prior_montecarlo

May 7, 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
```

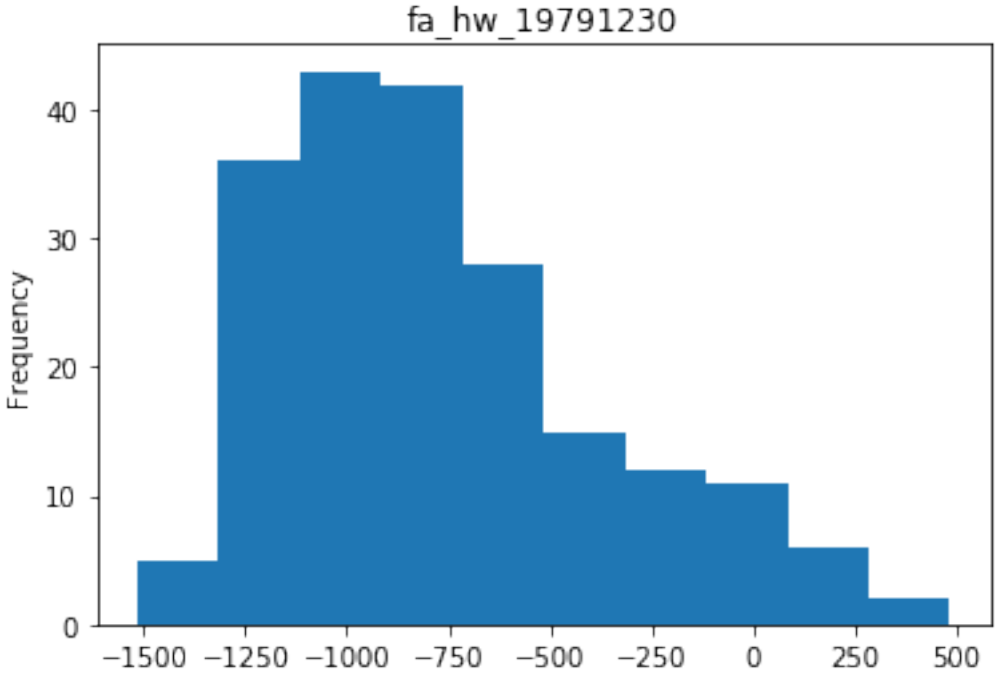
1.0.5 confirm which quantities were identified as forecasts

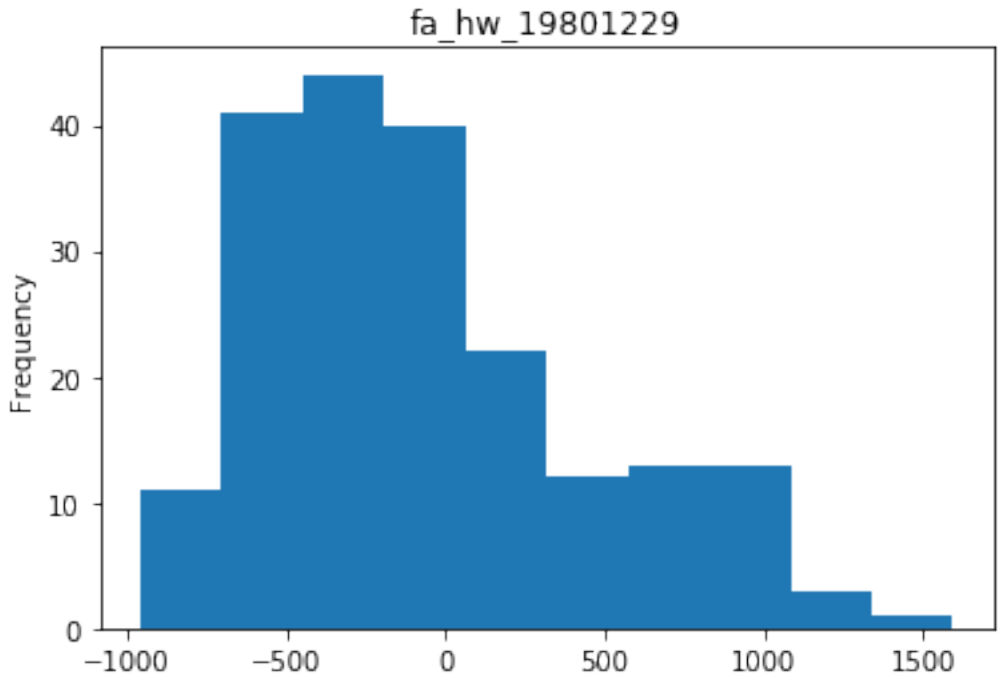
```
In [8]: fnames = pst.pestpp_options["forecasts"].split(',')
        fnames
```

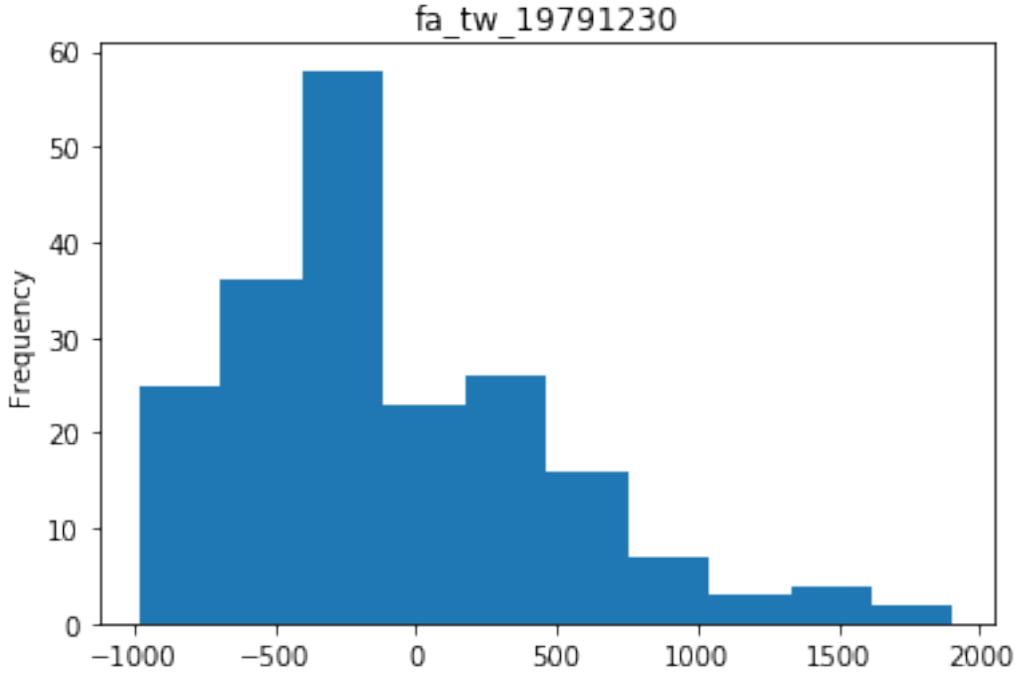
```
Out[8]: ['fa_hw_19791230',
         'fa_hw_19801229',
         'fa_tw_19791230',
         'fa_tw_19801229',
         'hds_00_013_002_000',
         'hds_00_013_002_001',
         'part_time',
         'part_status']
```

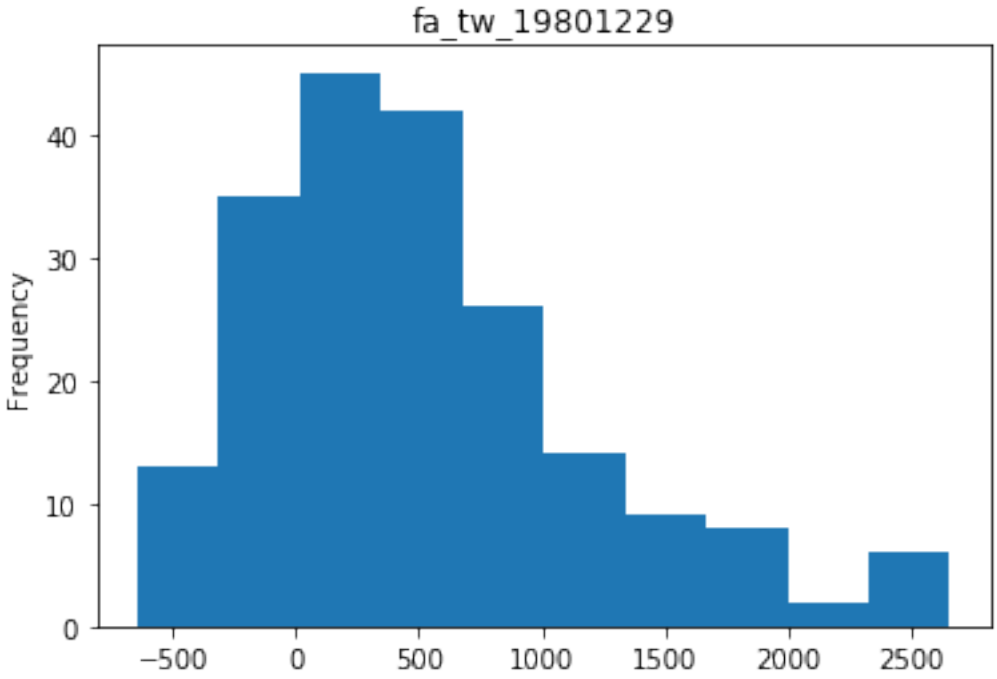
1.0.6 now we can plot the distributions of each forecast

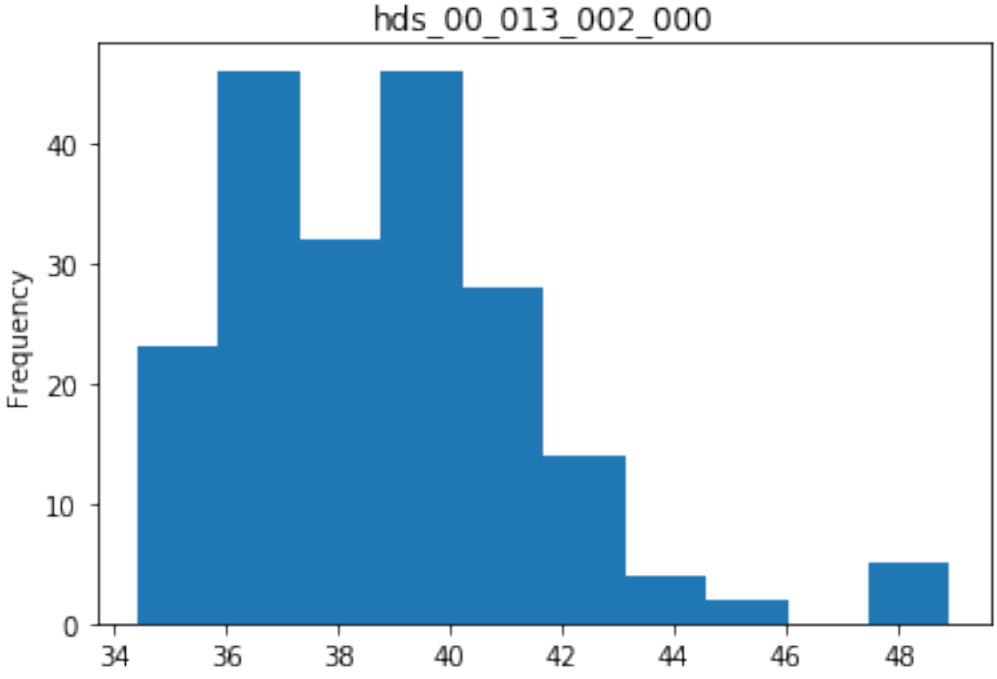
```
In [9]: for forecast in fnames:
            plt.figure()
            ax = obs_df.loc[:,forecast].plot(kind="hist")
            ax.set_title(forecast)
        plt.show()
```

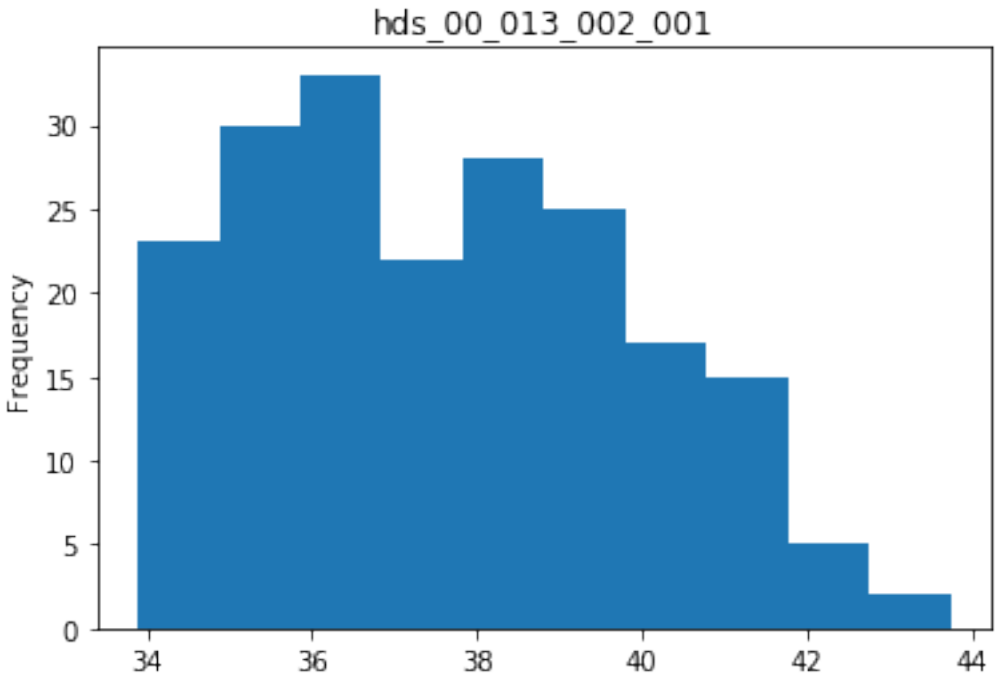


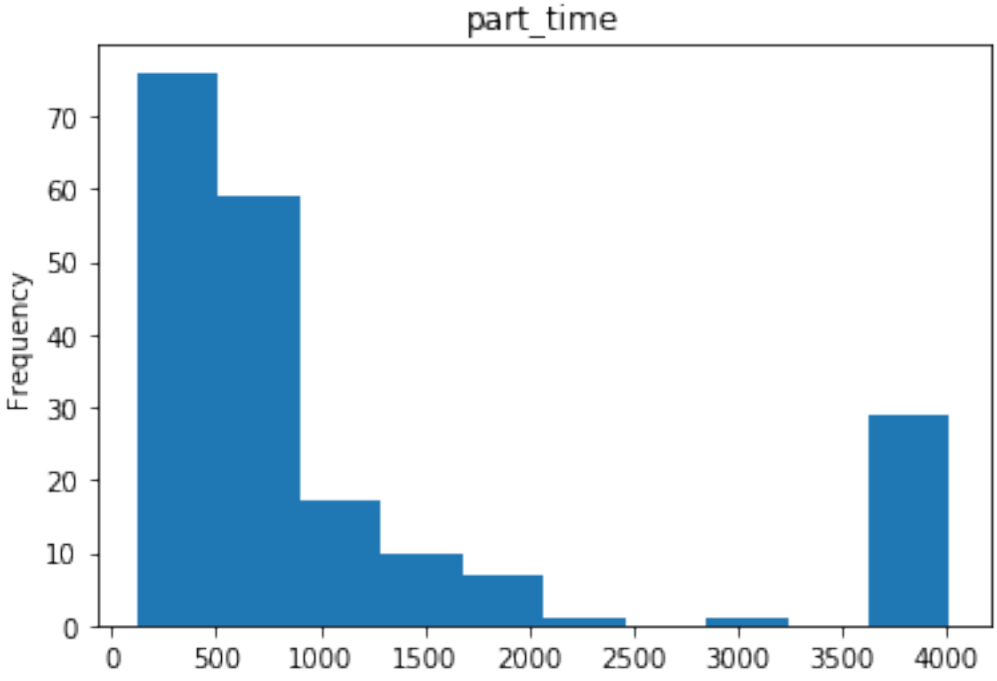

fa_hw_19801229
Frequency
40
30
20
10
0
−1000
−500
0
500
1000
1500

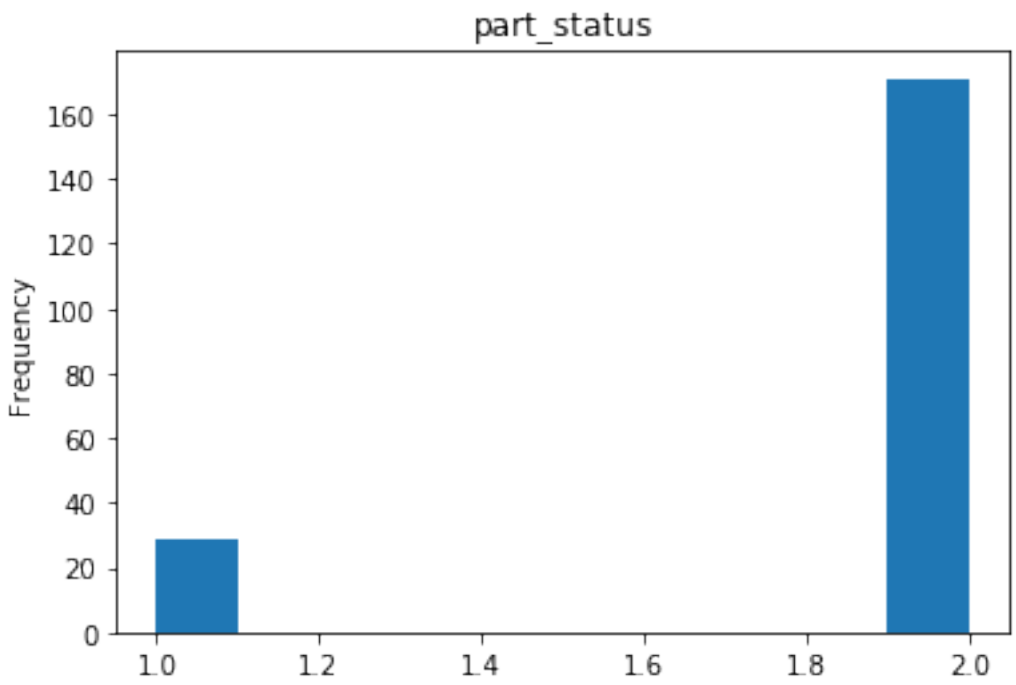

fa_tw_19791230
Frequency
60
50
40
30
20
10
0
−1000
−500
0
500
1000
1500
2000


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


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

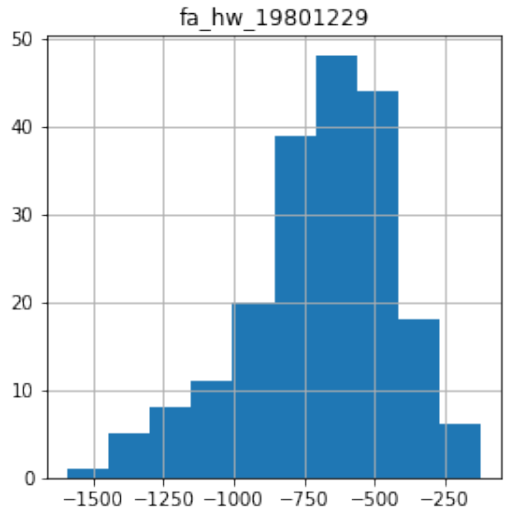

hds_00_013_002_001
