prior_montecarlo

May 8, 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
```

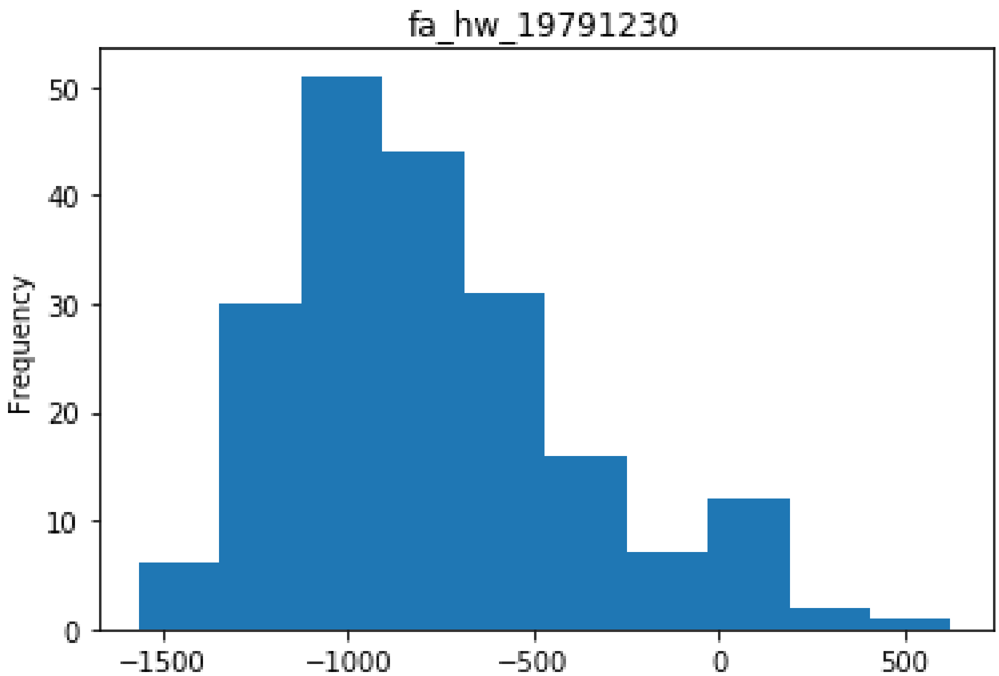
1.0.5 confirm which quantities were identified as forecasts

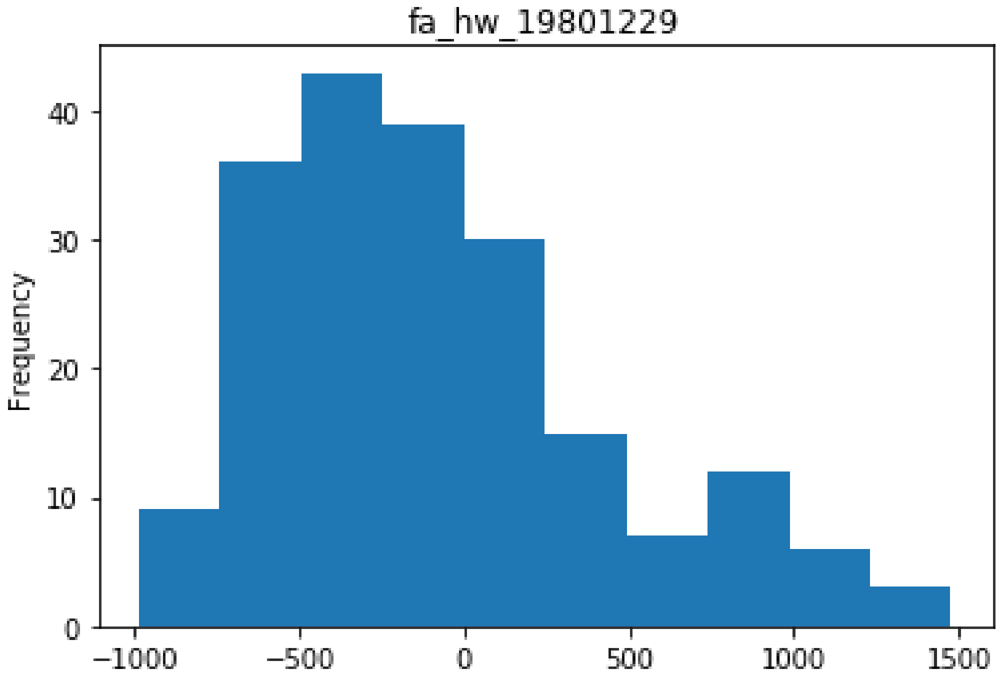
```
In [8]: fnames = pst.pestpp_options["forecasts"].split(',')
        fnames
```

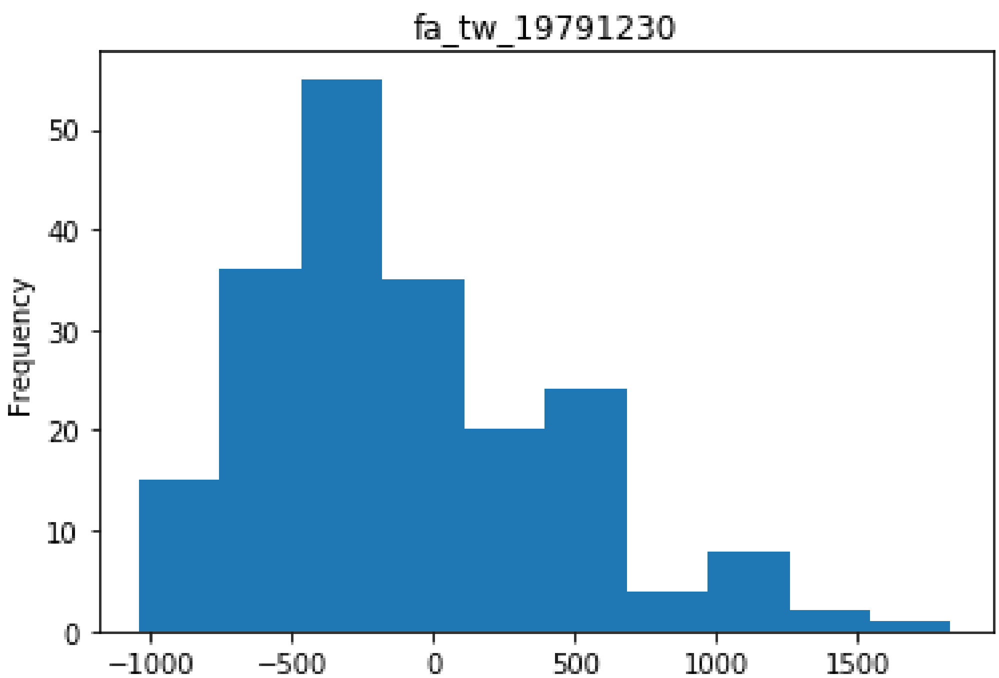
```
Out[8]: ['fa_hw_19791230',
         'fa_hw_19801229',
         'fa_tw_19791230',
         'fa_tw_19801229',
         'hds_00_013_002_000',
         'hds_00_013_002_001',
         'part_time',
         'part_status']
```

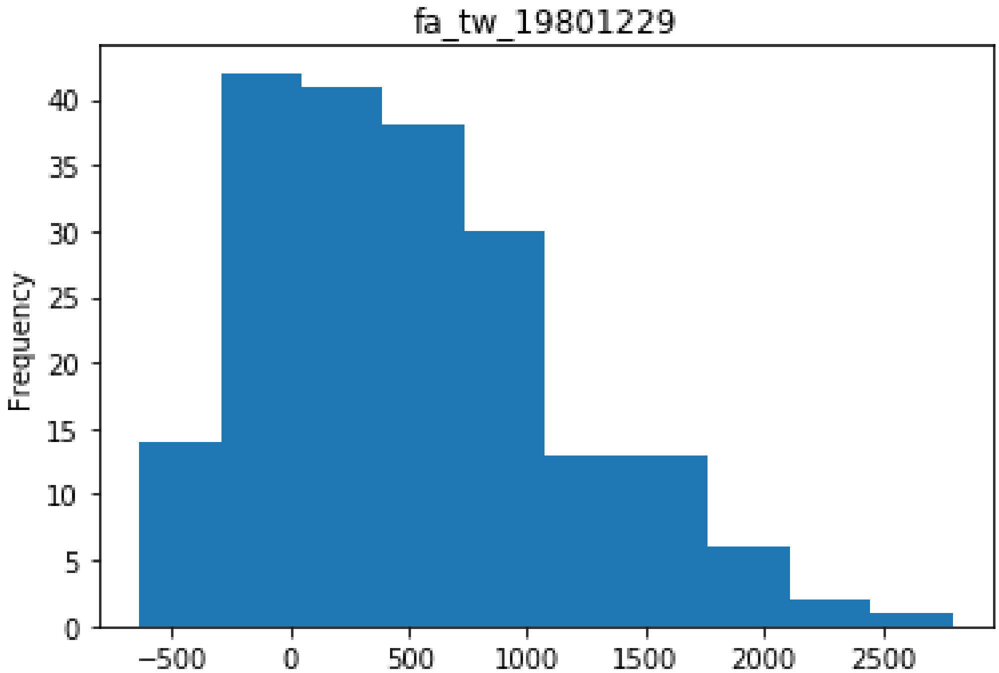
1.0.6 now we can plot the distributions of each forecast

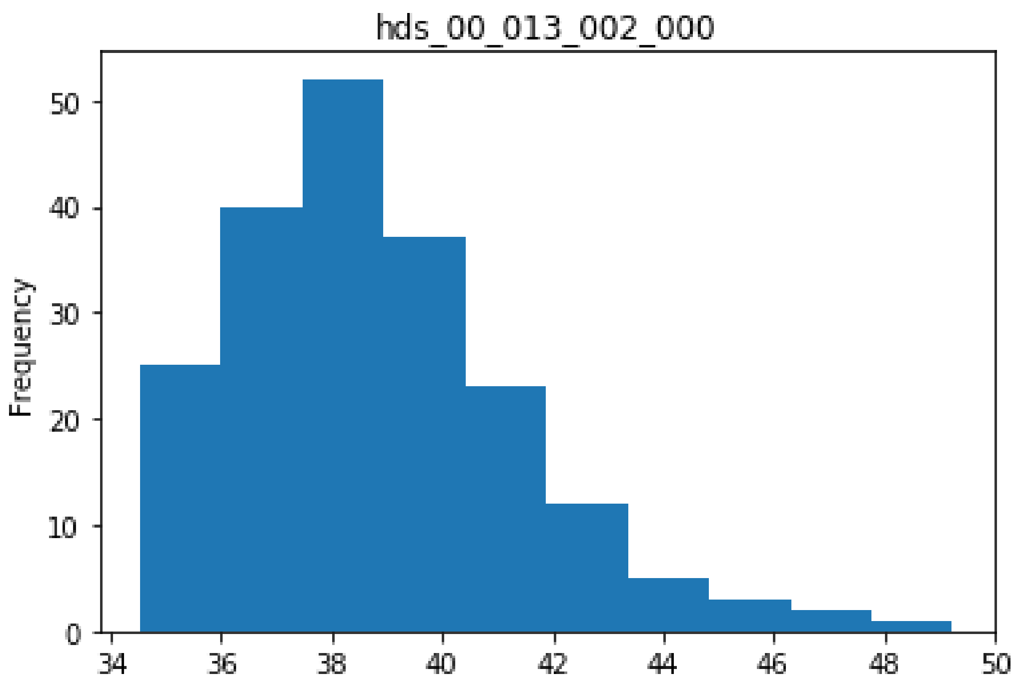
```
In [9]: for forecast in fnames:
            plt.figure()
            ax = obs_df.loc[:,forecast].plot(kind="hist")
            ax.set_title(forecast)
        plt.show()
```

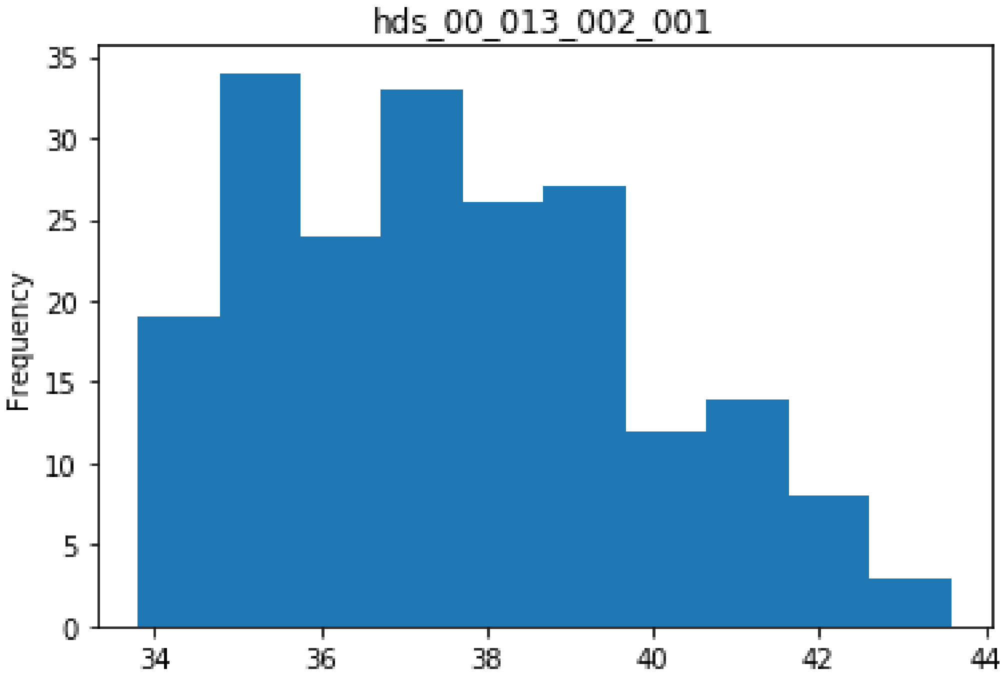


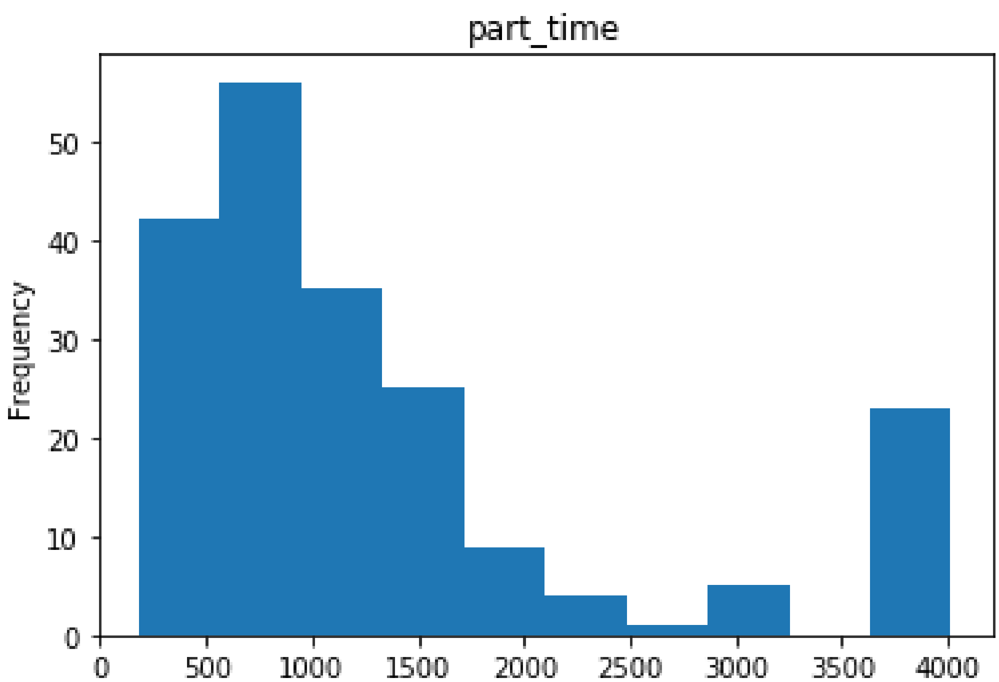

fa_hw_19801229
Frequency
0
10
20
30
40
−1000
−500
0
500
1000
1500

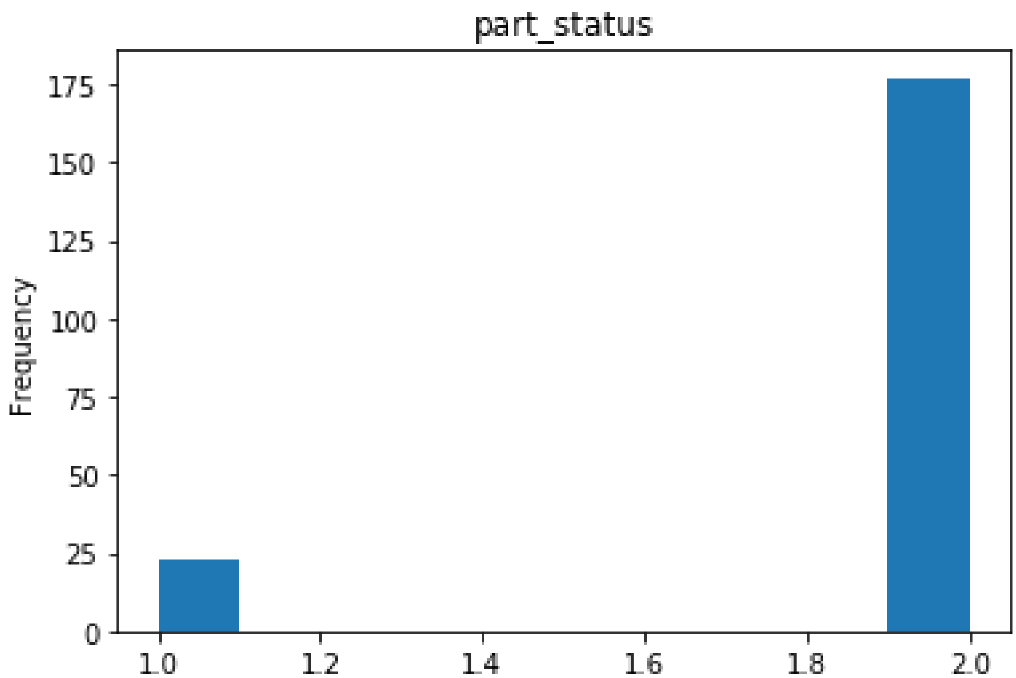

fa_tw_19791230
Frequency
0
10
20
30
40
50
−1000
−500
0
500
1000
1500


fa_tw_19801229
Frequency
0
5
10
15
20
25
30
35
40
−500
0
500
1000
1500
2000
2500


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

