds_00_021_010_000   -0.015136
         hds_00_022_015_000   -0.010322
         hds_00_024_004_000    0.041060
         hds_00_026_006_000    0.014404
         hds_00_029_015_000    0.145427
         hds_00_033_007_000    0.076104
         hds_00_034_010_000    0.012168
         Name: weight, dtype: float64
```

Then we write this out to a new file and run `pestpp-ies` to see how the objective function looks

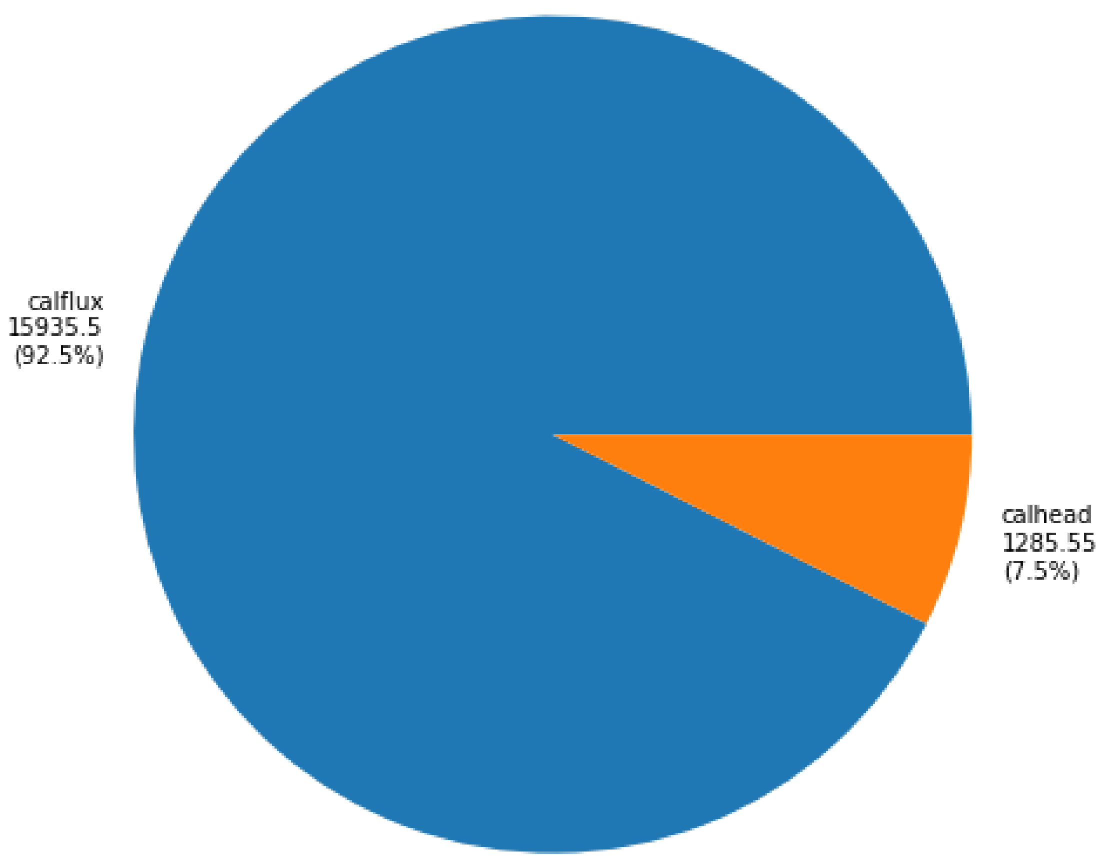
```
In [16]: pst.write(os.path.join(t_d,"freyberg.pst"))
         pyemu.os_utils.run("pestpp-ies freyberg.pst",cwd=t_d)
```

```
noptmax:0, npar_adj:14819, nnz_obs:14
```

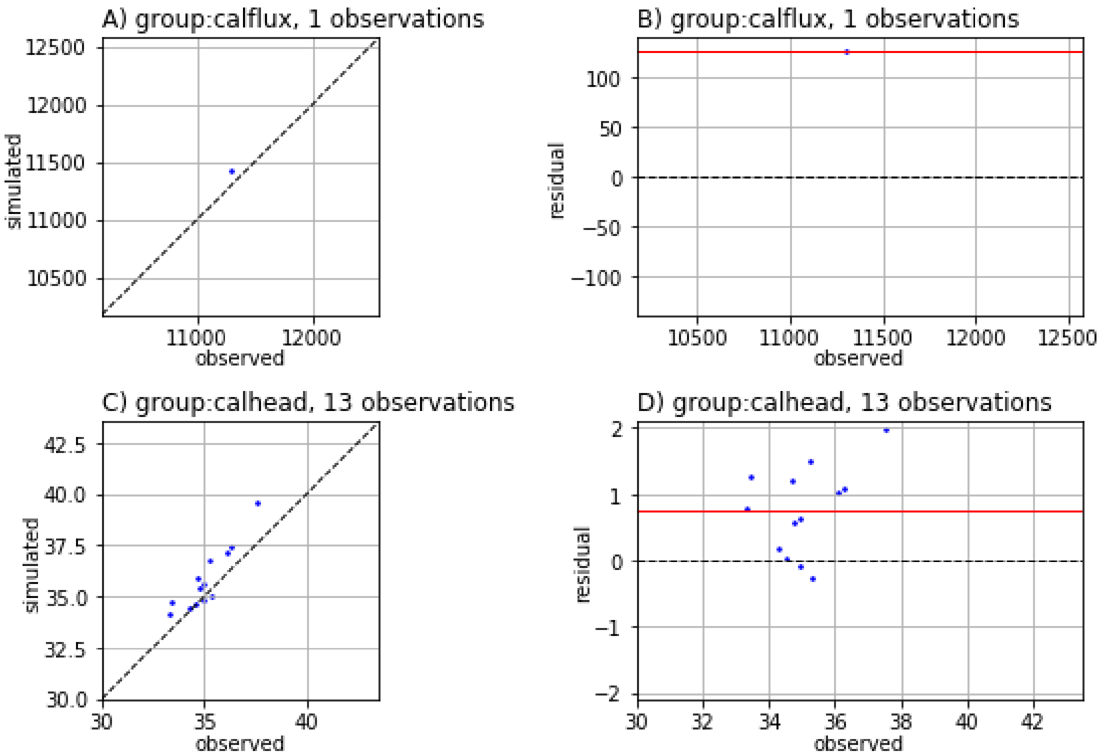
Now we can read in the results and make some figures showing residuals and the balance of the objective function

```
In [17]: pst = pyemu.Pst(os.path.join(t_d,"freyberg.pst"))
         print(pst.phi)
         plt.figure()
         pst.plot(kind='phi_pie')
         print('Here are the non-zero weighted observation names')

         figs = pst.plot(kind="1to1")
         plt.show()
         pst.res.loc[pst.nnz_obs_names,:]
```

```
17221.065640613586
Here are the non-zero weighted observation names


<Figure size 432x288 with 0 Axes>
```



```
<Figure size 576x756 with 0 Axes>
```



```
Out[17]:                                    name    group      measured      modelled  \
         name
         fo_39_19791230           fo_39_19791230  calflux  11303.764052  11430.000000
         hds_00_002_009_000   hds_00_002_009_000  calhead     36.098140     37.107498
         hds_00_002_015_000   hds_00_002_015_000  calhead     35.310673     35.045185
         hds_00_003_008_000   hds_00_003_008_000  calhead     36.307601     37.397289
         hds_00_009_001_000   hds_00_009_001_000  calhead     37.576156     39.546417
         hds_00_013_010_000   hds_00_013_010_000  calhead     34.950978     35.571774
         hds_00_015_016_000   hds_00_015_016_000  calhead     34.933472     34.835716
         hds_00_021_010_000   hds_00_021_010_000  calhead     34.798989     35.386250
         hds_00_022_015_000   hds_00_022_015_000  calhead     34.541894     34.577492
         hds_00_024_004_000   hds_00_024_004_000  calhead     35.250571     36.760464
         hds_00_026_006_000   hds_00_026_006_000  calhead     34.695973     35.896149
         hds_00_029_015_000   hds_00_029_015_000  calhead     34.268329     34.453842
         hds_00_033_007_000   hds_00_033_007_000  calhead     33.421769     34.678810
         hds_00_034_010_000   hds_00_034_010_000  calhead     33.330023     34.118073