Frequency
0
5
10
15
20
25
30
34
36
38
40
42
44

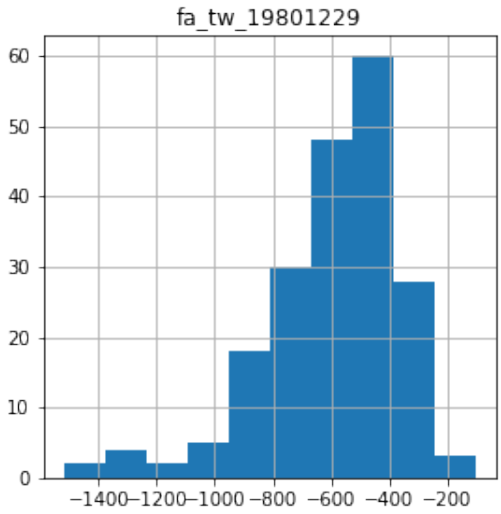

part_time
Frequency
0
10
20
30
40
50
60
70
0
500
1000
1500
2000
2500
3000
3500
4000

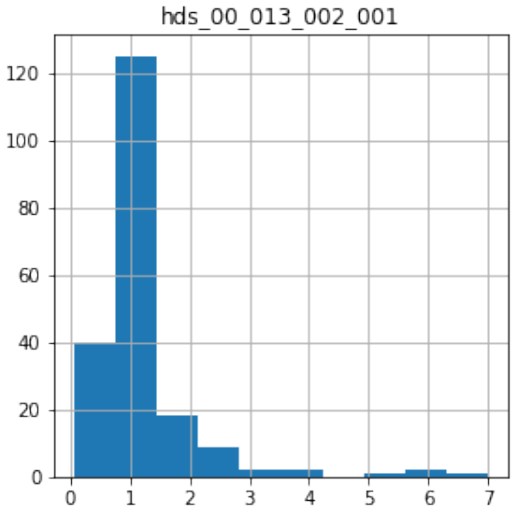


We see that under scenario conditions, many more realizations for the flow to the aquifer in the headwaters are postive (as expected). Lets difference these two:

```
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()
         idx = hist_swgw.index[100]
         idx
         hist_swgw
```

```
Out[11]: run_id
         21    -1515.022600
         5     -1478.211200
         182   -1429.960200
         20    -1370.134500
         11    -1337.385700
         116   -1308.621900
         114   -1300.427400
         38    -1292.823000
         178   -1290.769200
         61    -1268.275270
         138   -1266.314400
         49    -1250.714800
         130   -1242.871000
         170   -1242.660510
         186   -1239.799900
         26    -1239.114500
         44    -1227.066600
         65    -1221.035000
         22    -1218.391100
         48    -1216.842800
         128   -1211.274800
         113   -1209.880300
         185   -1199.719800
         2     -1184.331600
         146   -1166.464300
         46    -1165.863000
         159   -1156.649900
         134   -1155.403000
         166   -1148.670800