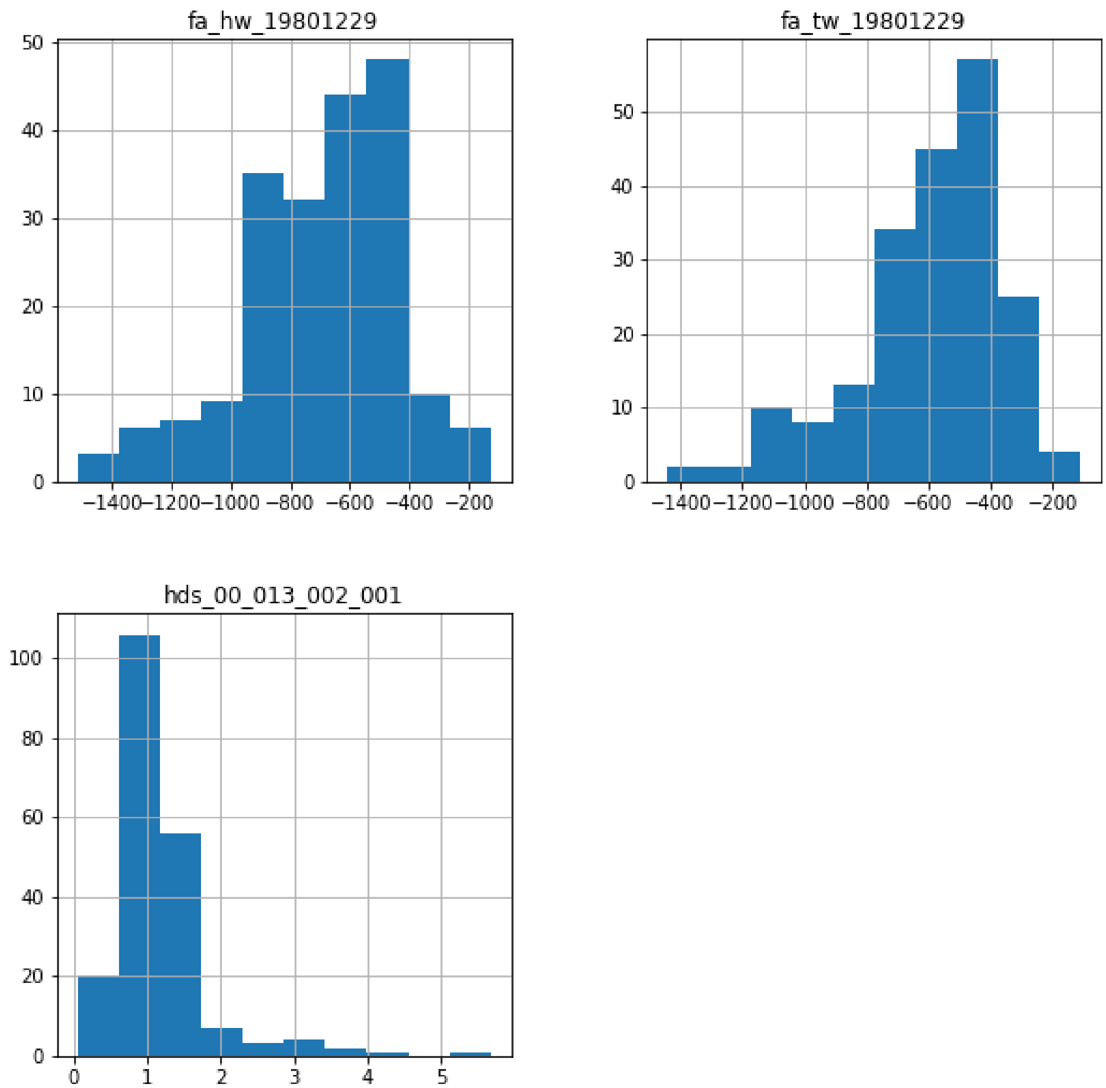

hds_00_013_002_001
Frequency
35
30
25
20
15
10
5
0
34
36
38
40
42
44


part_time
Frequency
50
40
30
20
10
0
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     184.1517
166     206.2137
77      276.1604
59      314.8956
100     331.3931
174     338.6796
35      343.6858
161     351.1038
120     365.6083
82      376.8029
0       384.3066
73      394.6332
98      398.3461
41      401.3468
21      402.4046
180     408.5494
52      420.0638
168     424.3355
57      446.0459
40      458.2126
3       462.9558
118     475.5129
132     477.4851
184     477.9743
117     479.2090
131     487.5205
37      502.1088
34      513.7058
56      521.4803
95      521.8308
          ...
4      2438.2690
178    2617.6400
115    2927.8600
116    2943.3860
32     3007.2270
83     3019.2510
158    3052.2840
17     4015.0000
5      4015.0000
24     4015.0000
43     4015.0000
25     4015.0000
147    4015.0000
```

```
12     4015.0000
165    4015.0000
69     4015.0000
96     4015.0000
157    4015.0000
159    4015.0000
51     4015.0000
175    4015.0000
173    4015.0000
55     4015.0000
78     4015.0000
76     4015.0000
137    4015.0000
64     4015.0000
65     4015.0000
108    4015.0000
169    4015.0000
Name: part_time, Length: 200, dtype: float64
```