                               residual  weight
         name
         fo_39_19791230     -126.235948     1.0
         hds_00_002_009_000   -1.009358    10.0
         hds_00_002_015_000    0.265488    10.0
         hds_00_003_008_000   -1.089689    10.0
         hds_00_009_001_000   -1.970261    10.0
         hds_00_013_010_000   -0.620795    10.0
         hds_00_015_016_000    0.097755    10.0
         hds_00_021_010_000   -0.587260    10.0
         hds_00_022_015_000   -0.035598    10.0
         hds_00_024_004_000   -1.509893    10.0
         hds_00_026_006_000   -1.200176    10.0
         hds_00_029_015_000   -0.185513    10.0
         hds_00_033_007_000   -1.257041    10.0
         hds_00_034_010_000   -0.788049    10.0
```

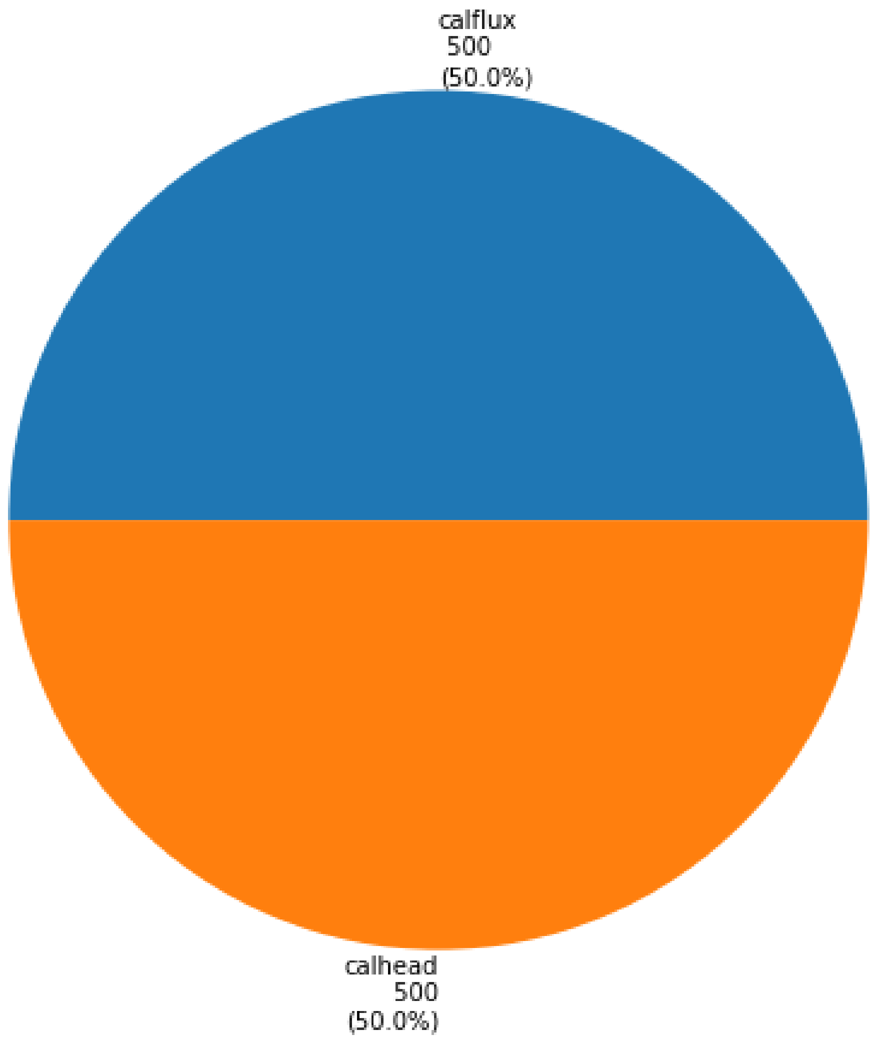
Publication ready figs - oh snap!

Depending on the truth you chose, we may have a problem - we set the weights for both the heads and the flux to reasonable values based on what we expect for measurement noise. But the contributions to total phi might be out of balance - if contribution of the flux measurement to total phi is too low, the history matching excersizes (coming soon!) will focus almost entirely on minimizing head residuals. So we need to balance the objective function. This is a subtle but very important step, especially since some of our forecasts deal with sw-gw exchange

```
In [18]: pc = pst.phi_components
         #target = {"calflux":0.3 * pc["calhead"]}
         target = {"calhead":500,"calflux":500}
```

```
pst.adjust_weights(obsgrp_dict=target)
pst.plot(kind='phi_pie')
```

Out[18]: <matplotlib.axes._subplots.AxesSubplot at 0x181d85e5c0>




Lets see what the new flux observation weight is:

In [19]:
```
pst.observation_data.loc[pst.nnz_obs_names,"weight"]
```

Out[19]:
```
obsnme
fo_39_19791230        0.177134
hds_00_002_009_000    6.236491
hds_00_002_015_000    6.236491
hds_00_003_008_000    6.236491
```

```
hds_00_009_001_000    6.236491
hds_00_013_010_000    6.236491
hds_00_015_016_000    6.236491
hds_00_021_010_000    6.236491
hds_00_022_015_000    6.236491
hds_00_024_004_000    6.236491
hds_00_026_006_000    6.236491
hds_00_029_015_000    6.236491
hds_00_033_007_000    6.236491
hds_00_034_010_000    6.236491
Name: weight, dtype: float64
```

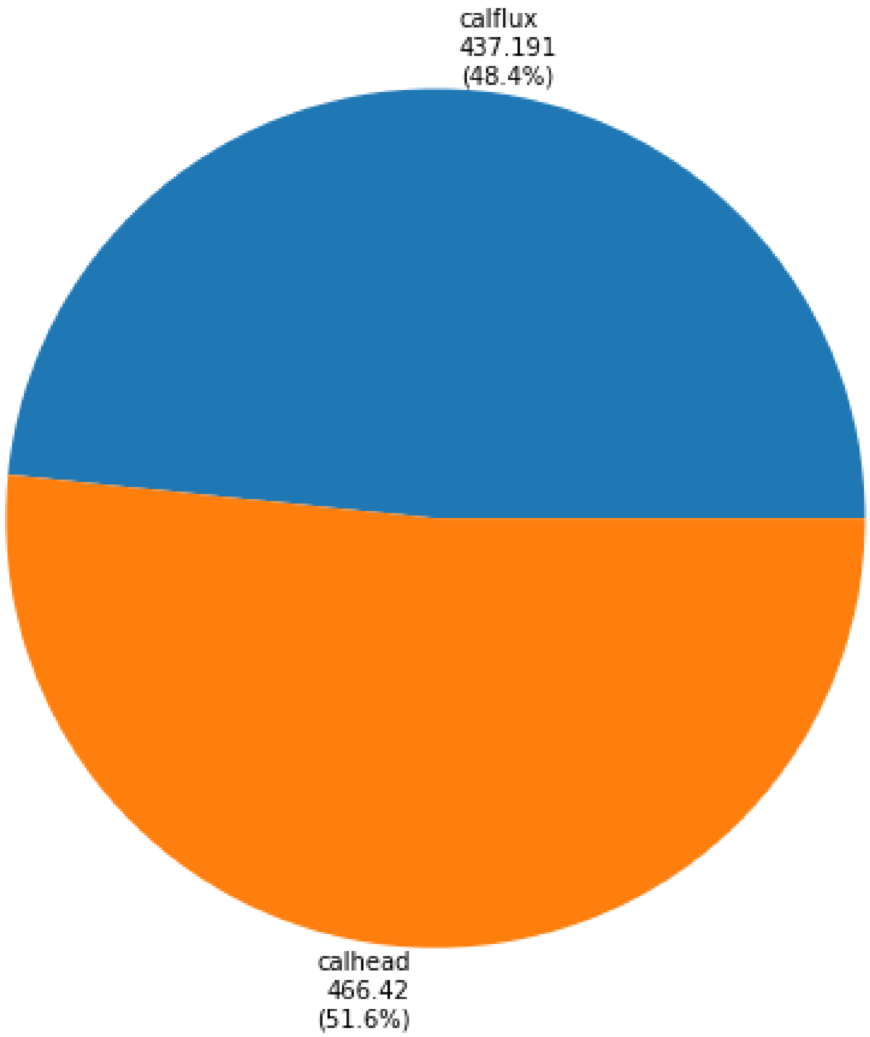
Now, for some super trickery: since we changed the weight, we need to generate the observation noise using these new weights for the error model (so meta!)

```
In [20]: obs = pst.observation_data
         np.random.seed(seed=0)
         snd = np.random.randn(pst.nnz_obs)
         noise = snd * 1./obs.loc[pst.nnz_obs_names,"weight"]
         obs.loc[:,"obsval"] = obs_df.loc[idx,pst.obs_names]
         pst.observation_data.loc[noise.index,"obsval"] += noise
         noise
```

```
Out[20]: obsnme
         fo_39_19791230        9.958857
         hds_00_002_009_000    0.064164
         hds_00_002_015_000    0.156937
         hds_00_003_008_000    0.359320
         hds_00_009_001_000    0.299457
         hds_00_013_010_000   -0.156703
         hds_00_015_016_000    0.152343
         hds_00_021_010_000   -0.024270
         hds_00_022_015_000   -0.016551
         hds_00_024_004_000    0.065838
         hds_00_026_006_000    0.023097
         hds_00_029_015_000    0.233188
         hds_00_033_007_000    0.122030
         hds_00_034_010_000    0.019510
         Name: weight, dtype: float64
```

```
In [21]: pst.write(os.path.join(t_d,"freyberg.pst"))
         pyemu.os_utils.run("pestpp-ies freyberg.pst",cwd=t_d)
         pst = pyemu.Pst(os.path.join(t_d,"freyberg.pst"))
         print(pst.phi)
         pst.plot(kind='phi_pie')
         plt.show()
```

```
noptmax:0, npar_adj:14819, nnz_obs:14
903.6102175392298
```




Whew! confused yet? Ok, let's leave all this confusion behind…its mostly academic, just to make sure we are using weights that are in harmony with the noise we added to the truth…Just to make sure we have everything working right, we should be able to load the truth parameters, run the model once and have a `phi` equivalent to the noise vector:

```
In [22]: par_df = pd.read_csv(os.path.join(m_d,"sweep_in.csv"),index_col=0)
         pst.parameter_data.loc[:,"parval1"] = par_df.loc[idx,pst.par_names]
         pst.write(os.path.join(m_d,"test.pst"))
```

```
noptmax:0, npar_adj:14819, nnz_obs:14
```

we will run this with `noptmax=0` to preform a single run. Pro-tip: you can use any of the `pestpp-###` binaries/executables to run `noptmax=0`

```
In [23]: pyemu.os_utils.run("pestpp-ies.exe test.pst",cwd=m_d)
         pst = pyemu.Pst(os.path.join(m_d,"test.pst"))
         print(pst.phi)
         pst.res.loc[pst.nnz_obs_names,:]
```