         69    -1148.229100
                  ...
         30     -307.996060
         98     -302.095600
         162    -294.096350
         89     -249.515060
         71     -208.660760
         147    -205.904900
         51     -199.145762
         165    -166.591800
         111    -165.552300
         189    -163.077070
         149    -119.544090
         181    -109.619790
         56      -83.603250
         105     -74.408900
         50      -57.105100
         36      -25.374384
```

```
126     -13.427900
31      -12.679864
155       1.307900
40       11.568782
17       23.331010
60       76.068821
0        84.979200
12      119.832260
139     139.525690
163     160.345500
90      164.420400
41      186.825430
16      425.030270
27      484.226980
Name: fa_hw_19791230, Length: 200, dtype: float64
```

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

```
Out[12]: fo_39_19791230        10597.000000
         hds_00_002_009_000       37.343391
         hds_00_002_015_000       34.760021
         hds_00_003_008_000       37.572289
         hds_00_009_001_000       39.558464
         hds_00_013_010_000       35.365974
         hds_00_015_016_000       34.653934
         hds_00_021_010_000       34.711166
         hds_00_022_015_000       34.419338
         hds_00_024_004_000       35.141888
         hds_00_026_006_000       34.682674
         hds_00_029_015_000       34.207253
         hds_00_033_007_000       34.075302
         hds_00_034_010_000       33.636864
         Name: 81, 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       -853.092900
         fa_hw_19801229       -210.374210
         fa_tw_19791230       -184.237020
         fa_tw_19801229        427.883580
         hds_00_013_002_000     39.466167
         hds_00_013_002_001     38.665234
         part_time             637.733900
         part_status             2.000000
         Name: 81, 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"] = 0.005
```

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        352.810469
         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
```

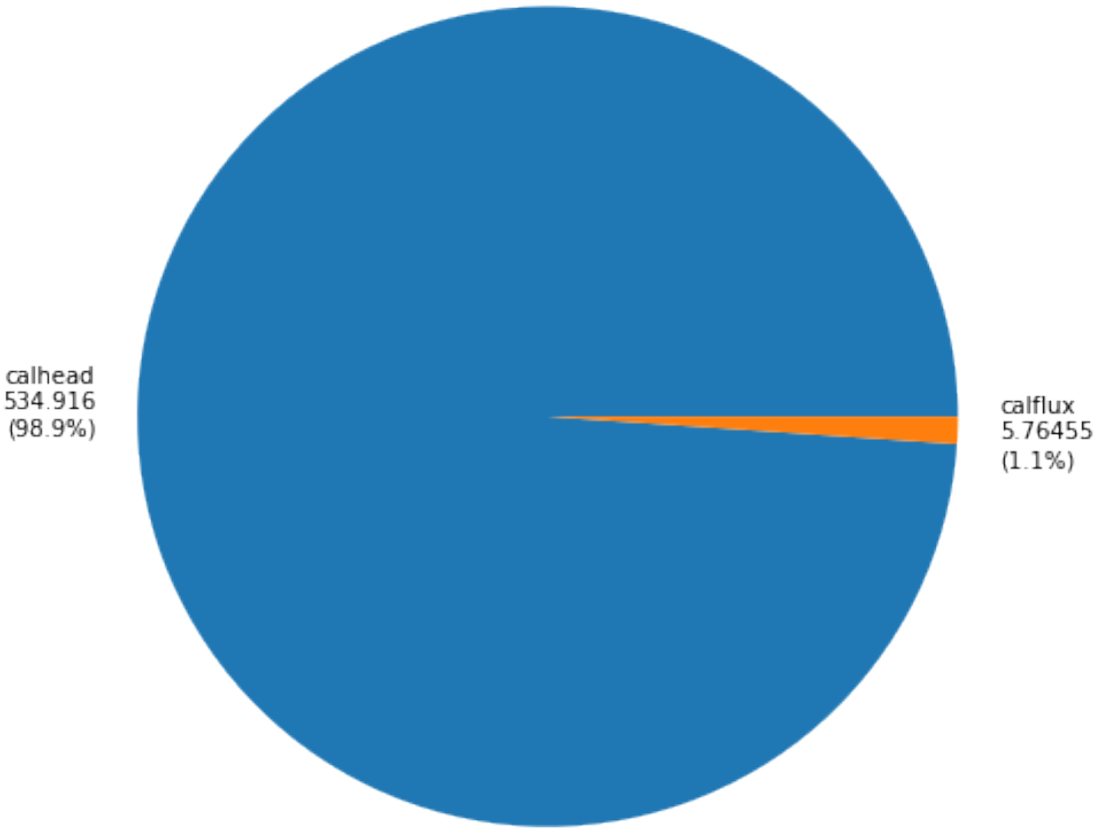
Then we write this out to a new file and run `pestpp-ies` to see how the objective function looks

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

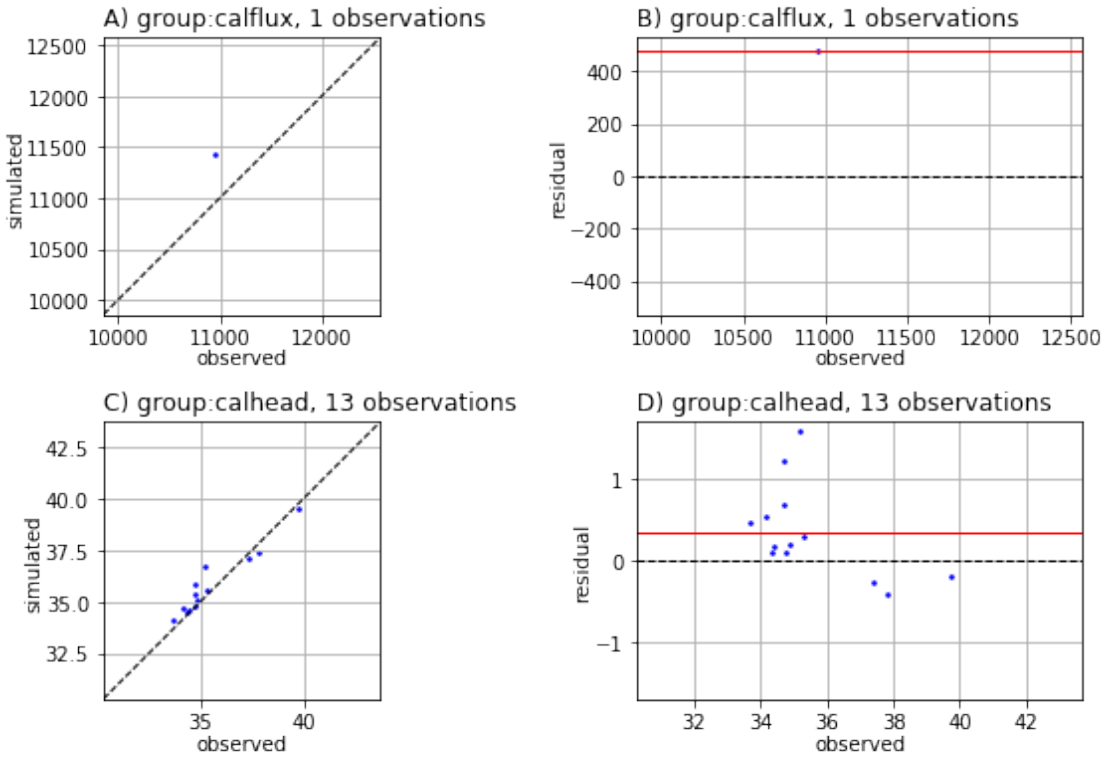
Now we can read in the results and make some figures showing residuals and the balance of the objective function

```
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,:]
```

```
540.6801963885084
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	10949.810469	11430.000000	

```