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

Out[12]:
```
fo_39_19791230        9714.600000
hds_00_002_009_000      35.826954
hds_00_002_015_000      34.983761
hds_00_003_008_000      35.923908
hds_00_009_001_000      36.820004
hds_00_013_010_000      34.999874
hds_00_015_016_000      34.566364
hds_00_021_010_000      34.772247
hds_00_022_015_000      34.603825
hds_00_024_004_000      34.965450
hds_00_026_006_000      34.759605
hds_00_029_015_000      34.272018
hds_00_033_007_000      34.105034
hds_00_034_010_000      33.770840
Name: 3, 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       -1123.553000
fa_hw_19801229        -197.152255
fa_tw_19791230          58.586980
fa_tw_19801229         631.809570
hds_00_013_002_000      36.341404
hds_00_013_002_001      35.233444
part_time              462.955800
part_status              2.000000
Name: 3, 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)
```

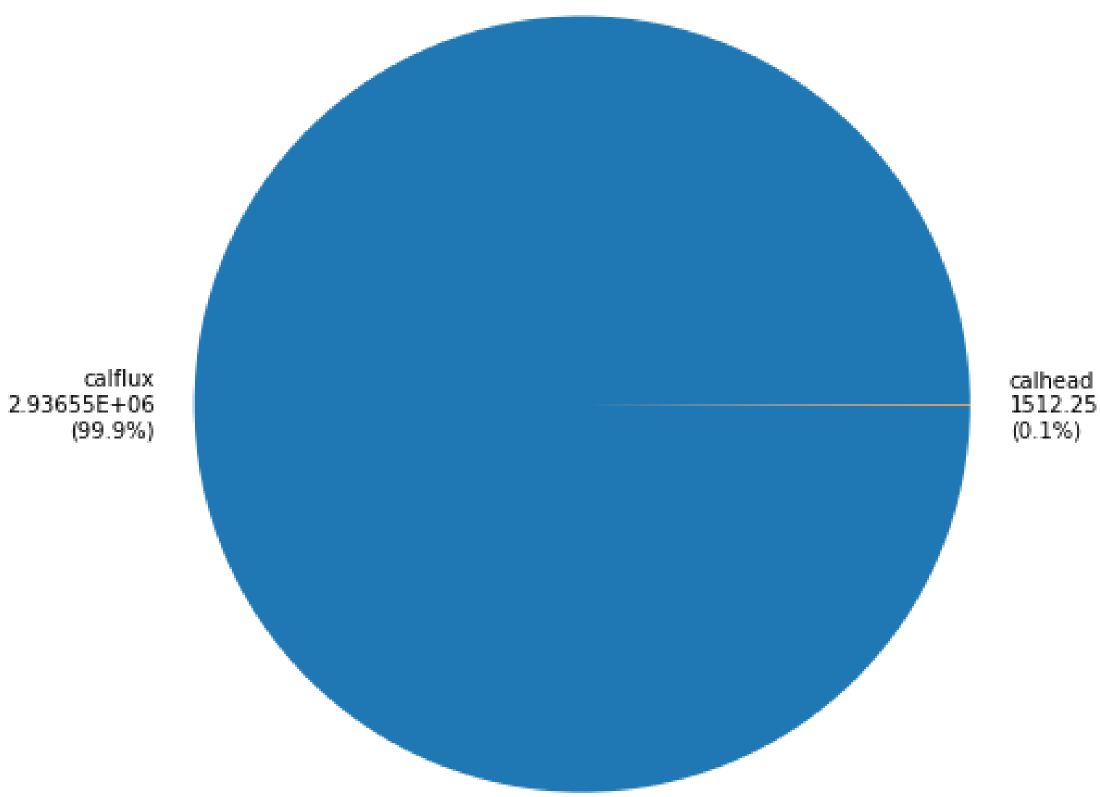
```
noptmax:0, npar_adj:14819, nnz_obs:14
```

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

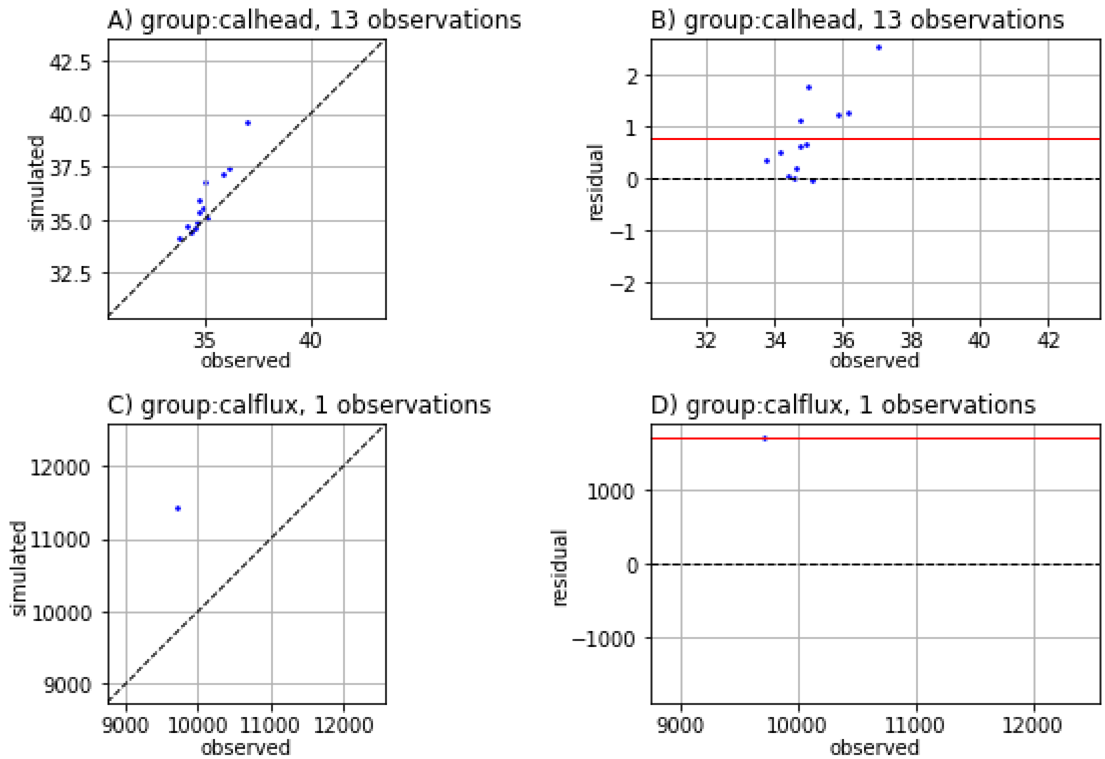
```
In [17]: pst = pyemu.Pst(os.path.join(t_d,"freyberg.pst"))
         print(pst.phi)
         plt.figure()
         pst.plot(kind='phi_pie')
         print('Here are the non-zero weighted observation names')

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

```
2938060.4131643856
Here are the non-zero weighted observation names
```

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



<Figure size 576x756 with 0 Axes>



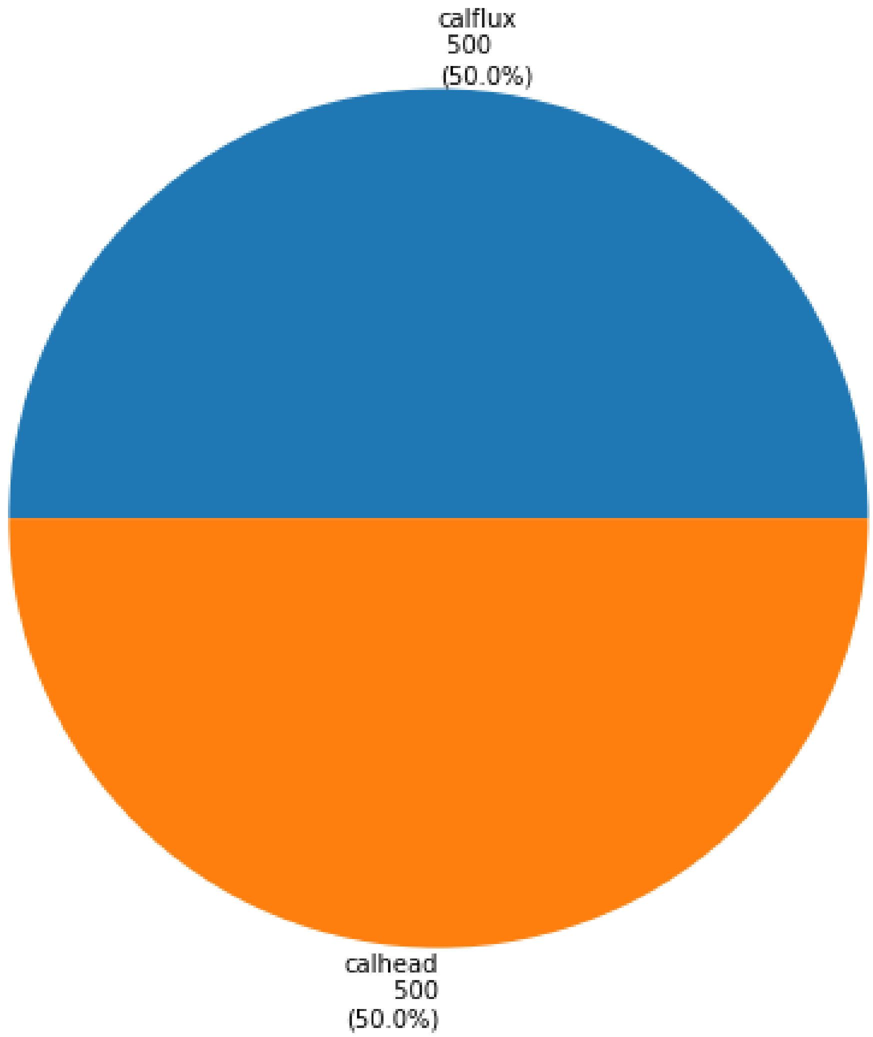
```
Out[17]:                                   name    group     measured      modelled  \
         name
         fo_39_19791230           fo_39_19791230  calflux  9716.364052  11430.000000
         hds_00_002_009_000   hds_00_002_009_000  calhead    35.866970     37.107498
         hds_00_002_015_000   hds_00_002_015_000  calhead    35.081635     35.045185
         hds_00_003_008_000   hds_00_003_008_000  calhead    36.147998     37.397289
         hds_00_009_001_000   hds_00_009_001_000  calhead    37.006759     39.546417
         hds_00_013_010_000   hds_00_013_010_000  calhead    34.902146     35.571774
         hds_00_015_016_000   hds_00_015_016_000  calhead    34.661373     34.835716
         hds_00_021_010_000   hds_00_021_010_000  calhead    34.757112     35.386250
         hds_00_022_015_000   hds_00_022_015_000  calhead    34.593503     34.577492
         hds_00_024_004_000   hds_00_024_004_000  calhead    35.006510     36.760464
         hds_00_026_006_000   hds_00_026_006_000  calhead    34.774010     35.896149
         hds_00_029_015_000   hds_00_029_015_000  calhead    34.417446     34.453842
         hds_00_033_007_000   hds_00_033_007_000  calhead    34.181138     34.678810
         hds_00_034_010_000   hds_00_034_010_000  calhead    33.783007     34.118073

                                residual  weight
         name
         fo_39_19791230     -1713.635948     1.0
         hds_00_002_009_000    -1.240529    10.0
         hds_00_002_015_000     0.036450    10.0
         hds_00_003_008_000    -1.249292    10.0
         hds_00_009_001_000    -2.539658    10.0
         hds_00_013_010_000    -0.669627    10.0
         hds_00_015_016_000    -0.174343    10.0
         hds_00_021_010_000    -0.629138    10.0
         hds_00_022_015_000     0.016011    10.0
         hds_00_024_004_000    -1.753954    10.0
         hds_00_026_006_000    -1.122139    10.0
         hds_00_029_015_000    -0.036396    10.0
         hds_00_033_007_000    -0.497672    10.0
         hds_00_034_010_000    -0.335065    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 0x18264b24e0>
```



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         0.013049
         hds_00_002_009_000     5.750067
         hds_00_002_015_000     5.750067
         hds_00_003_008_000     5.750067
         hds_00_009_001_000     5.750067
         hds_00_013_010_000     5.750067
         hds_00_015_016_000     5.750067
         hds_00_021_010_000     5.750067
         hds_00_022_015_000     5.750067
```

```
hds_00_024_004_000    5.750067
hds_00_026_006_000    5.750067
hds_00_029_015_000    5.750067
hds_00_033_007_000    5.750067
hds_00_034_010_000    5.750067
Name: weight, dtype: float64
```