```
17.52884697222985
```

```
Out[23]:                                  name    group      measured      modelled  \
         name
         fo_39_19791230          fo_39_19791230  calflux  11311.958857  11302.000000
         hds_00_002_009_000  hds_00_002_009_000  calhead     36.122288     36.058125
         hds_00_002_015_000  hds_00_002_015_000  calhead     35.369736     35.212799
         hds_00_003_008_000  hds_00_003_008_000  calhead     36.442831     36.083511
         hds_00_009_001_000  hds_00_009_001_000  calhead     37.688857     37.389400
         hds_00_013_010_000  hds_00_013_010_000  calhead     34.892003     35.048706
         hds_00_015_016_000  hds_00_015_016_000  calhead     34.990806     34.838463
         hds_00_021_010_000  hds_00_021_010_000  calhead     34.789855     34.814125
         hds_00_022_015_000  hds_00_022_015_000  calhead     34.535665     34.552216
         hds_00_024_004_000  hds_00_024_004_000  calhead     35.275349     35.209511
         hds_00_026_006_000  hds_00_026_006_000  calhead     34.704665     34.681568
         hds_00_029_015_000  hds_00_029_015_000  calhead     34.356090     34.122902
         hds_00_033_007_000  hds_00_033_007_000  calhead     33.467695     33.345665
         hds_00_034_010_000  hds_00_034_010_000  calhead     33.337366     33.317856

                             residual    weight
         name
         fo_39_19791230      9.958857  0.177134
         hds_00_002_009_000  0.064164  6.236491
         hds_00_002_015_000  0.156937  6.236491
         hds_00_003_008_000  0.359320  6.236491
         hds_00_009_001_000  0.299457  6.236491
         hds_00_013_010_000 -0.156703  6.236491
         hds_00_015_016_000  0.152343  6.236491
         hds_00_021_010_000 -0.024270  6.236491
         hds_00_022_015_000 -0.016551  6.236491
         hds_00_024_004_000  0.065838  6.236491
         hds_00_026_006_000  0.023097  6.236491
         hds_00_029_015_000  0.233188  6.236491
         hds_00_033_007_000  0.122030  6.236491
         hds_00_034_010_000  0.019510  6.236491
```

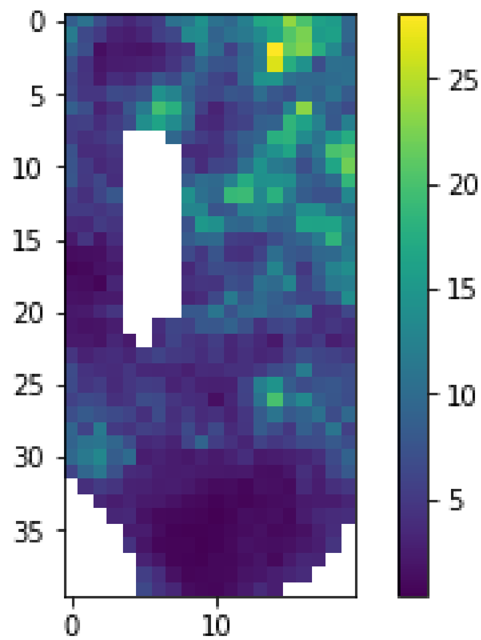
The residual should be exactly the noise values from above.Lets load the model (that was just run using the true pars) and check some things

```
In [24]: m = flopy.modflow.Modflow.load("freyberg.nam",model_ws=m_d)
```

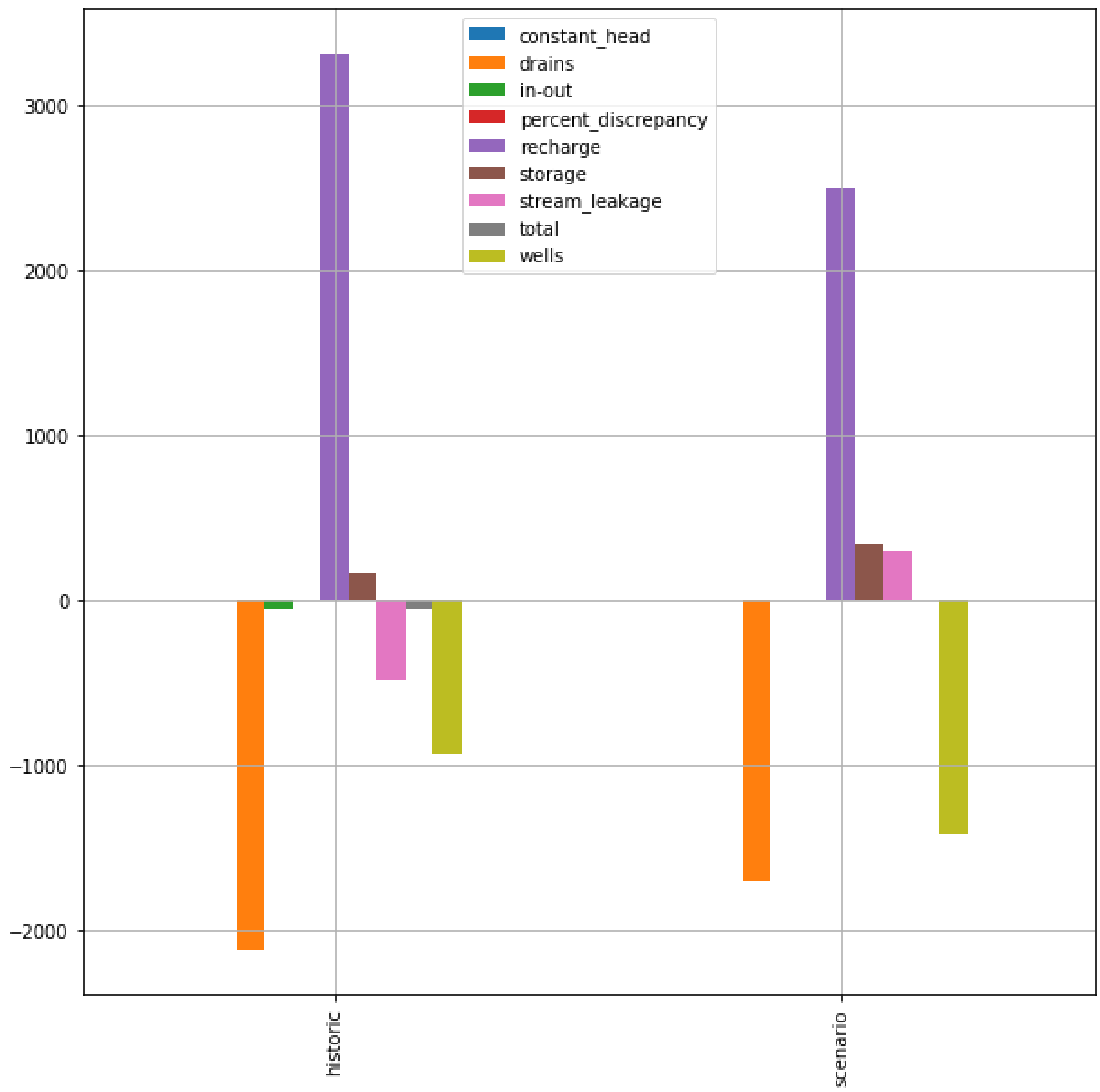
```
In [25]: a = m.upw.hk[0].array
         #a = m.rch.rech[0].array
```

```
a = np.ma.masked_where(m.bas6.ibound[0].array==0,a)
print(a.min(),a.max())
c = plt.imshow(a)
plt.colorbar()
plt.show()
```