hds_00_002_009_000  hds_00_002_009_000  calhead     37.383407     37.107498
hds_00_002_015_000  hds_00_002_015_000  calhead     34.857895     35.045185
hds_00_003_008_000  hds_00_003_008_000  calhead     37.796378     37.397289
hds_00_009_001_000  hds_00_009_001_000  calhead     39.745220     39.546417
hds_00_013_010_000  hds_00_013_010_000  calhead     35.268247     35.571774
hds_00_015_016_000  hds_00_015_016_000  calhead     34.748943     34.835716
hds_00_021_010_000  hds_00_021_010_000  calhead     34.696031     35.386250
hds_00_022_015_000  hds_00_022_015_000  calhead     34.409016     34.577492
hds_00_024_004_000  hds_00_024_004_000  calhead     35.182948     36.760464
hds_00_026_006_000  hds_00_026_006_000  calhead     34.697079     35.896149
hds_00_029_015_000  hds_00_029_015_000  calhead     34.352680     34.453842
hds_00_033_007_000  hds_00_033_007_000  calhead     34.151406     34.678810
hds_00_034_010_000  hds_00_034_010_000  calhead     33.649031     34.118073
```

name	residual	weight
fo_39_19791230	-480.189531	0.005
hds_00_002_009_000	0.275909	10.000
hds_00_002_015_000	-0.187290	10.000
hds_00_003_008_000	0.399089	10.000
hds_00_009_001_000	0.198803	10.000
hds_00_013_010_000	-0.303527	10.000
hds_00_015_016_000	-0.086773	10.000
hds_00_021_010_000	-0.690219	10.000
hds_00_022_015_000	-0.168475	10.000
hds_00_024_004_000	-1.577516	10.000