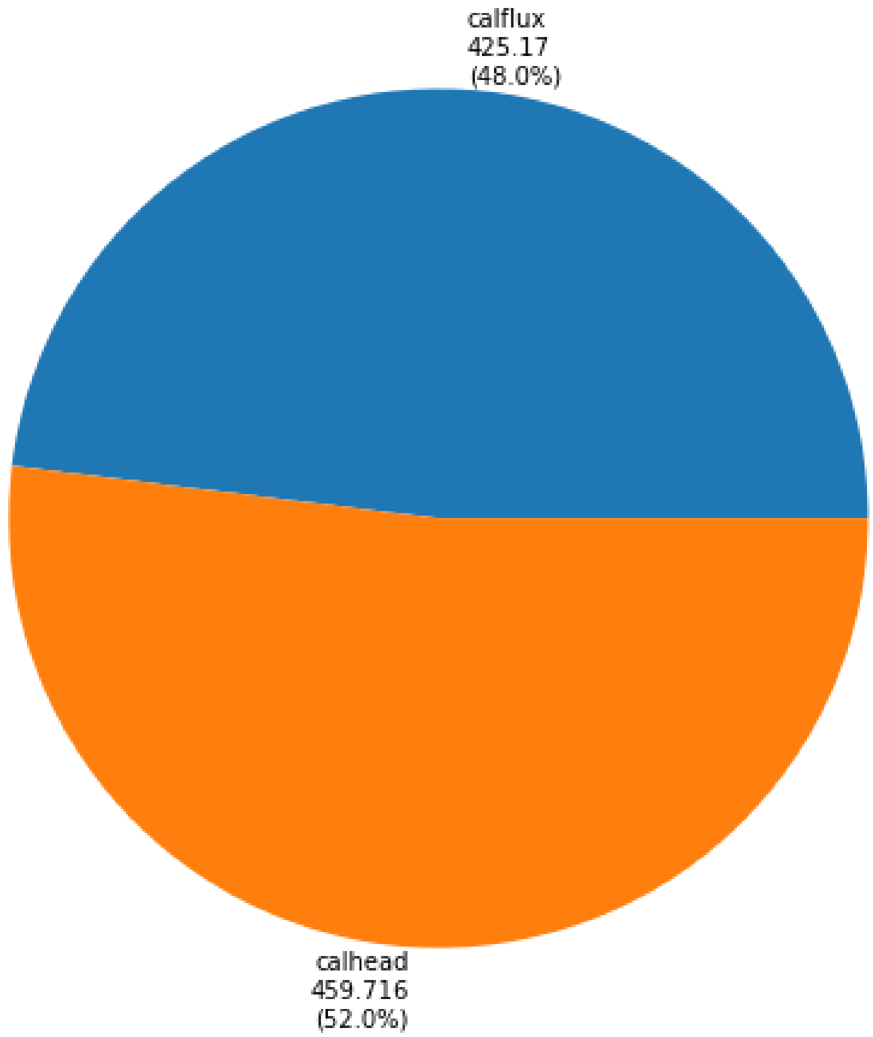
Now, for some super trickery: since we changed the weight, we need to generate the observation noise using these new weights for the error model (so meta!)

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        135.190144
hds_00_002_009_000      0.069592
hds_00_002_015_000      0.170213
hds_00_003_008_000      0.389716
hds_00_009_001_000      0.324789
hds_00_013_010_000     -0.169959
hds_00_015_016_000      0.165231
hds_00_021_010_000     -0.026323
hds_00_022_015_000     -0.017951
hds_00_024_004_000      0.071408
hds_00_026_006_000      0.025051
hds_00_029_015_000      0.252914
hds_00_033_007_000      0.132353
hds_00_034_010_000      0.021161
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
884.8855030468067
```



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,:]
```

```
17.528847226654747
```

```
Out[23]:                                   name    group     measured     modelled  \
         name
         fo_39_19791230          fo_39_19791230  calflux  9849.790144  9714.600000
         hds_00_002_009_000  hds_00_002_009_000  calhead    35.896546    35.826954
         hds_00_002_015_000  hds_00_002_015_000  calhead    35.153974    34.983761
         hds_00_003_008_000  hds_00_003_008_000  calhead    36.313624    35.923908
         hds_00_009_001_000  hds_00_009_001_000  calhead    37.144792    36.820004
         hds_00_013_010_000  hds_00_013_010_000  calhead    34.829915    34.999874
         hds_00_015_016_000  hds_00_015_016_000  calhead    34.731595    34.566364
         hds_00_021_010_000  hds_00_021_010_000  calhead    34.745925    34.772247
         hds_00_022_015_000  hds_00_022_015_000  calhead    34.585874    34.603825
         hds_00_024_004_000  hds_00_024_004_000  calhead    35.036858    34.965450
         hds_00_026_006_000  hds_00_026_006_000  calhead    34.784656    34.759605
         hds_00_029_015_000  hds_00_029_015_000  calhead    34.524933    34.272018
         hds_00_033_007_000  hds_00_033_007_000  calhead    34.237387    34.105034
         hds_00_034_010_000  hds_00_034_010_000  calhead    33.792000    33.770840

                               residual    weight
         name
         fo_39_19791230      135.190144  0.013049
         hds_00_002_009_000    0.069592  5.750067
         hds_00_002_015_000    0.170213  5.750067
         hds_00_003_008_000    0.389716  5.750067
         hds_00_009_001_000    0.324789  5.750067
         hds_00_013_010_000   -0.169959  5.750067
         hds_00_015_016_000    0.165231  5.750067
         hds_00_021_010_000   -0.026323  5.750067
         hds_00_022_015_000   -0.017951  5.750067
         hds_00_024_004_000    0.071408  5.750067
         hds_00_026_006_000    0.025051  5.750067
         hds_00_029_015_000    0.252914  5.750067
         hds_00_033_007_000    0.132353  5.750067
         hds_00_034_010_000    0.021161  5.750067
```

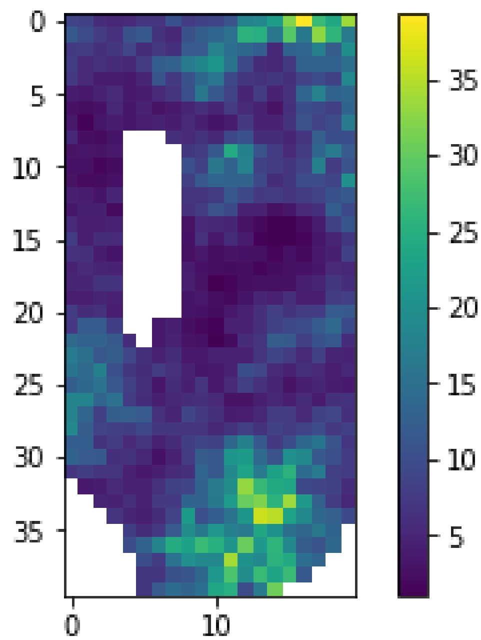
The residual should be exactly the noise values from above.Lets load the model (that was just run using the true pars) and check some things

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

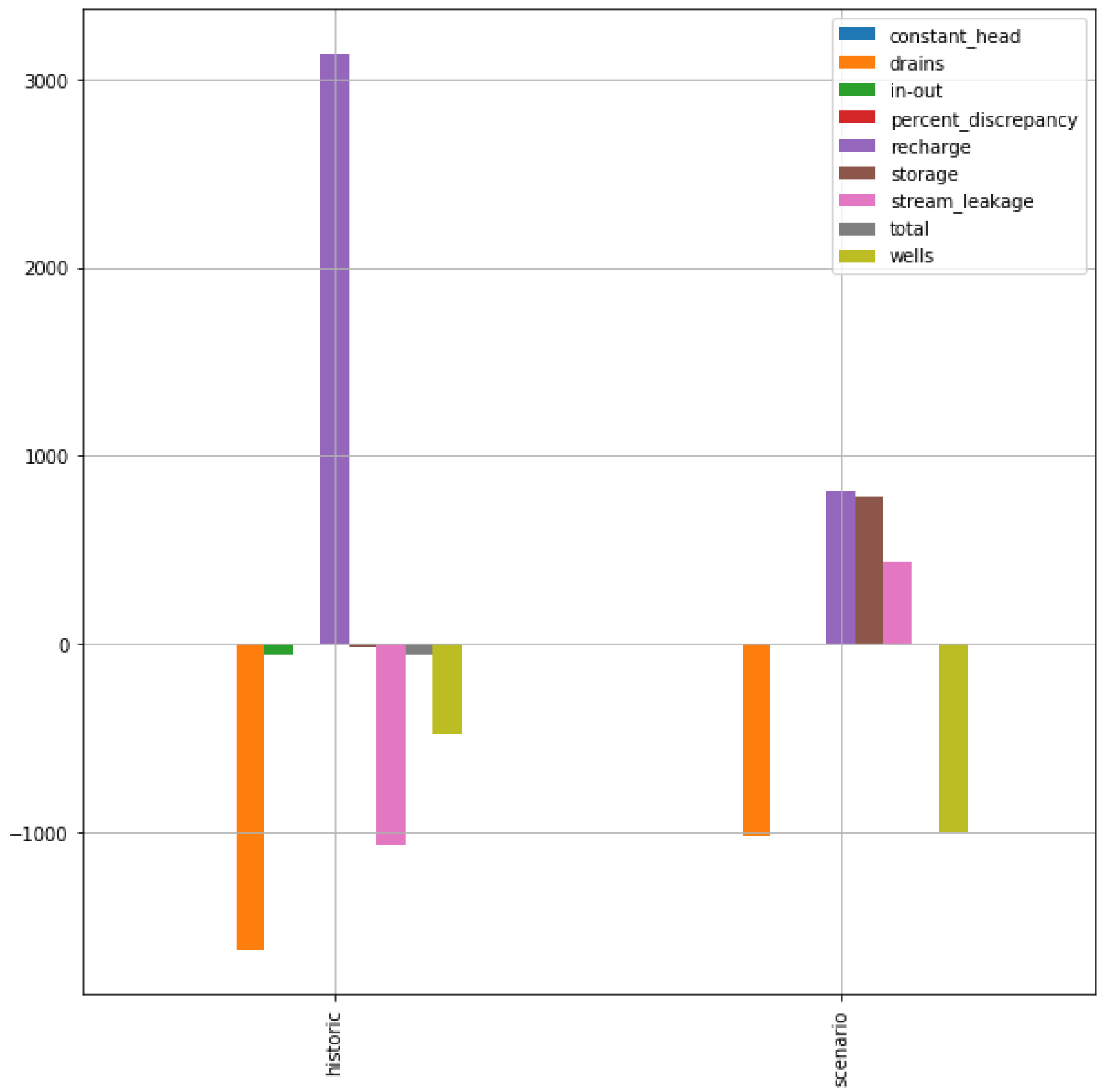
```
In [25]: a = m.upw.hk[0].array
         #a = m.rch.rech[0].array
```

```
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()
```

```
1.017649 39.28789
```