```
0.4185674 28.04684
```



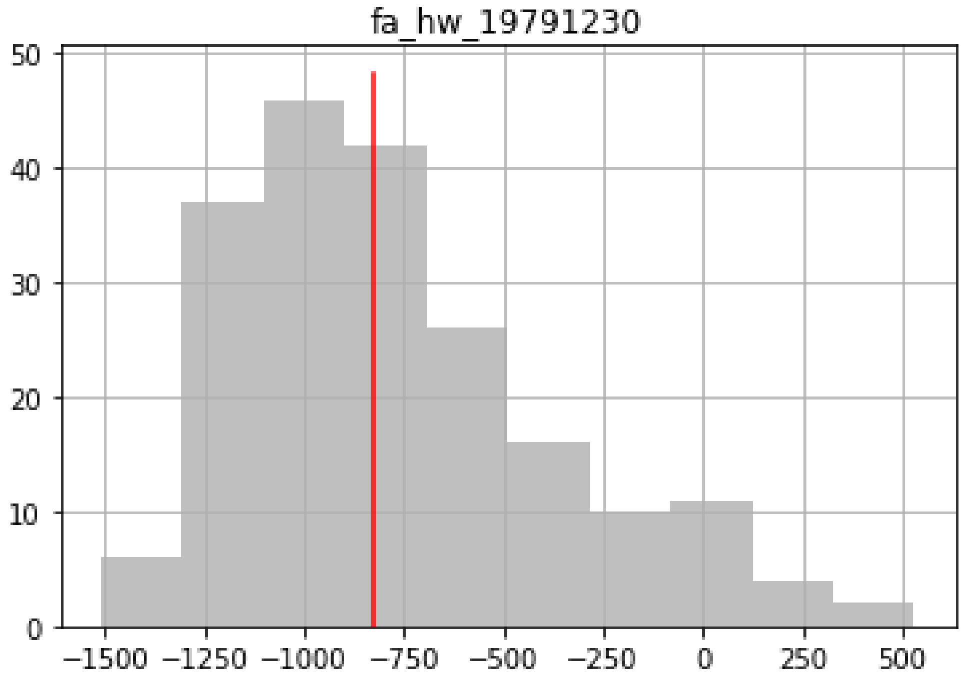

```
In [26]: lst = flopy.utils.MfListBudget(os.path.join(m_d,"freyberg.list"))
         df = lst.get_dataframes(diff=True)[0]
         ax = df.plot(kind="bar",figsize=(10,10), grid=True)
         a = ax.set_xticklabels(["historic","scenario"],rotation=90)
         plt.show(ax)
```

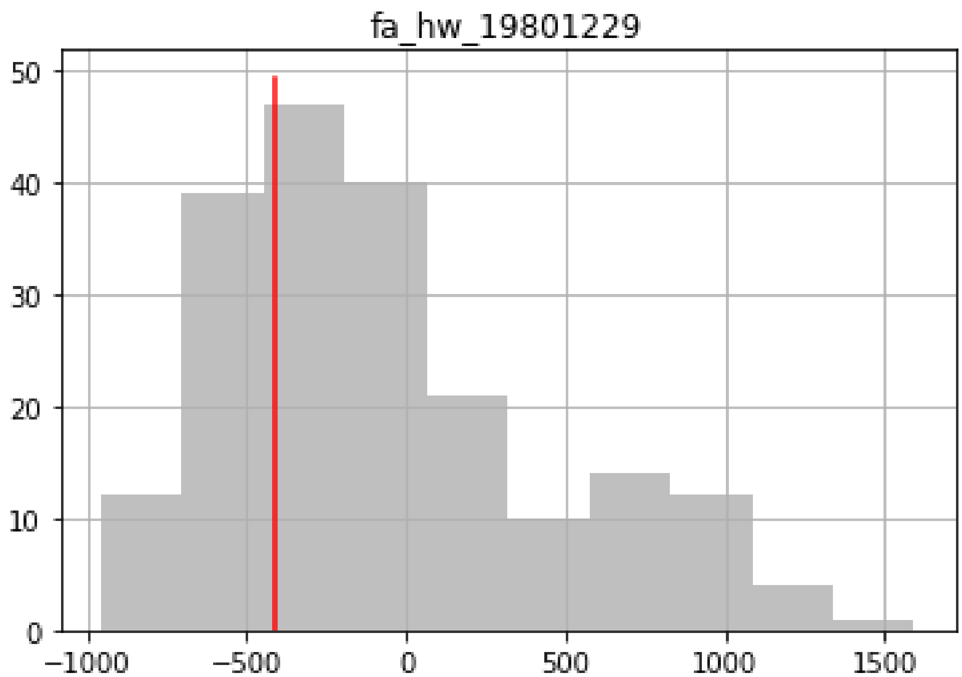


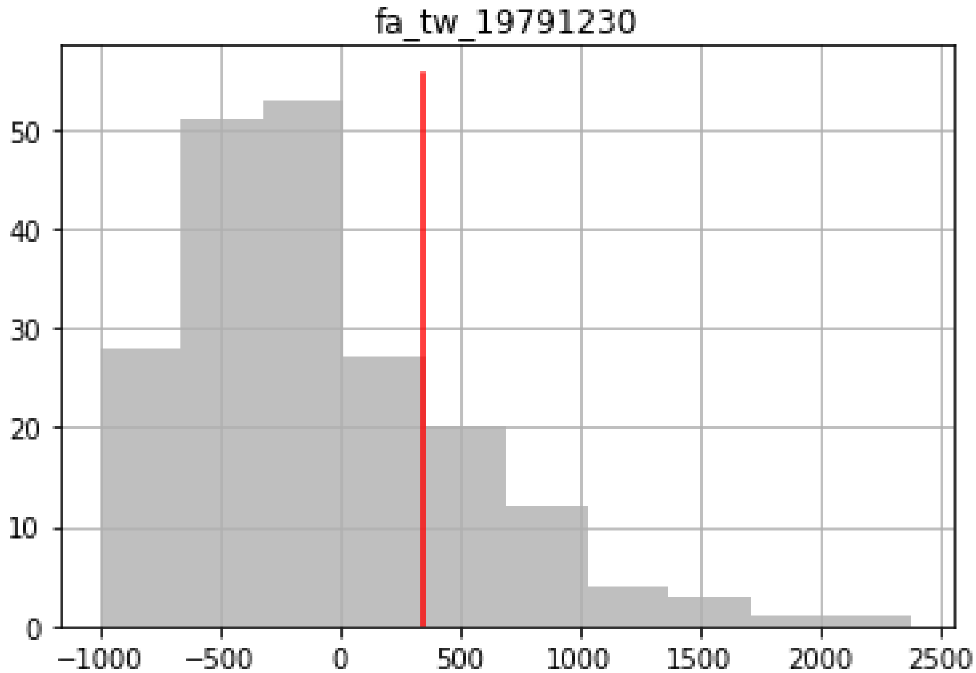

### 1.0.8 see how our existing observation ensemble compares to the truth

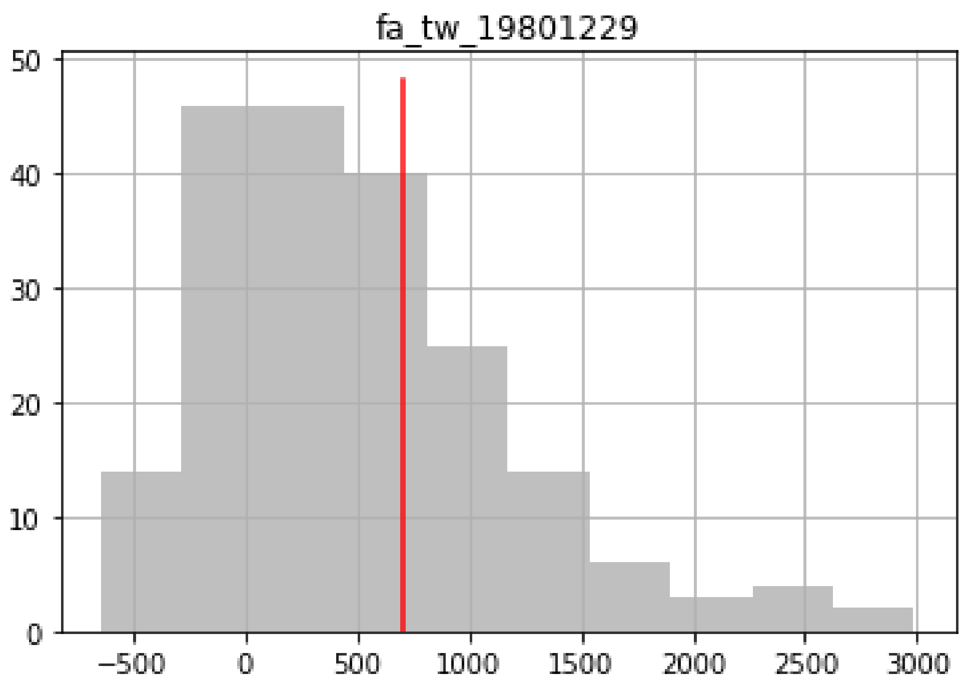
forecasts:

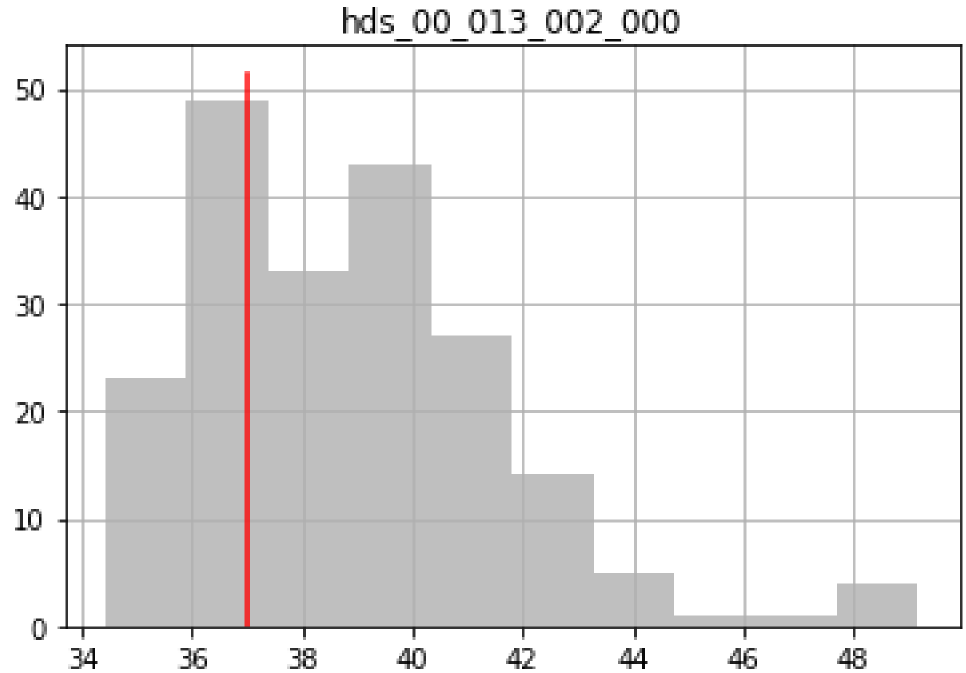
```
In [27]: obs = pst.observation_data
         plt.figure()
         for forecast in fnames:
             ax = plt.subplot(111)
             obs_df.loc[:,forecast].hist(ax=ax,color="0.5",alpha=0.5)
             ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r")
             ax.set_title(forecast)
             plt.show()
```

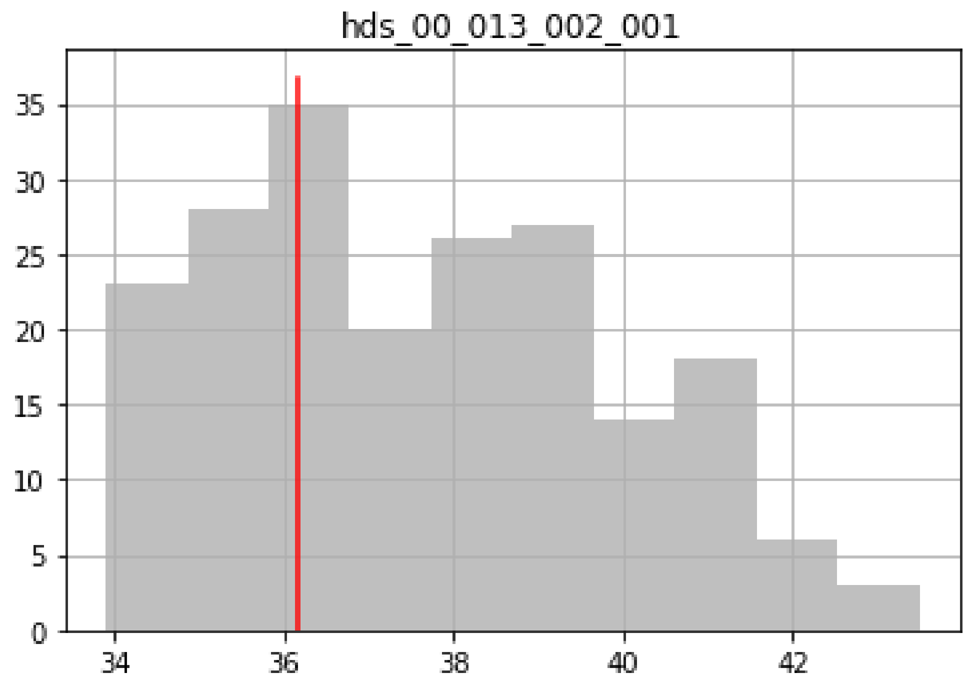

fa_hw_19791230
50
40
30
20
10
0
−1500
−1250
−1000
−750
−500
−250
0
250
500

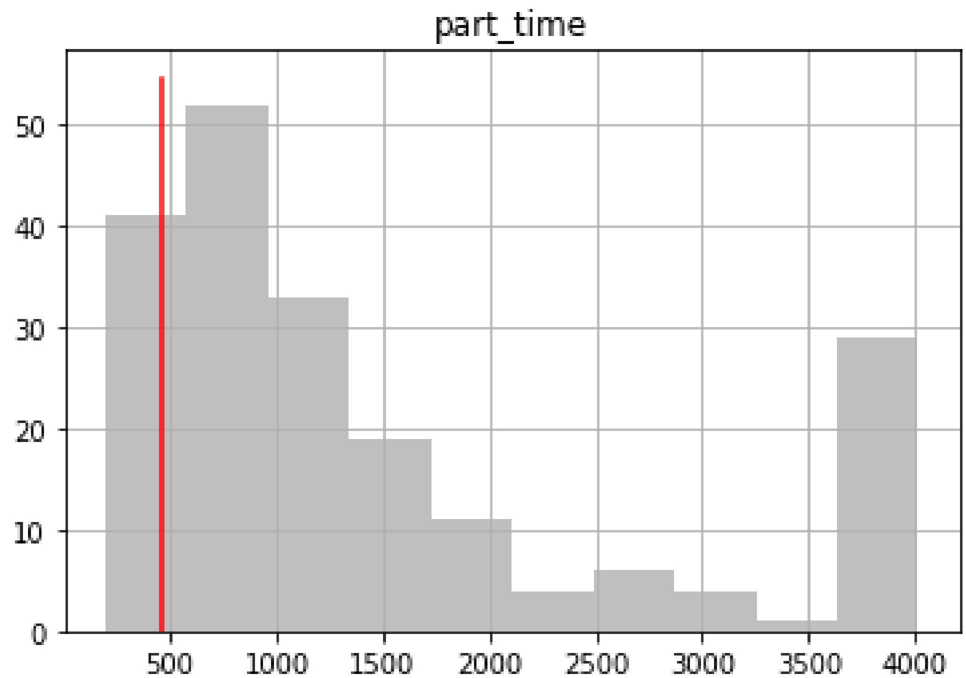

fa_hw_19801229
50
40
30
20
10
0
−1000
−500
0
500
1000
1500

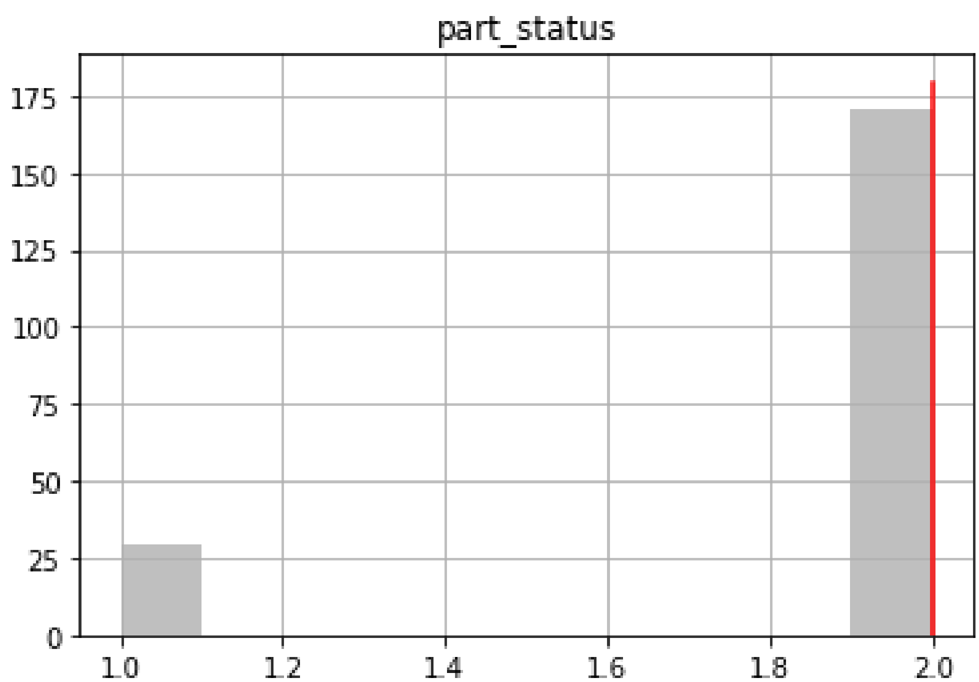

fa_tw_19791230
50
40
30
20
10
0
−1000
−500
0
500
1000
1500
2000
2500


fa_tw_19801229
50
40
30
20
10
0
−500
0
500
1000
1500
2000
2500
3000


hds_00_013_002_000
50
40
30
20
10
0
34
36
38
40
42
44
46
48

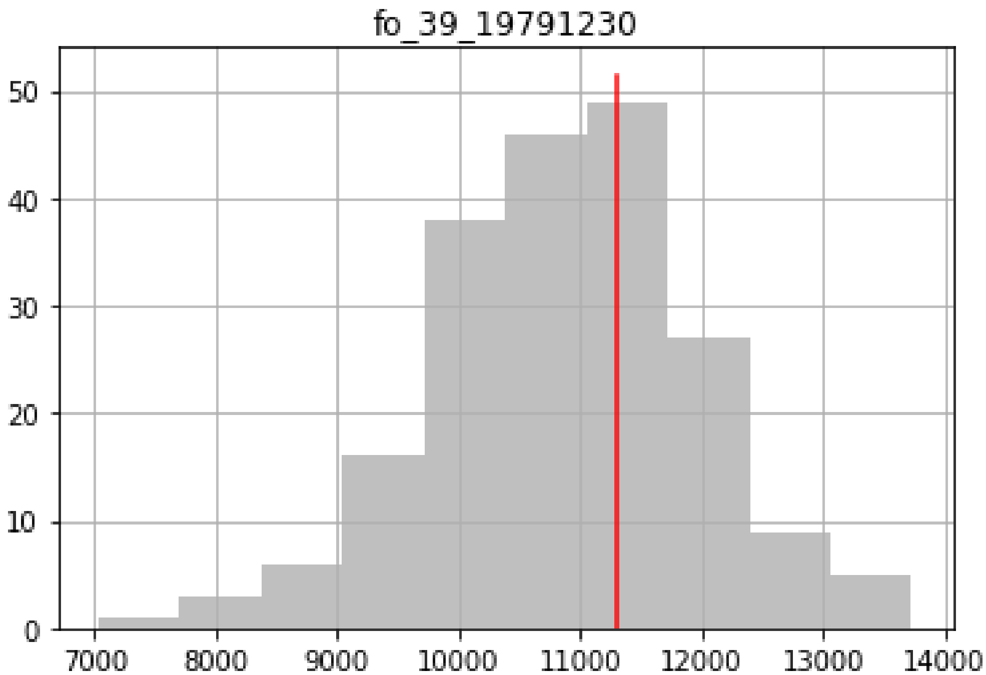

hds_00_013_002_001
35
30
25
20
15
10
5
0
34
36
38
40
42

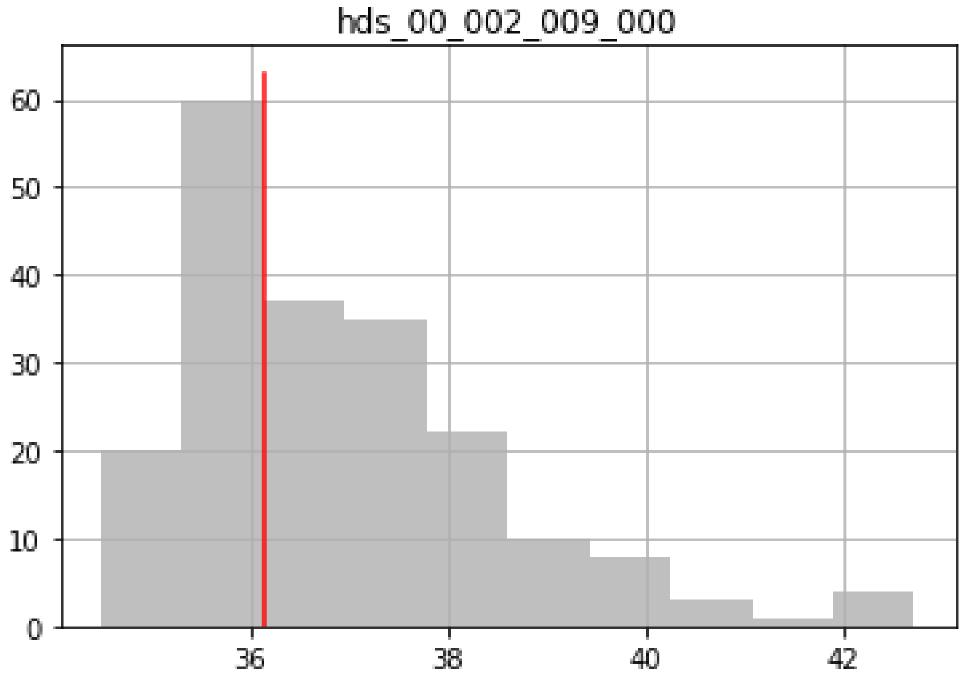


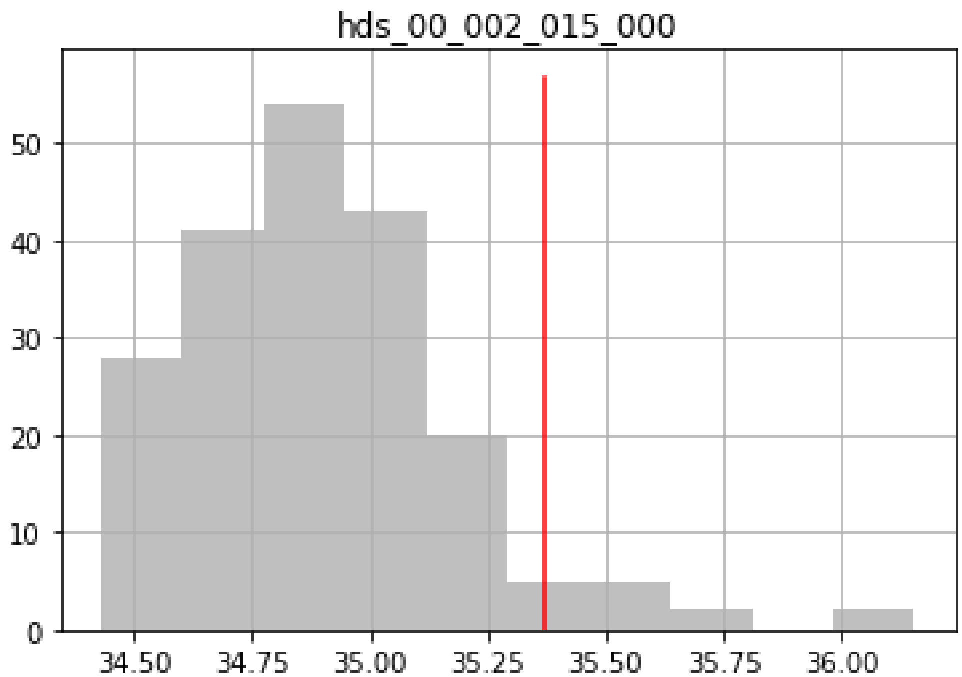




observations:

```
In [28]: for oname in pst.nnz_obs_names:
             ax = plt.subplot(111)
             obs_df.loc[:,oname].hist(ax=ax,color="0.5",alpha=0.5)
             ax.plot([obs.loc[oname,"obsval"],obs.loc[oname,"obsval"]],ax.get_ylim(),"r")
             ax.set_title(oname)
             plt.show()
```




hds_00_002_009_000
60
50
40
30
20
10
0
36
38
40
42


hds_00_002_015_000
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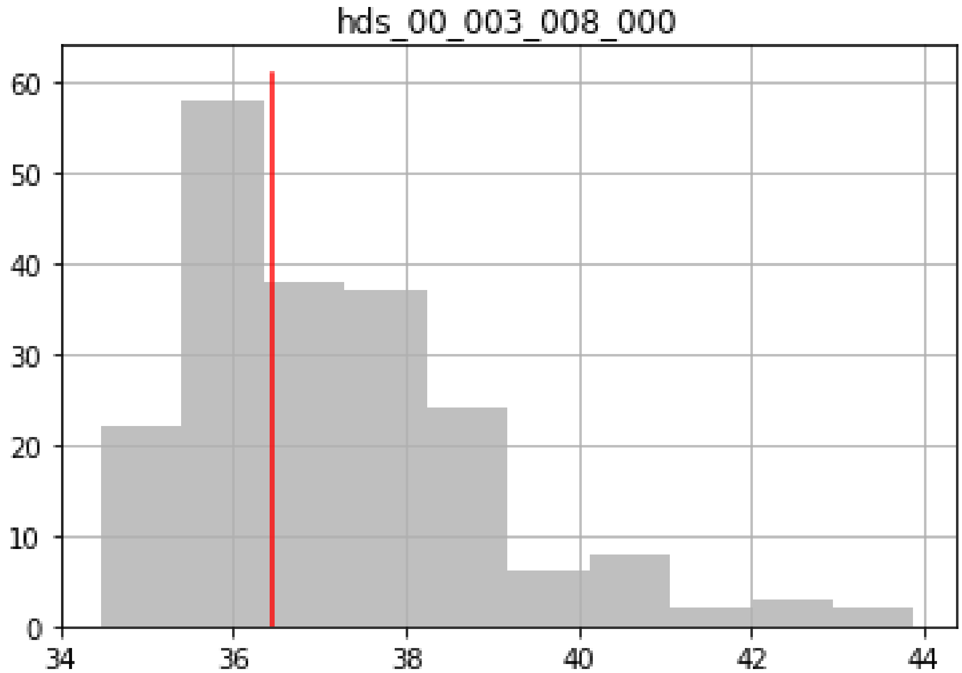
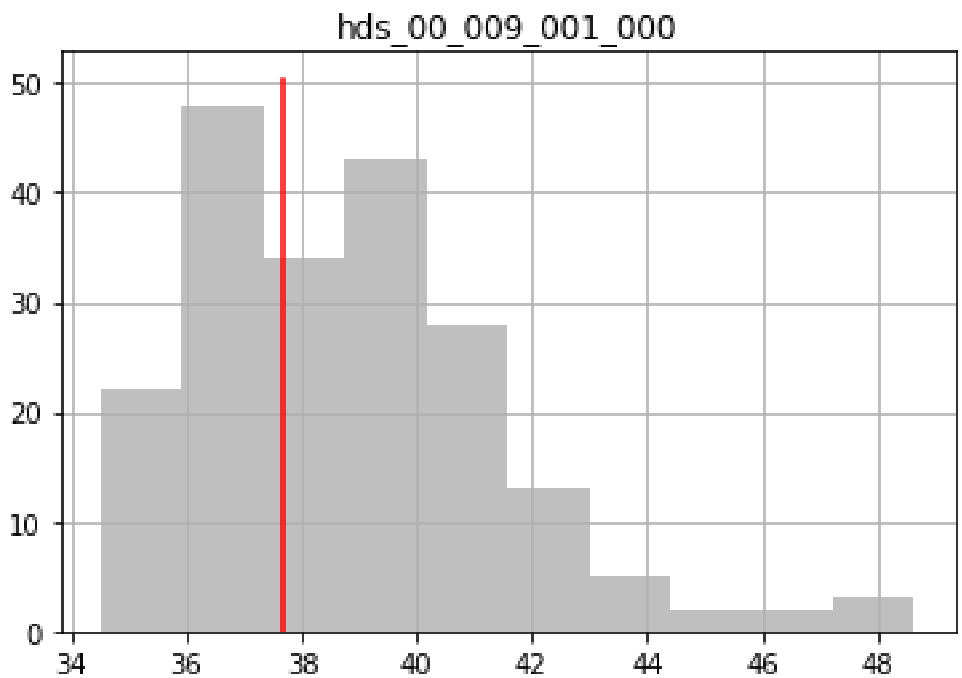
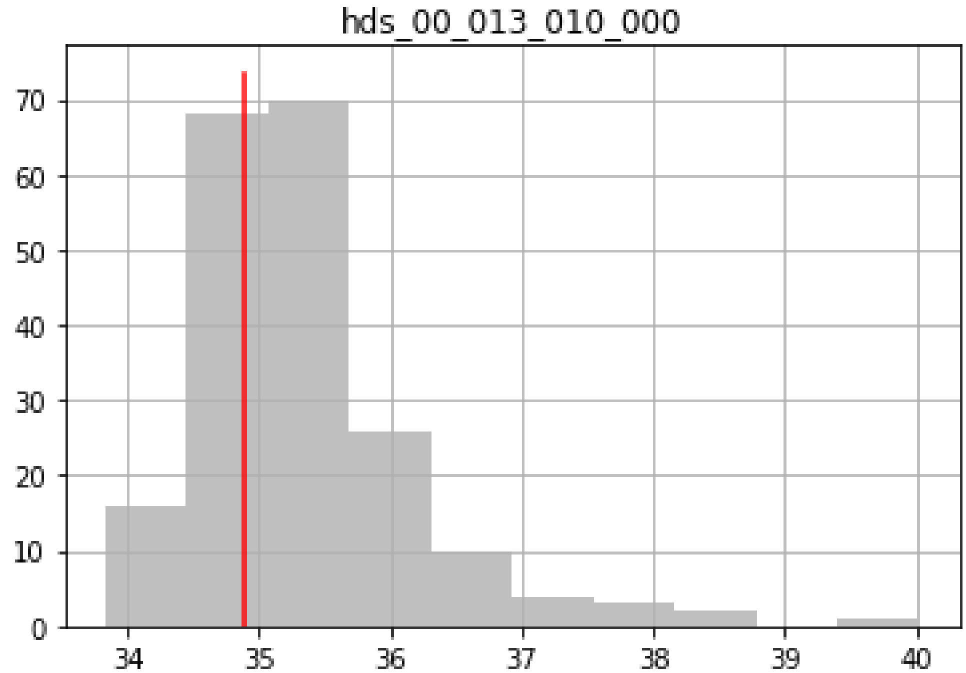
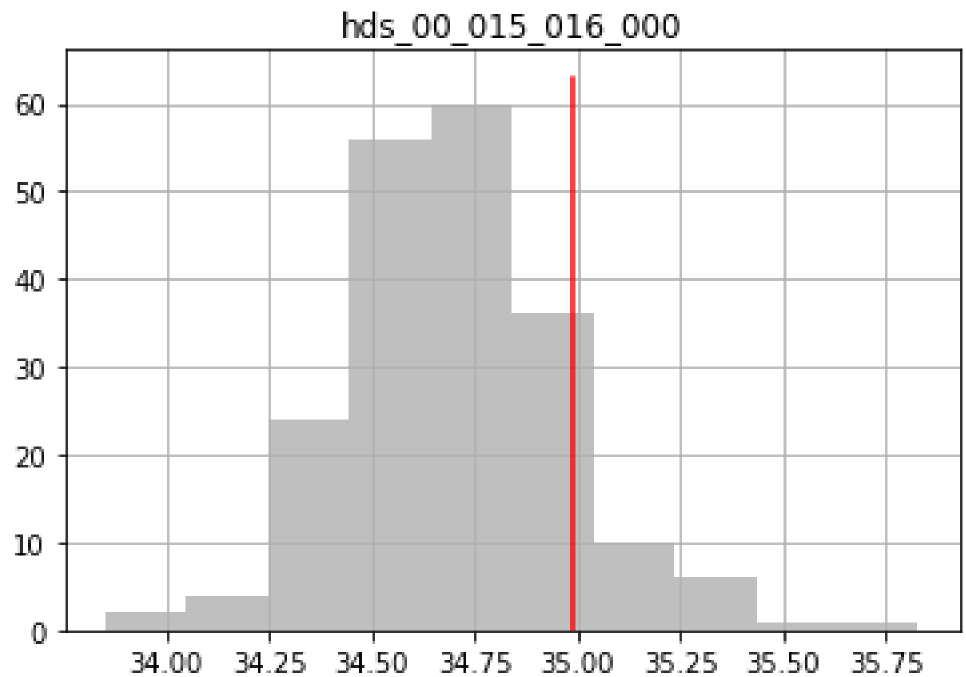
40
30
20
10
0
34.50
34.75
35.00
35.25
35.50
35.75