hds_00_026_006_000	-1.199070	10.000
hds_00_029_015_000	-0.101162	10.000
hds_00_033_007_000	-0.527404	10.000
hds_00_034_010_000	-0.469041	10.000

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"]}
#pst.adjust_weights(obsgrp_dict=target)
#pst.plot(kind='phi_pie')
```

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 [19]:
```
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"))
```

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 [20]: 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,:]
```

```
17.528847215722436
```

Out[20]:

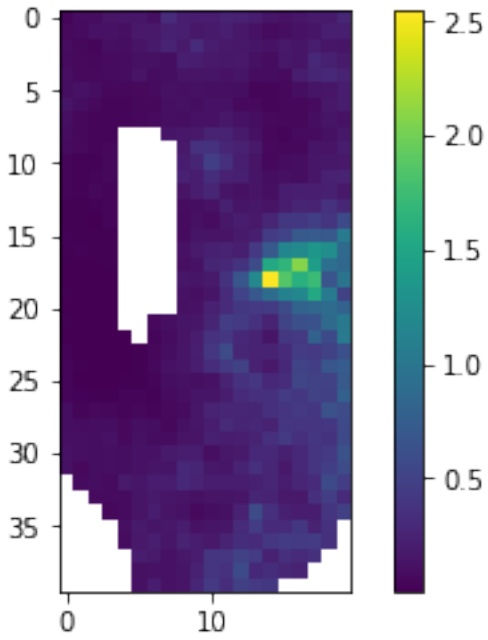
	name	group	measured	modelled	residual	weight
name						
fo_39_19791230	fo_39_19791230	calflux	10949.810469	10597.000000	352.810469	0.005
hds_00_002_009_000	hds_00_002_009_000	calhead	37.383407	37.343391	0.040016	10.000
hds_00_002_015_000	hds_00_002_015_000	calhead	34.857895	34.760021	0.097874	10.000
hds_00_003_008_000	hds_00_003_008_000	calhead	37.796378	37.572289	0.224089	10.000
hds_00_009_001_000	hds_00_009_001_000	calhead	39.745220	39.558464	0.186756	10.000
hds_00_013_010_000	hds_00_013_010_000	calhead	35.268247	35.365974	-0.097728	10.000
hds_00_015_016_000	hds_00_015_016_000	calhead	34.748943	34.653934	0.095009	10.000
hds_00_021_010_000	hds_00_021_010_000	calhead	34.696031	34.711166	-0.015136	10.000