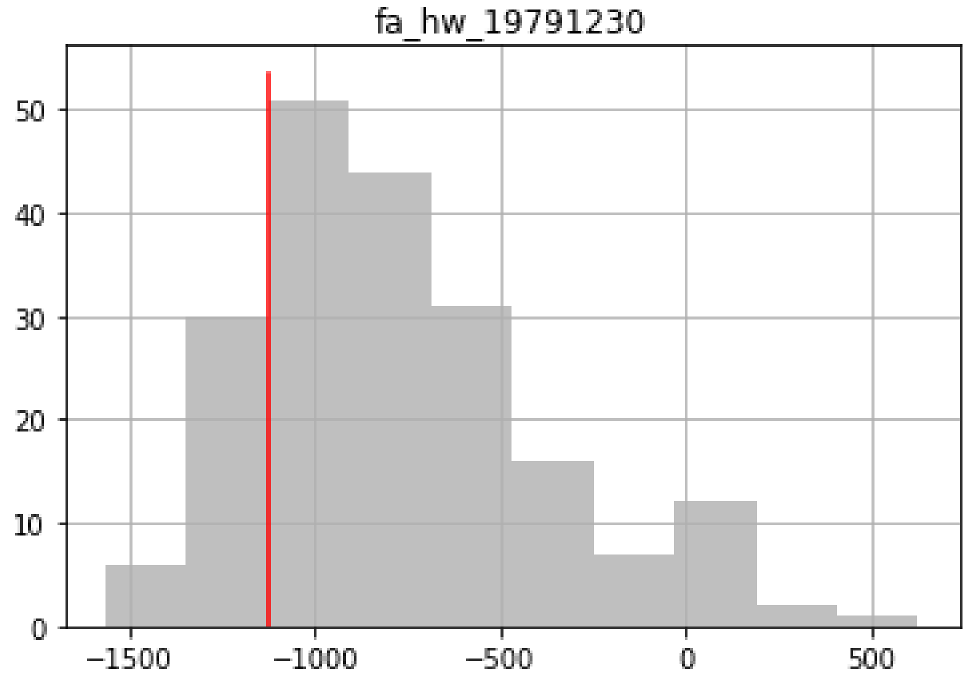

```
In [26]: lst = flopy.utils.MfListBudget(os.path.join(m_d,"freyberg.list"))
         df = lst.get_dataframes(diff=True)[0]
         ax = df.plot(kind="bar",figsize=(10,10), grid=True)
         a = ax.set_xticklabels(["historic","scenario"],rotation=90)
         plt.show(ax)
```

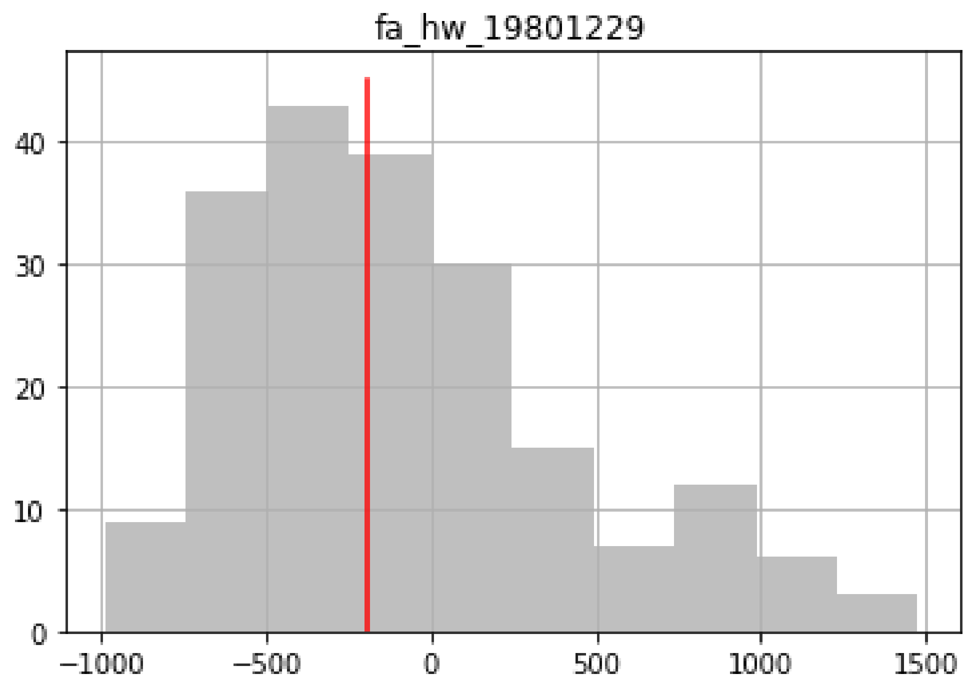


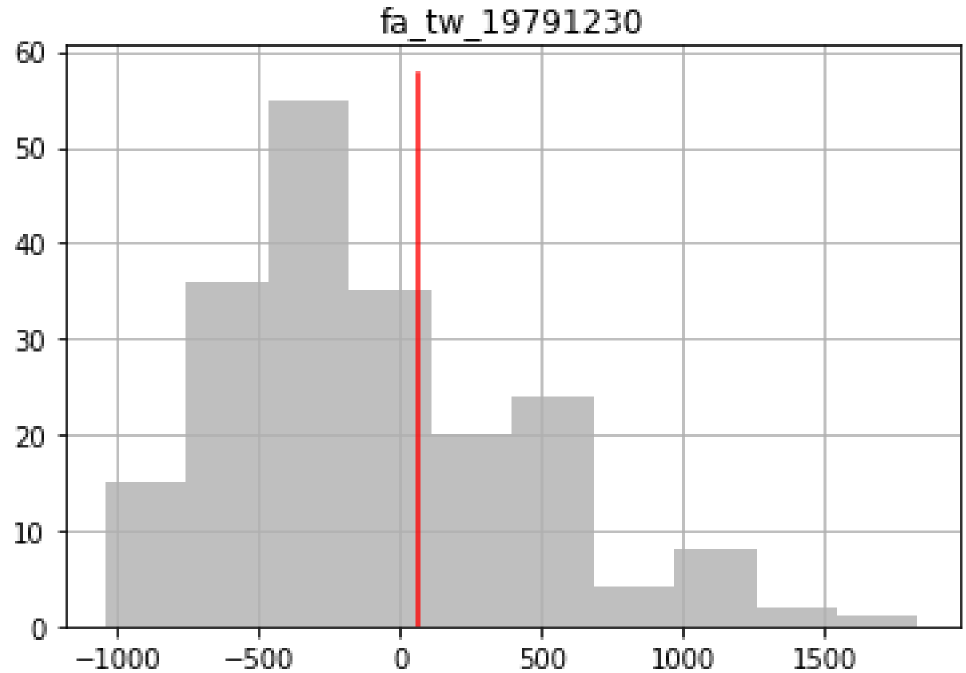
1.0.8 see how our existing observation ensemble compares to the truth

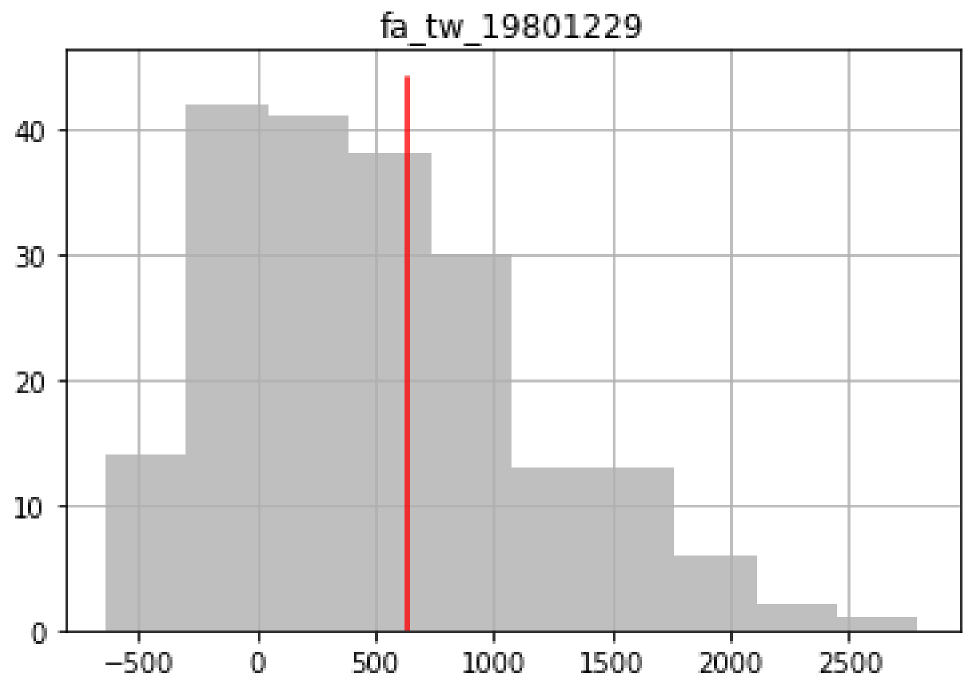
forecasts:

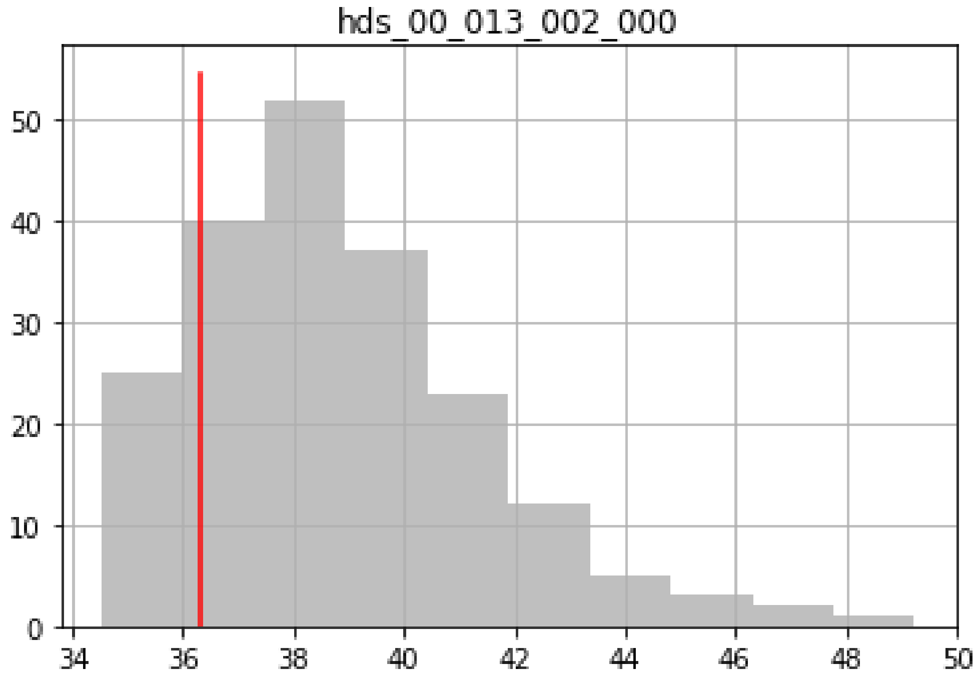
```
In [27]: obs = pst.observation_data
         plt.figure()
         for forecast in fnames:
             ax = plt.subplot(111)
             obs_df.loc[:,forecast].hist(ax=ax,color="0.5",alpha=0.5)
             ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r")
    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

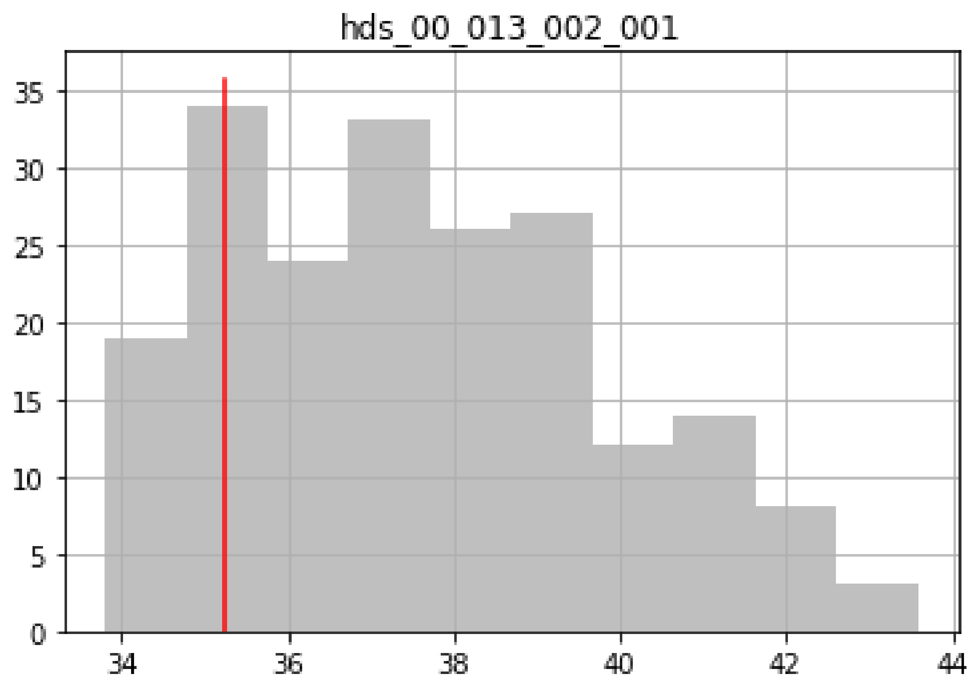

fa_hw_19791230
50
40
30
20
10
0
−1500
−1000
−500
0
500

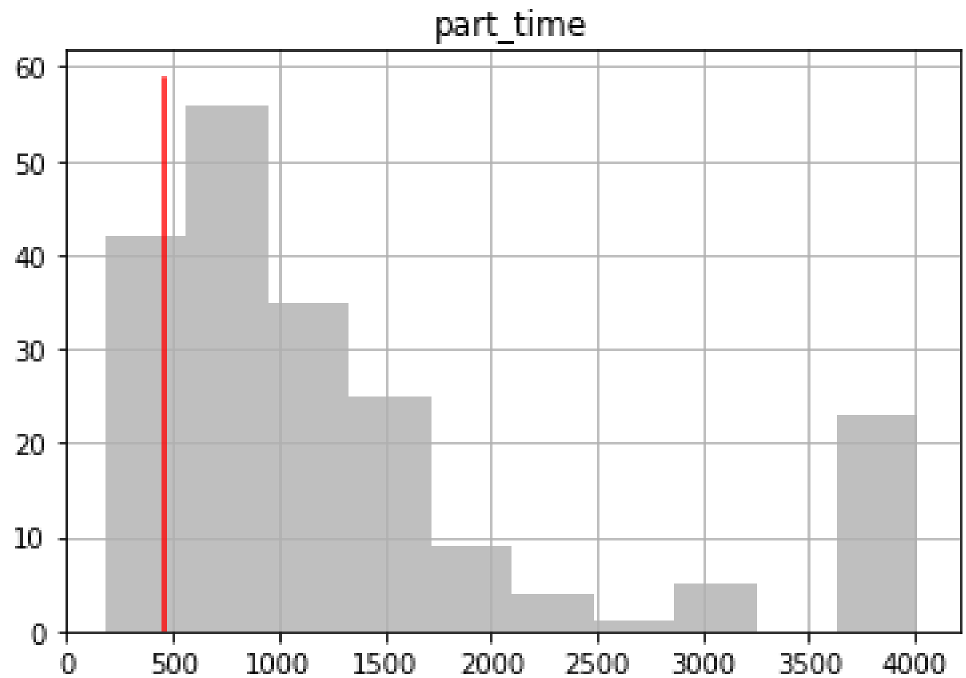

fa_hw_19801229
40
30
20
10
0
−1000
−500
0
500
1000
1500

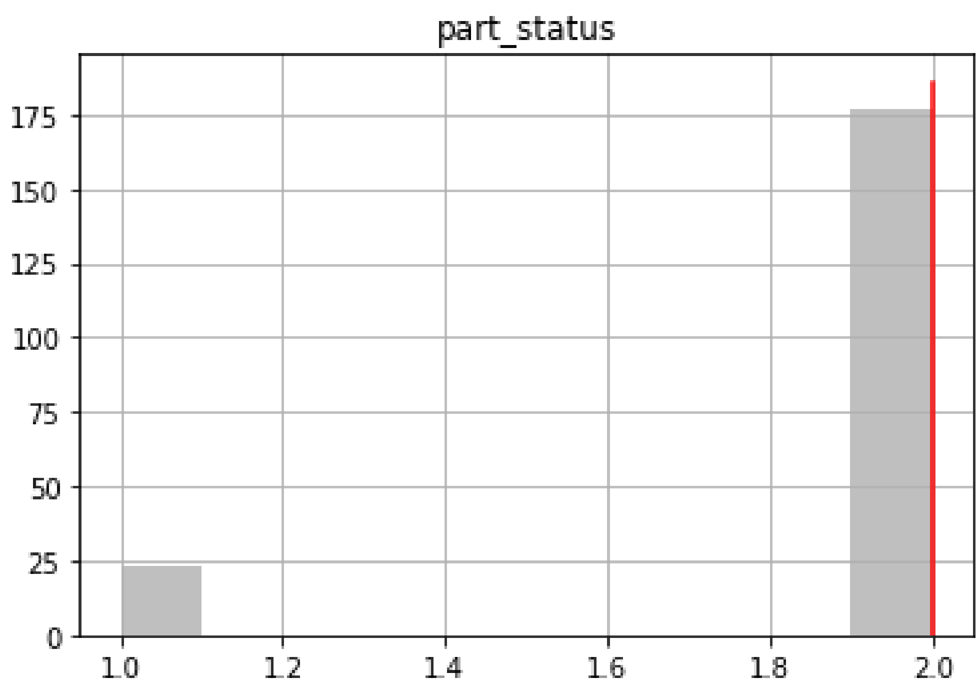

fa_tw_19791230
60
50
40
30
20
10
0
−1000
−500
0
500
1000
1500


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


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

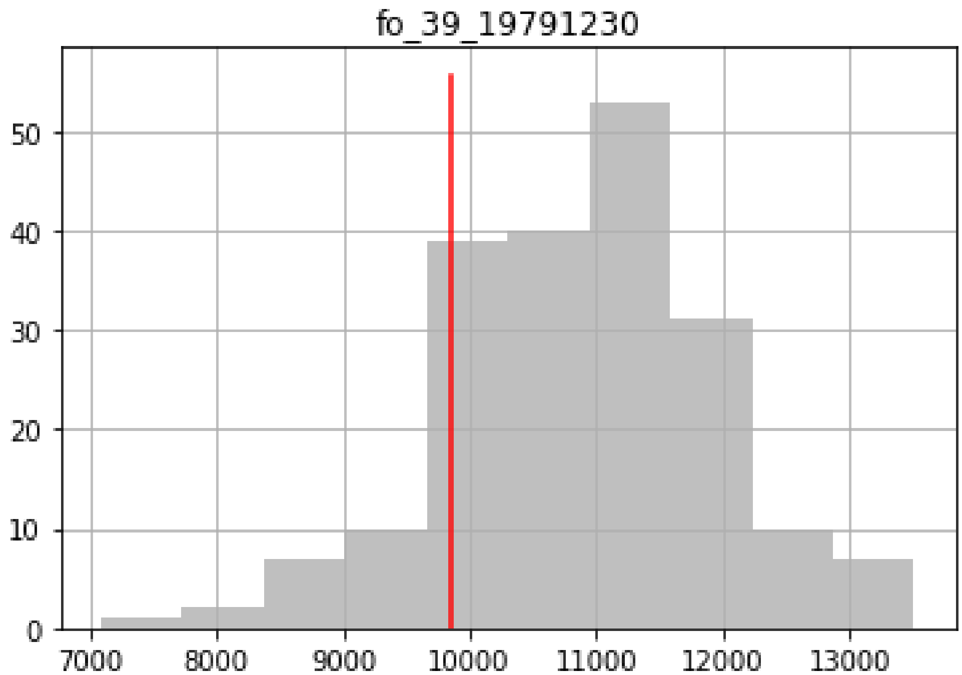

hds_00_013_002_001
0
5
10
15
20
25
30
35
34
36
38
40
42
44

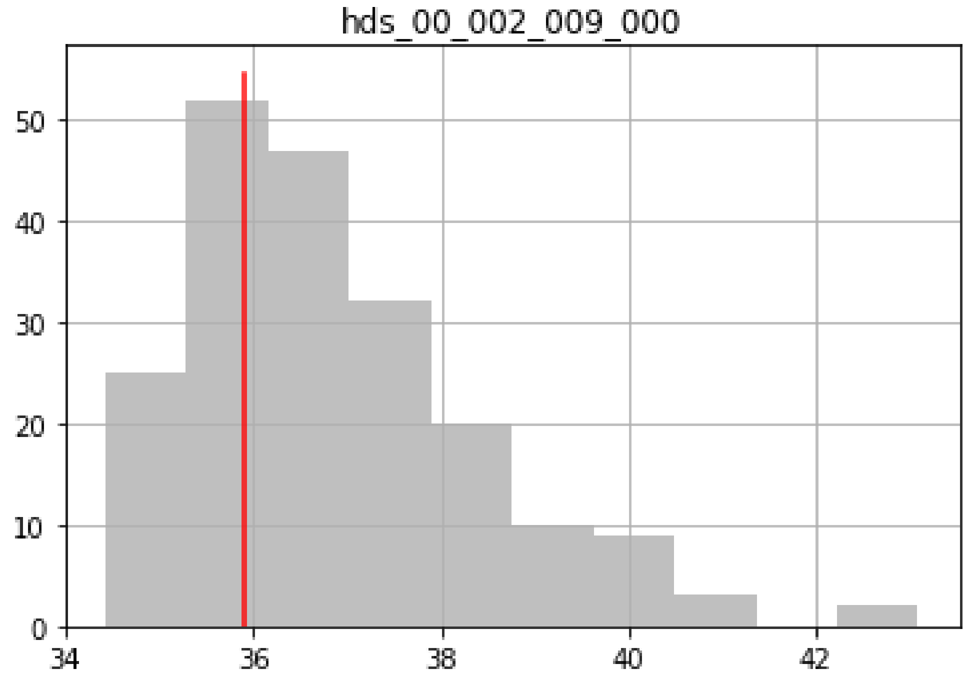