36.00


hds_00_003_008_000
60
50
40
30
20
10
0
34
36
38
40
42
44


hds_00_009_001_000
50
40
30
20
10
0
34
36
38
40
42
44
46
48


hds_00_013_010_000
70
60
50
40
30
20
10
0
34
35
36
37
38
39
40


hds_00_015_016_000
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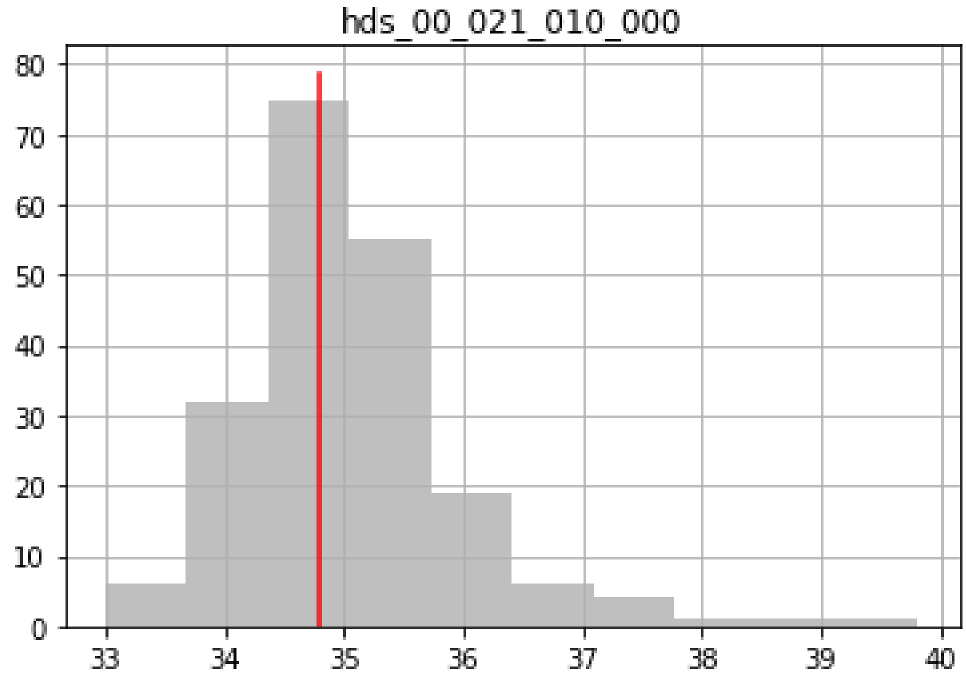
50
40
30
20
10
0
34.00
34.25
34.50
34.75
35.00
35.25
35.50
35.75


hds_00_021_010_000
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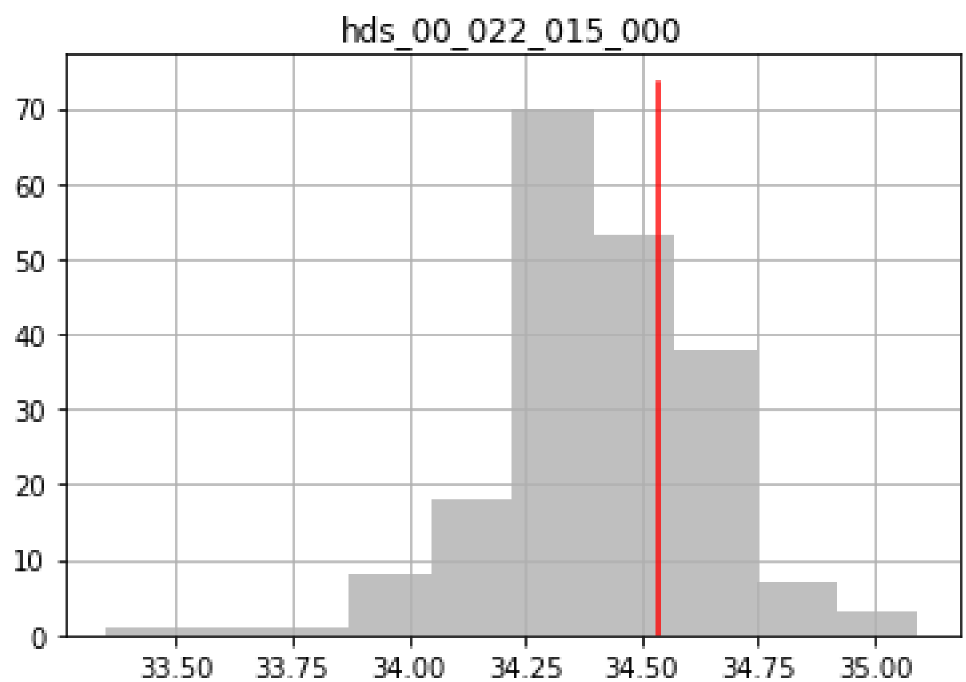
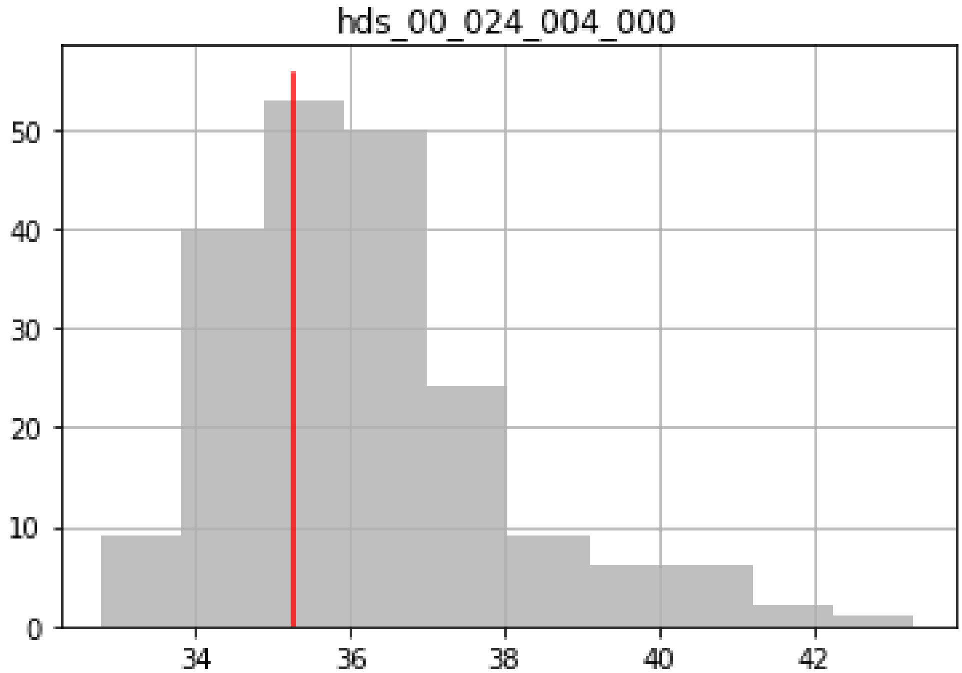
20
30
40
50
60
70
80
33
34
35
36
37
38
39
40


hds_00_022_015_000
0
10
20
30
40
50
60
70
33.50
33.75
34.00
34.25