hds_00_022_015_000	hds_00_022_015_000	calhead	34.409016	34.419338	-0.010322	10.000
hds_00_024_004_000	hds_00_024_004_000	calhead	35.182948	35.141888	0.041060	10.000
hds_00_026_006_000	hds_00_026_006_000	calhead	34.697079	34.682674	0.014404	10.000
hds_00_029_015_000	hds_00_029_015_000	calhead	34.352680	34.207253	0.145427	10.000
hds_00_033_007_000	hds_00_033_007_000	calhead	34.151406	34.075302	0.076104	10.000
hds_00_034_010_000	hds_00_034_010_000	calhead	33.649031	33.636864	0.012168	10.000

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

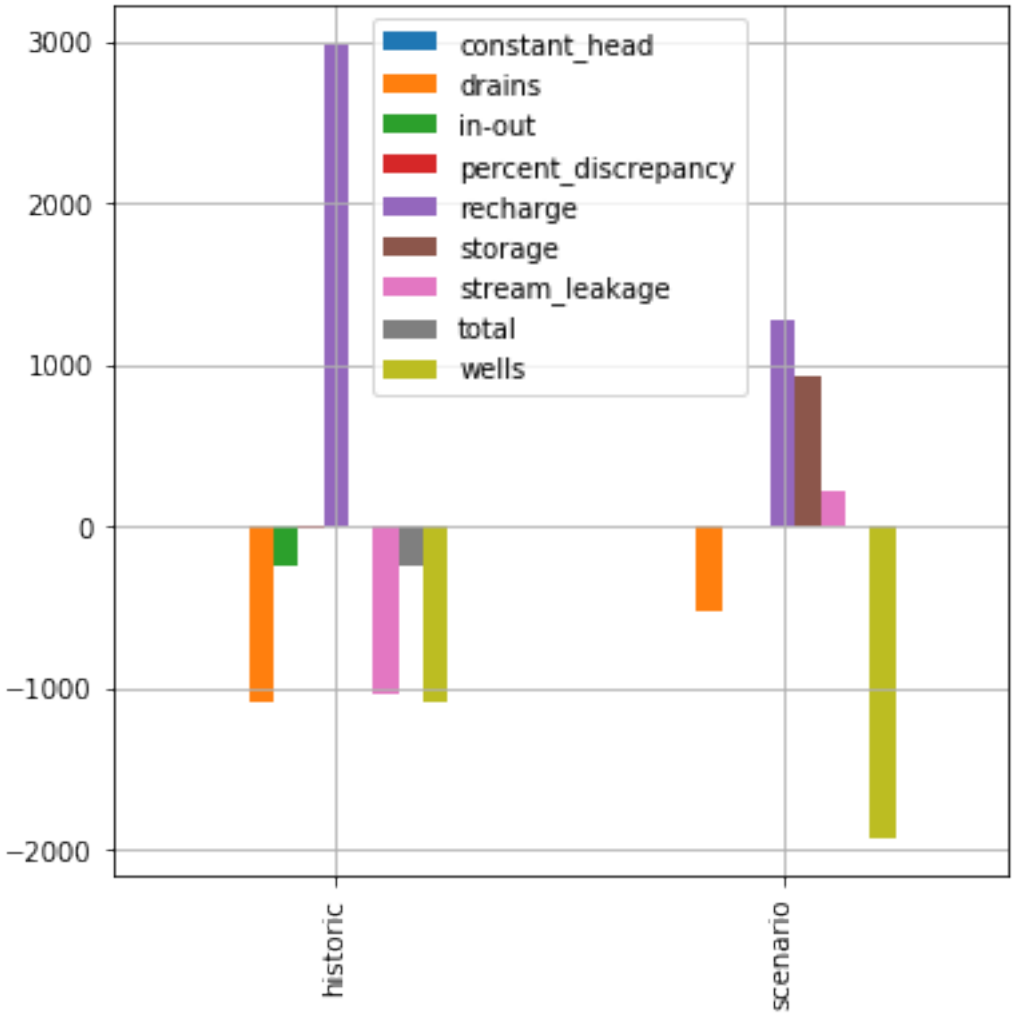
```
In [21]: m = flopy.modflow.Modflow.load("freyberg.nam",model_ws=m_d)
```

In [22]:
```
a = m.upw.vka[1].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()
```

```
0.00231499 2.546079
```



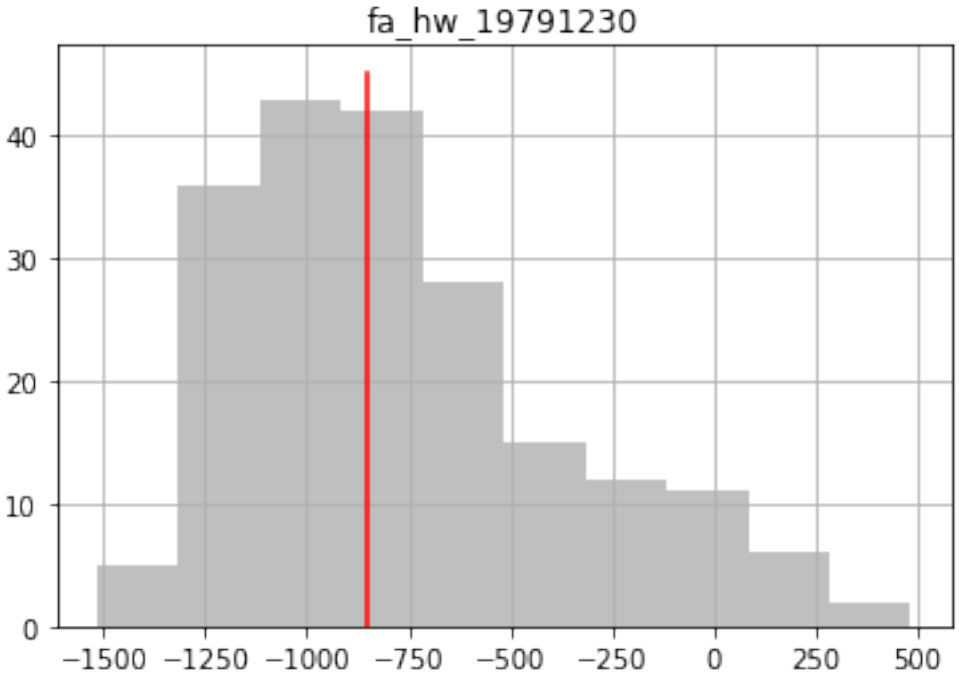
In [23]:
```
lst = flopy.utils.MfListBudget(os.path.join(m_d,"freyberg.list"))
df = lst.get_dataframes(diff=True)[0]
ax = df.plot(kind="bar",figsize=(6,6), grid=True)
a = ax.set_xticklabels(["historic","scenario"],rotation=90)
plt.show(ax)
```



1.0.8 see how our existing observation ensemble compares to the truth

forecasts:

```
In [24]: 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()
```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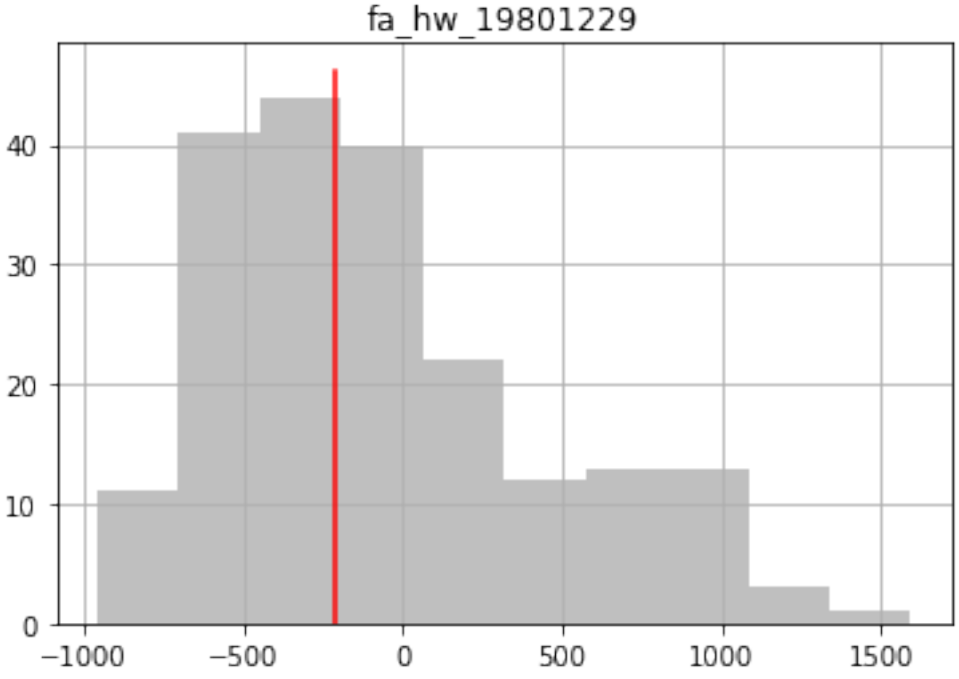
−1500
−1250
−1000
−750
−500
−250
0
250