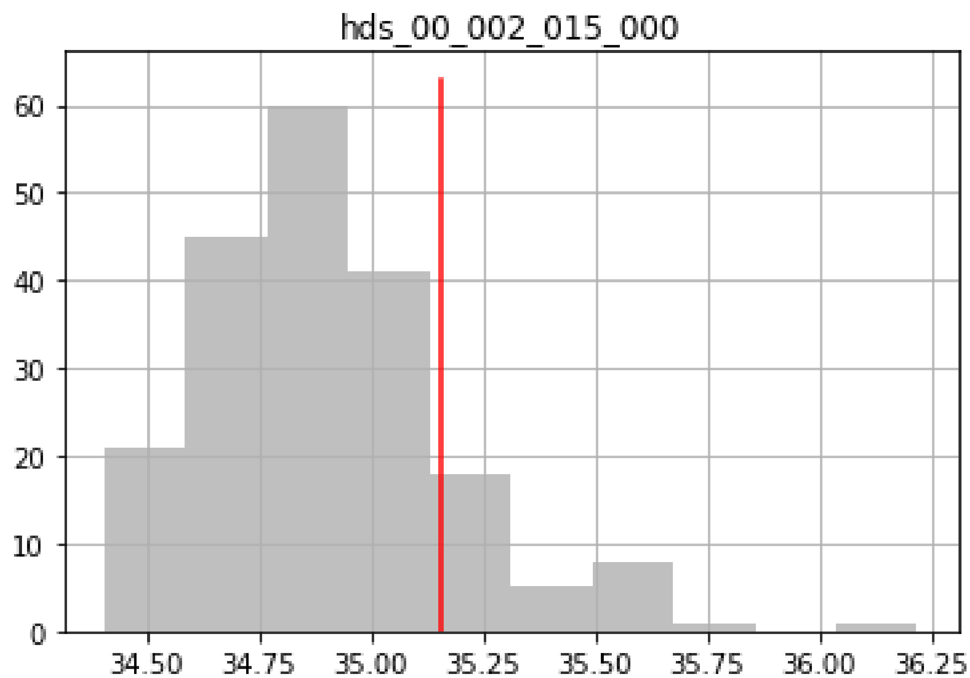


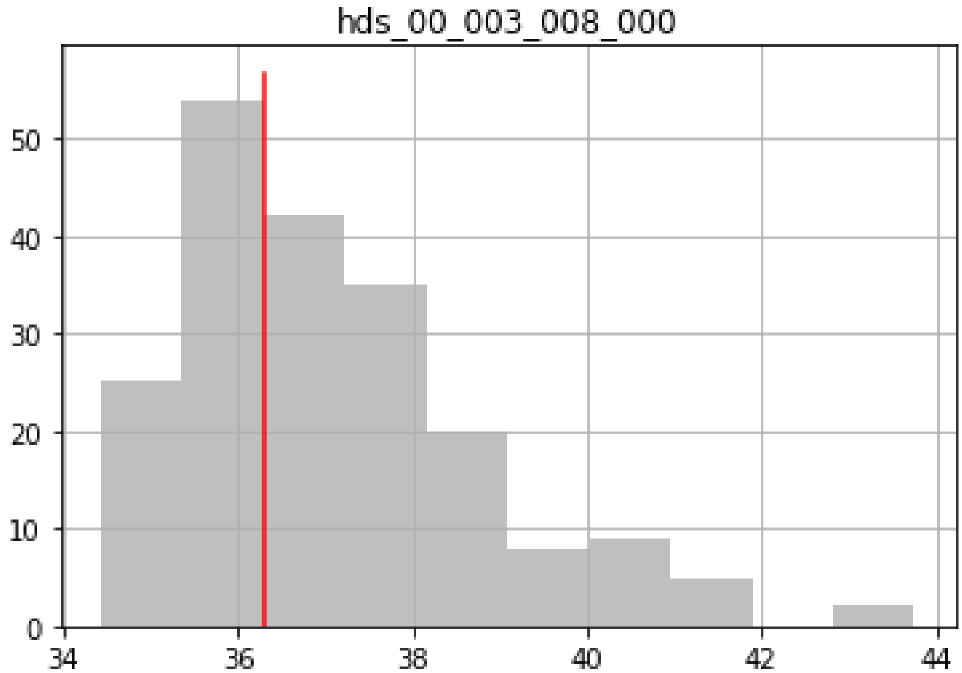
observations:

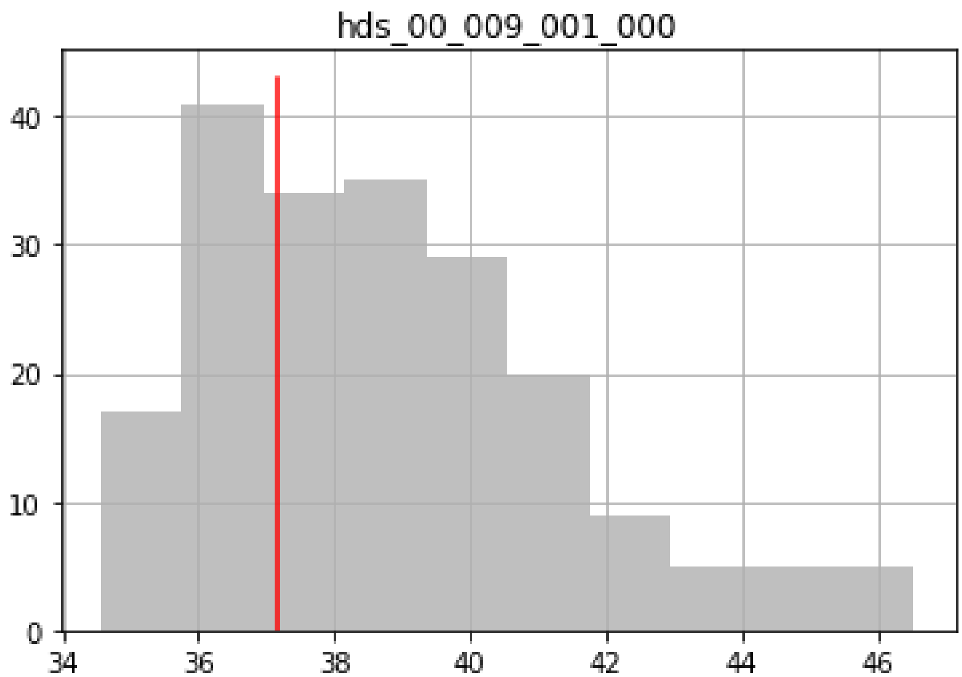
In [28]:
```
for oname in pst.nnz_obs_names:
    ax = plt.subplot(111)
    obs_df.loc[:,oname].hist(ax=ax,color="0.5",alpha=0.5)
    ax.plot([obs.loc[oname,"obsval"],obs.loc[oname,"obsval"]],ax.get_ylim(),"r")
    ax.set_title(oname)
    plt.show()
```

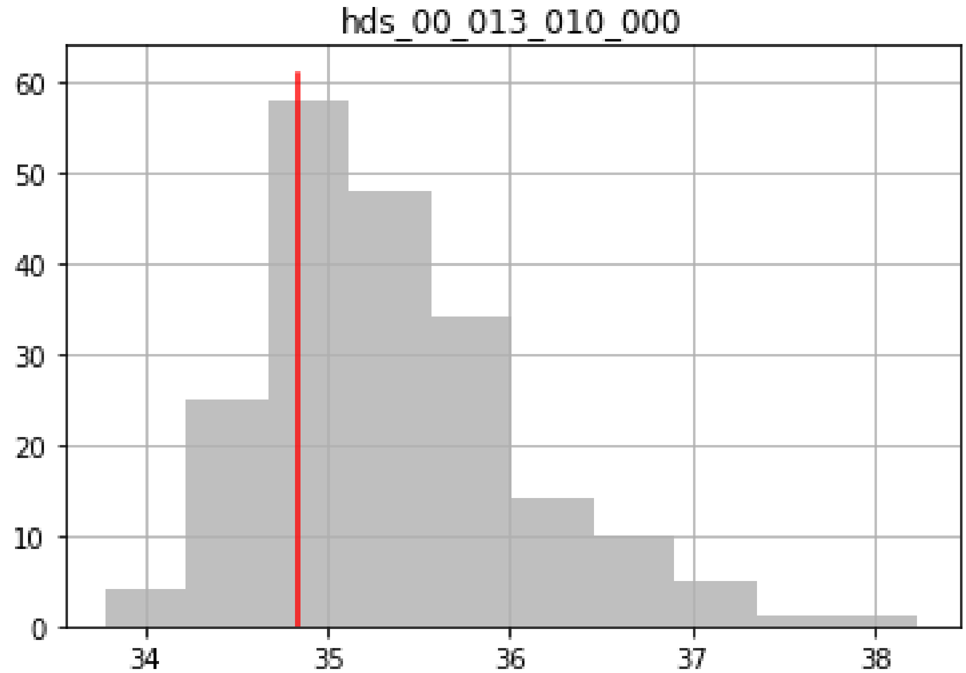



hds_00_002_009_000
0
10
20
30
40
50
34
36
38
40
42


hds_00_002_015_000
0
10
20
30
40
50
60
34.50
34.75
35.00
35.25
35.50
35.75
36.00
36.25


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


hds_00_009_001_000
0
10
20
30
40
34
36
38
40
42
44
46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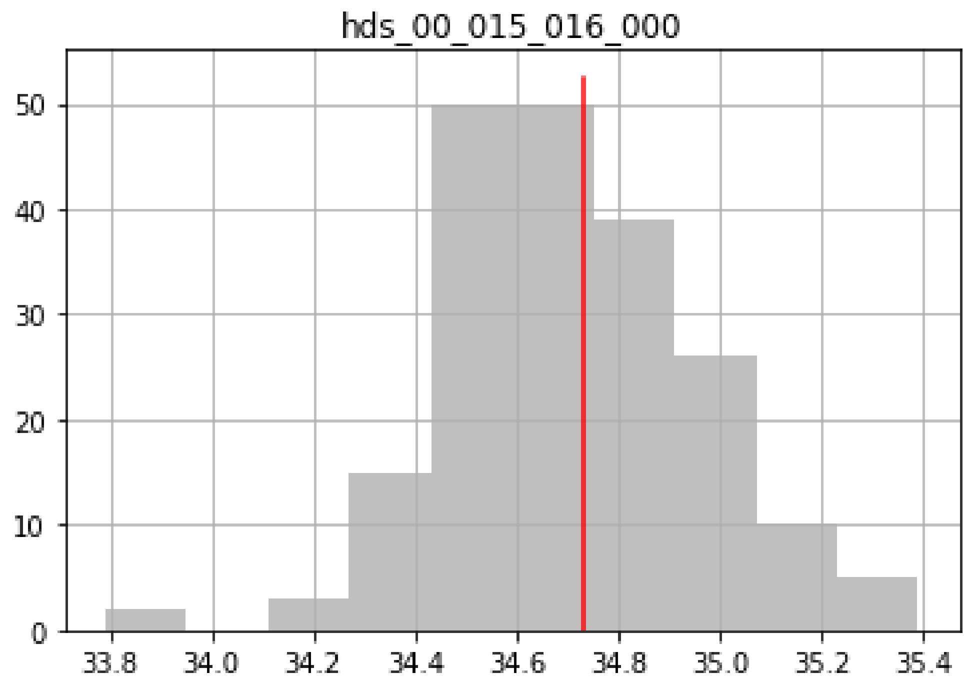
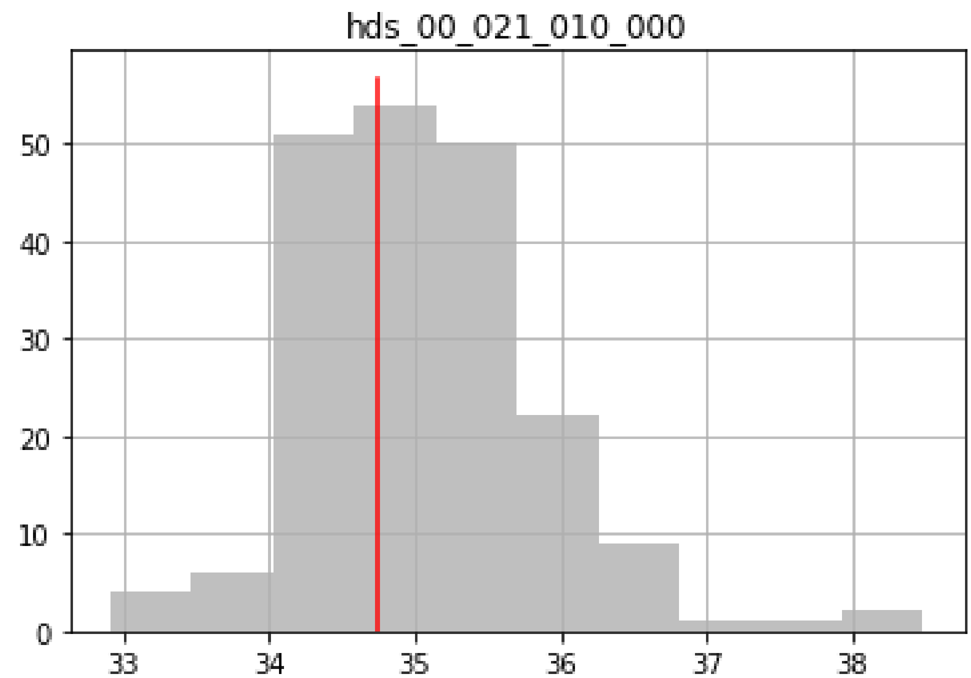
50
40
30
20
10
0
34
35
36
37
38


hds_00_015_016_000
50
40
30
20
10
0
33.8
34.0
34.2
34.4
34.6
34.8