34.50
34.75
35.00


hds_00_024_004_000
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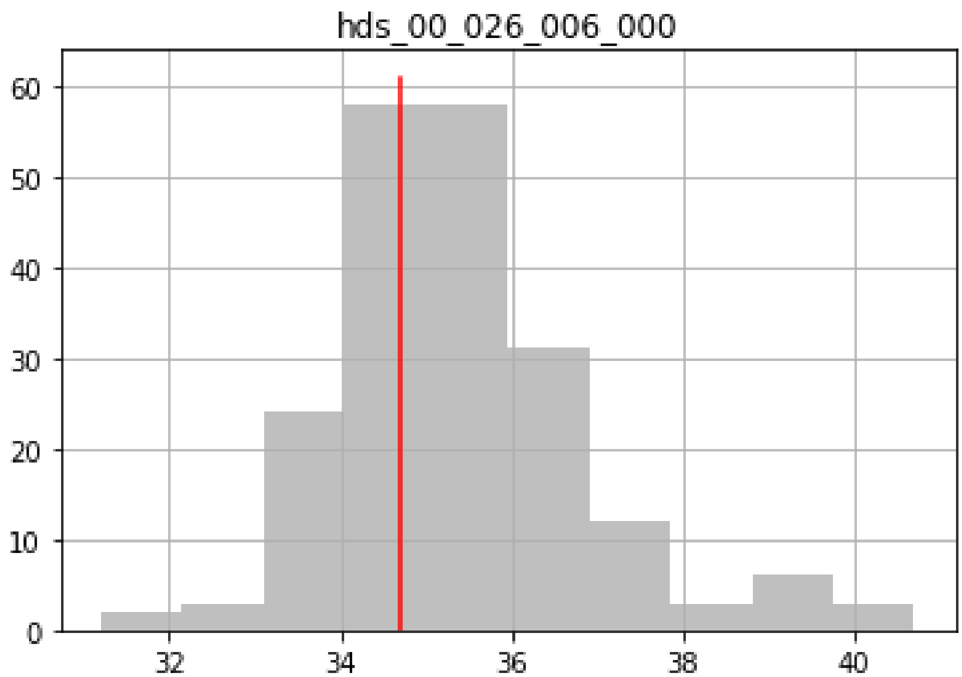
40
30
20
10
0
34
36
38
40
42


hds_00_026_006_000
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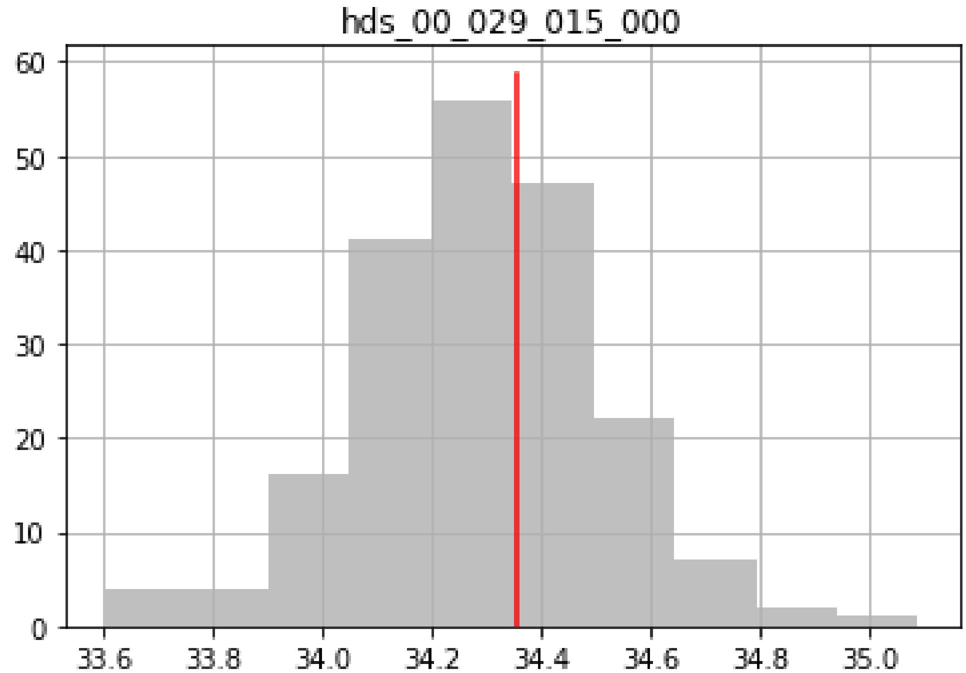
50
40
30
20
10
0
32
34
36
38
40


hds_00_029_015_000
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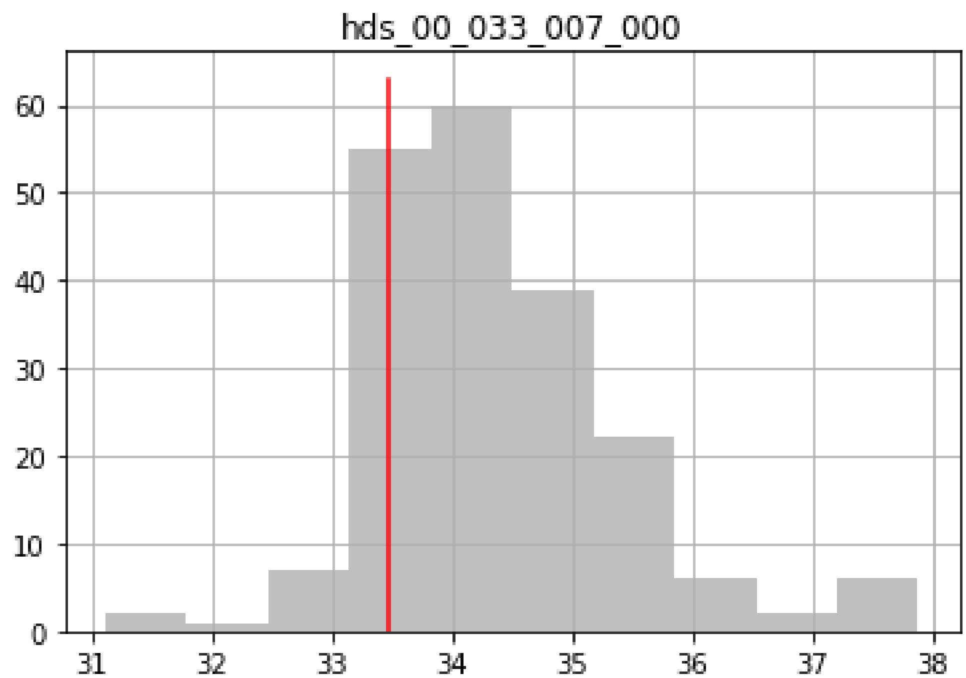
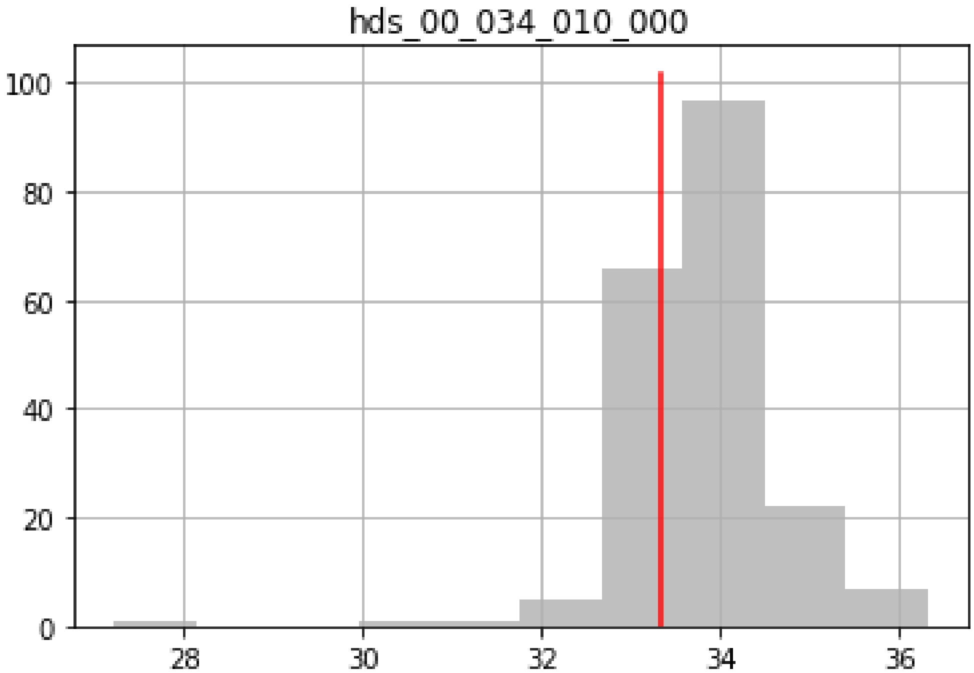
50
40
30
20
10
0
33.6
33.8
34.0
34.2
34.4
34.6
34.8
35.0


hds_00_033_007_000
60
50
40
30
20
10
0
31
32
33
34
35
36
37
38


hds_00_034_010_000
100
80
60
40
20
0
28
30
32
34
36