35.0
35.2
35.4



hds_00_021_010_000
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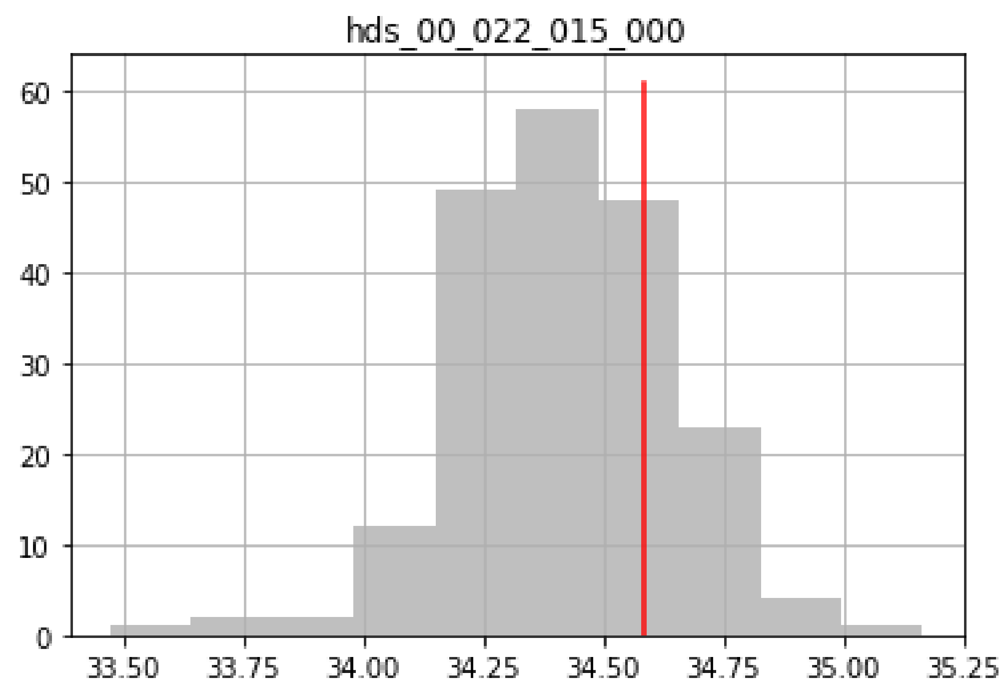
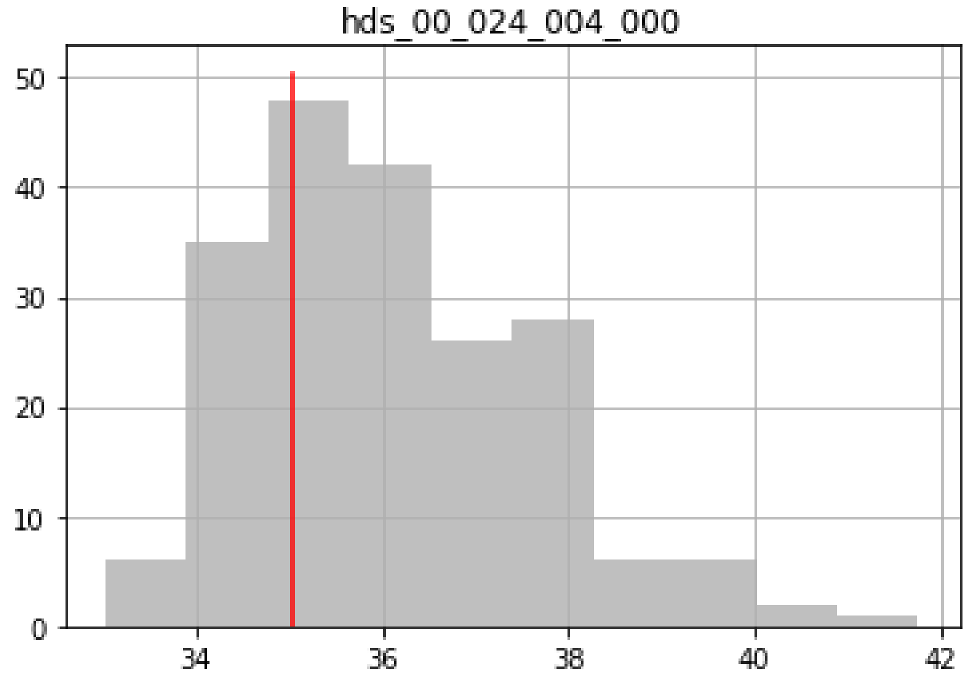
20
30
40
50
33
34
35
36
37
38



hds_00_022_015_000
0
10
20
30
40
50
60
33.50
33.75
34.00
34.25
34.50
34.75
35.00
35.25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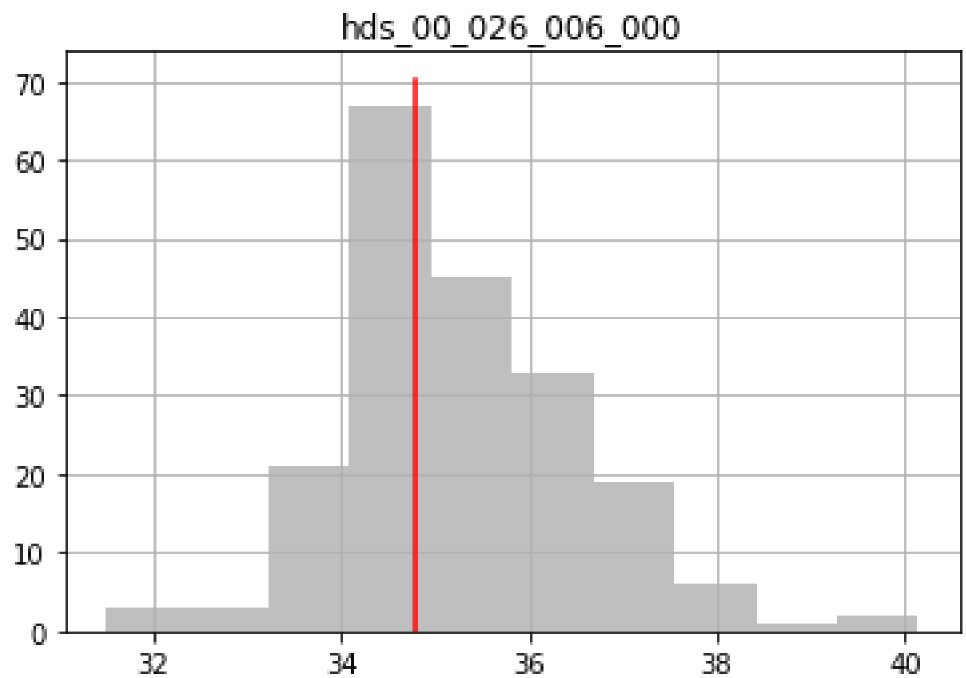
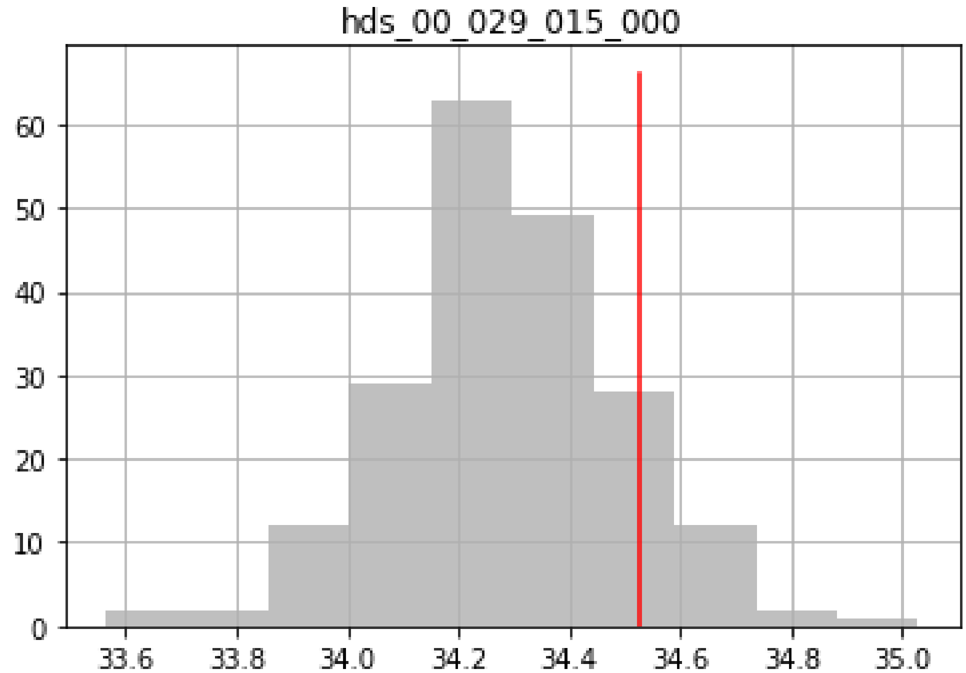
0
10
20
30
40
50
34
36
38
40
42


hds_00_026_006_000
0
10
20
30
40
50
60
70
32
34
36
38
40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30
20
10
0
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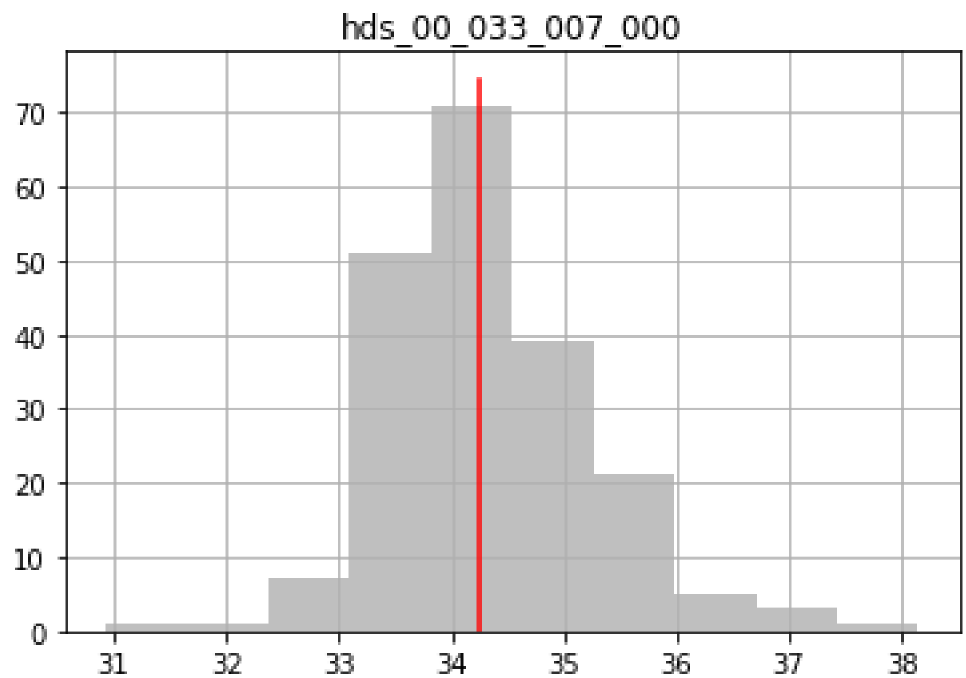
33.8
34.0
34.2
34.4
34.6
34.8
35.0


hds_00_033_007_000
70
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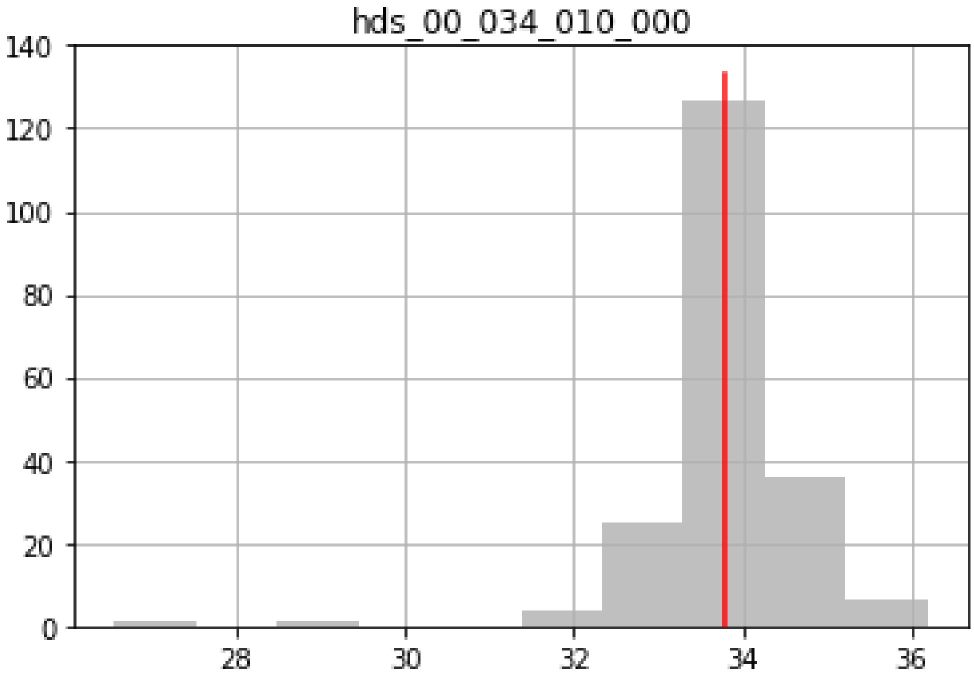
50
40
30
20
10
0
31
32
33
34
35
36
37
38


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