500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30
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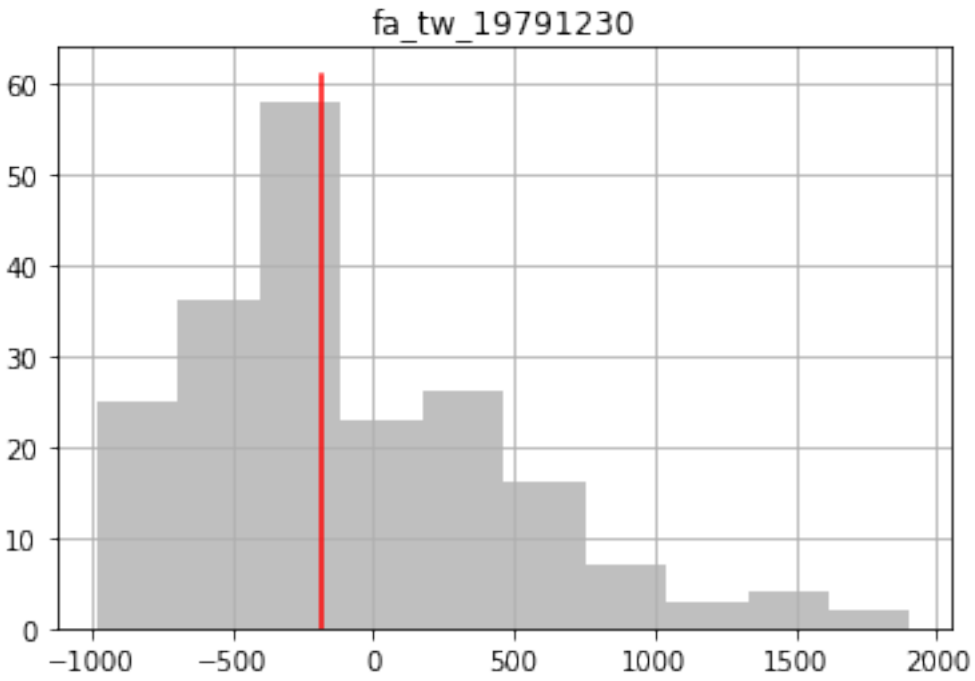
10
0
−1000
−500
0
500
1000
1500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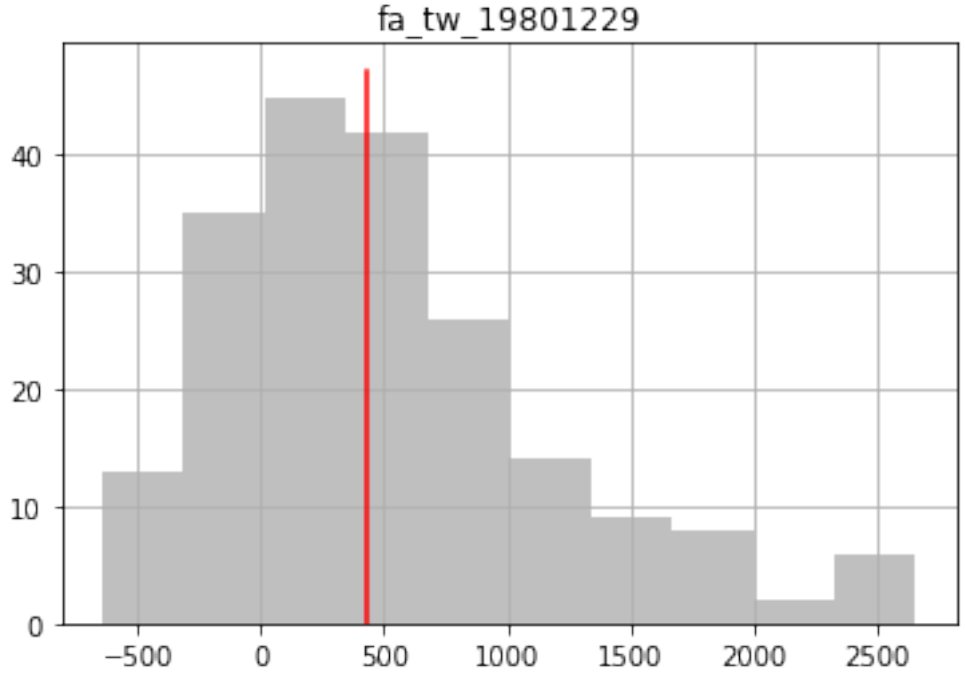
0
−1000
−500
0
500
1000
1500
2000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−500
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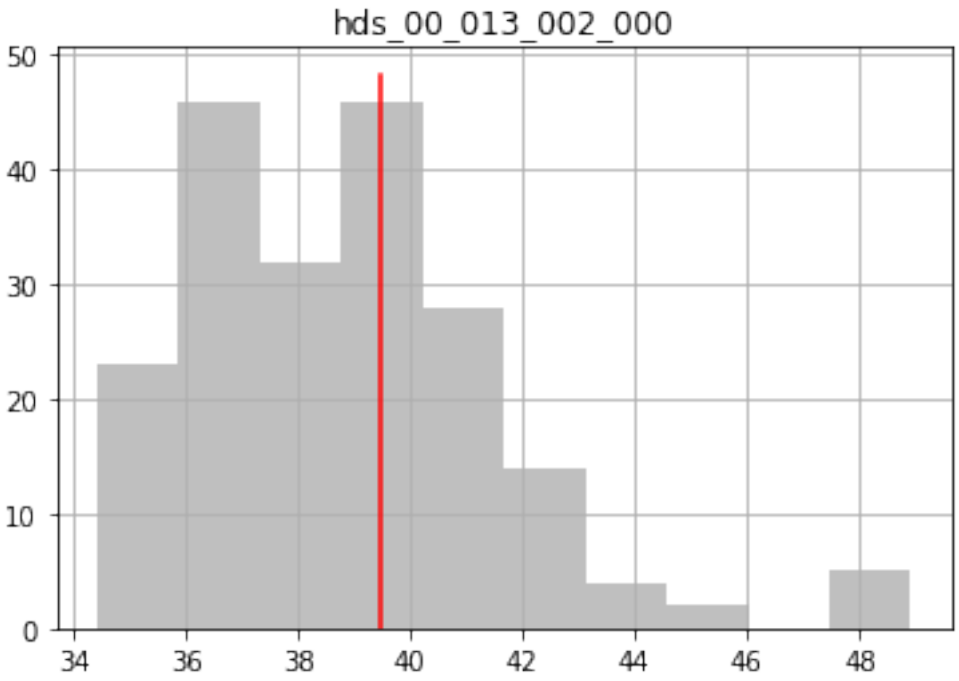
1000
1500
2000
2500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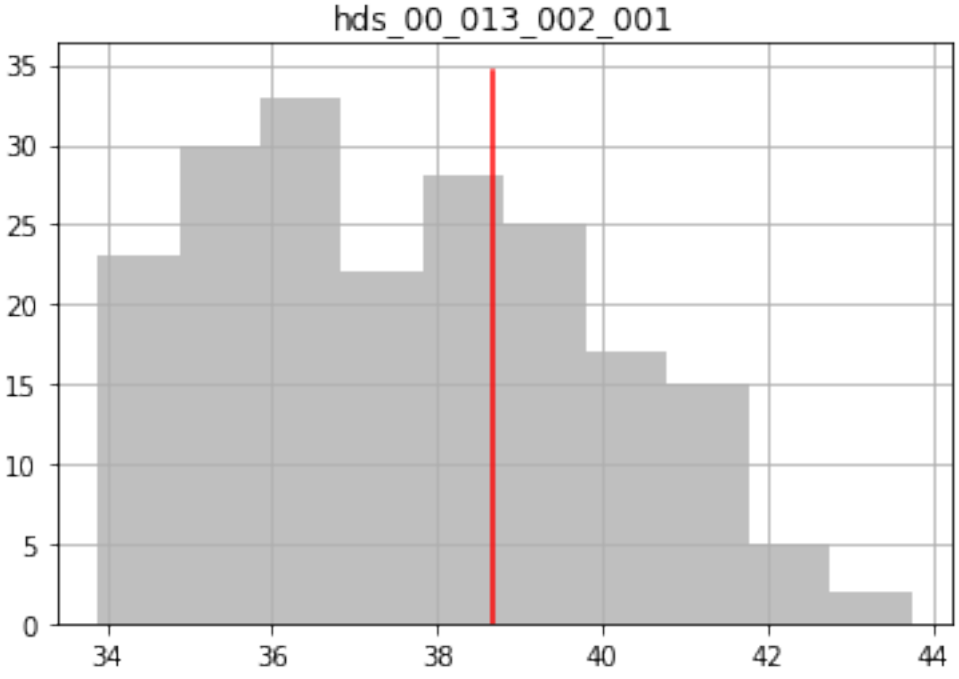
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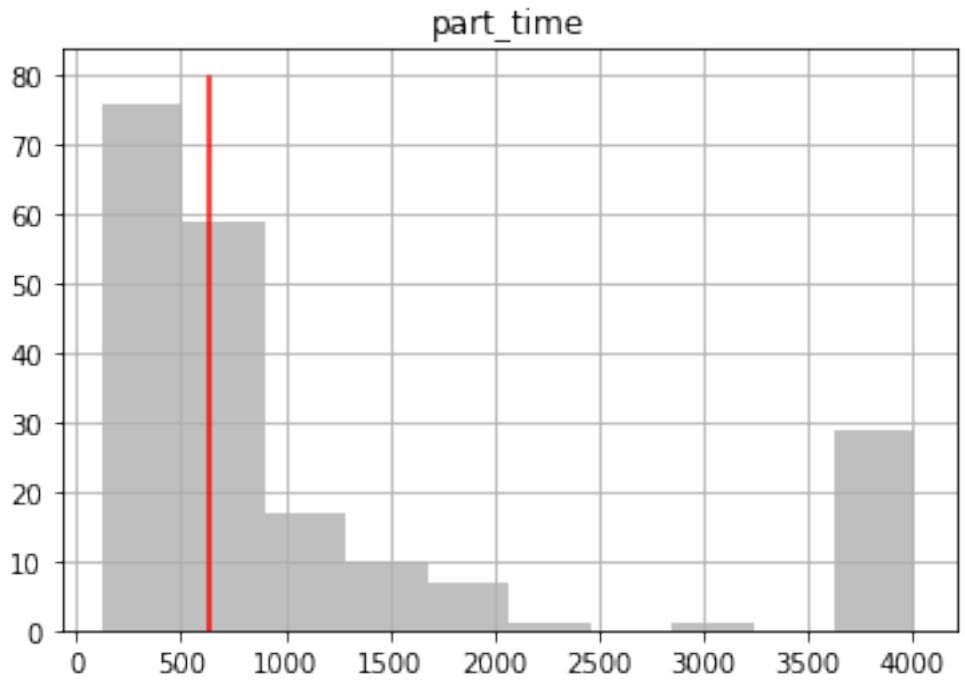
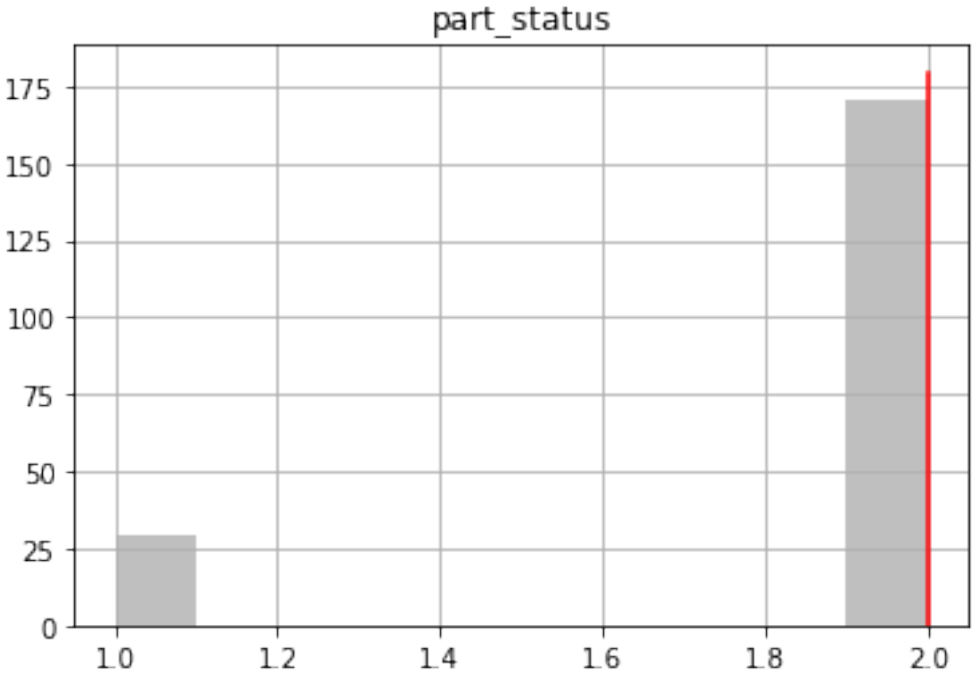
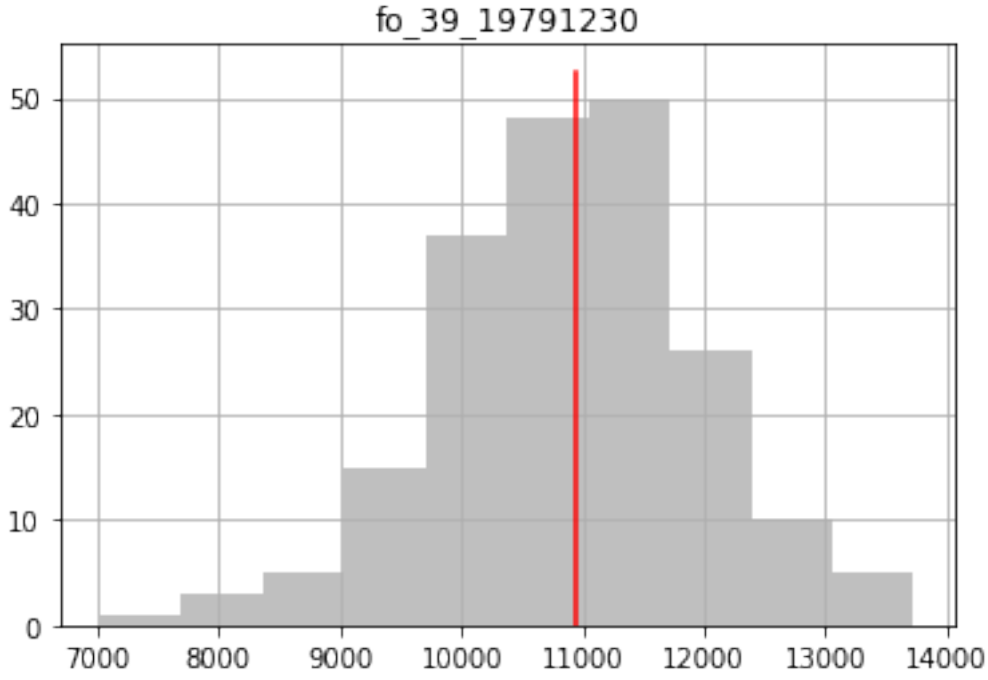
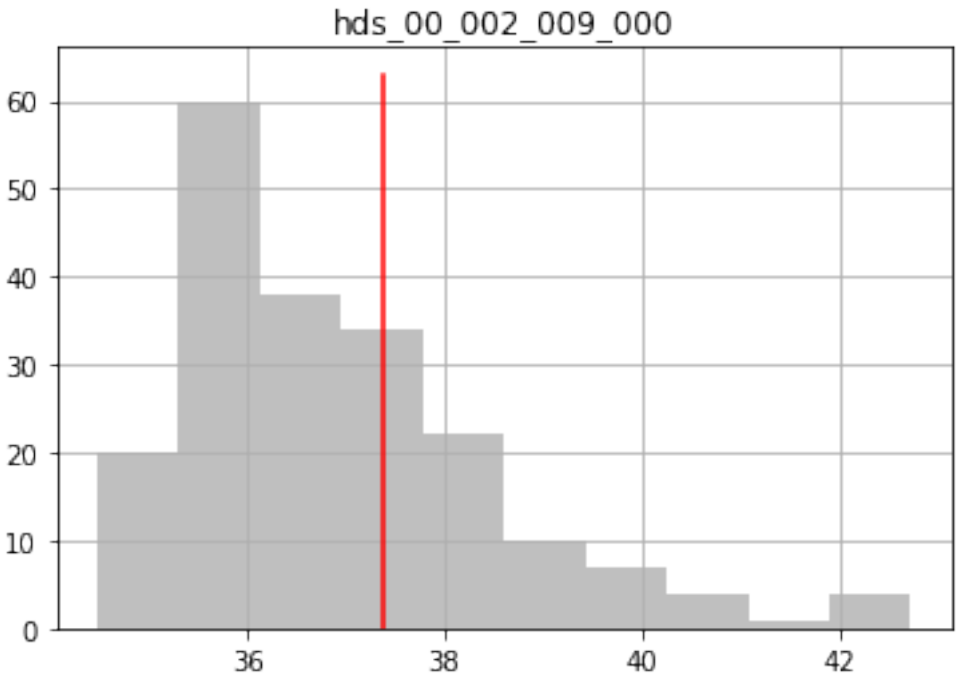




observations:

In [25]:
```
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()
```

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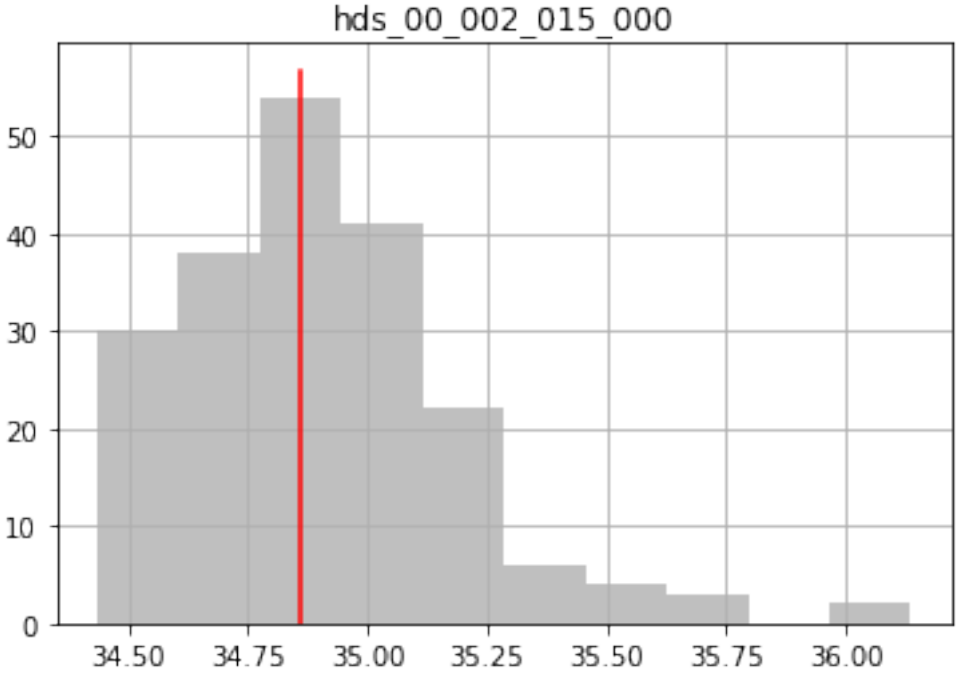
38
40
42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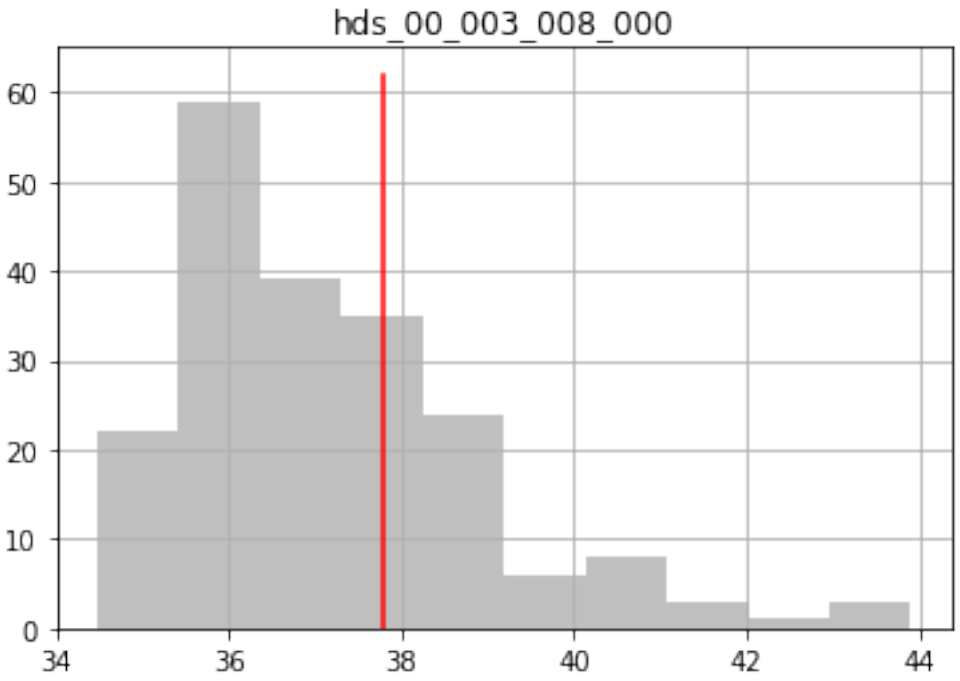
35.50
35.75
36.00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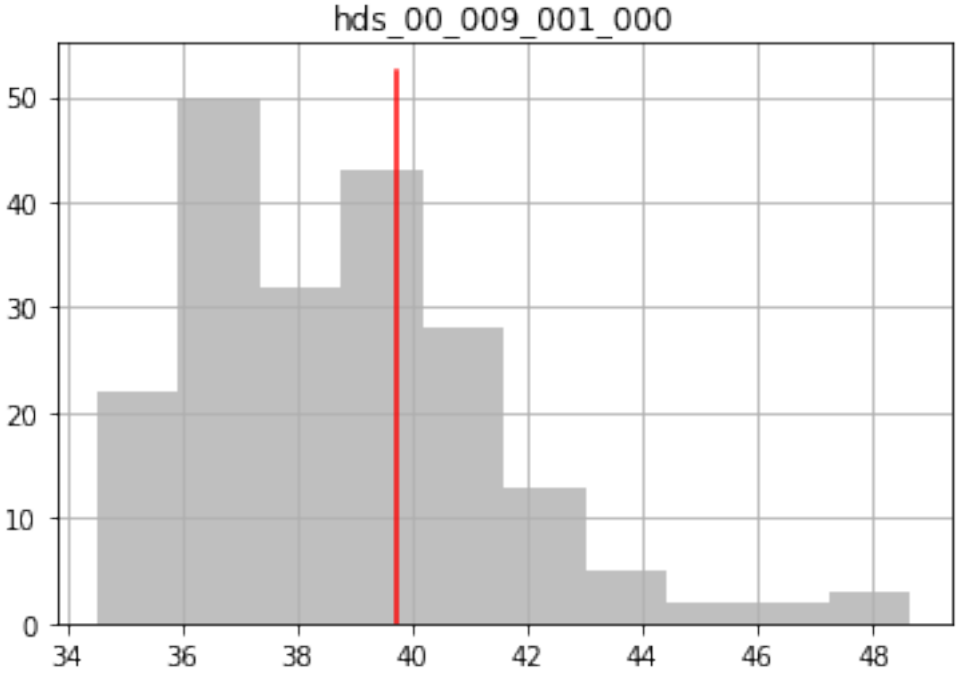
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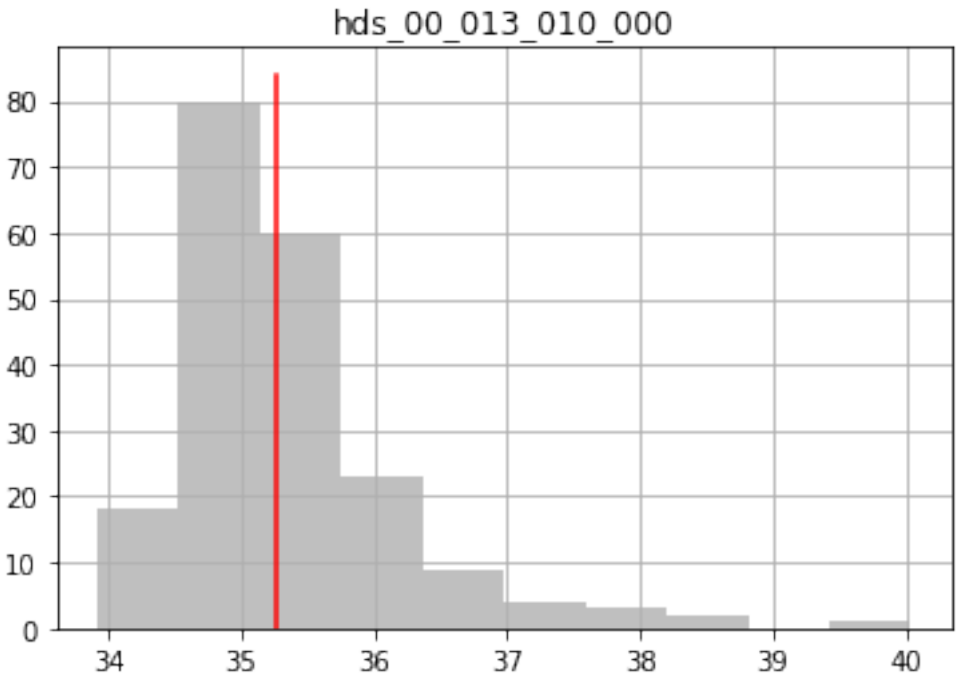
44
46
48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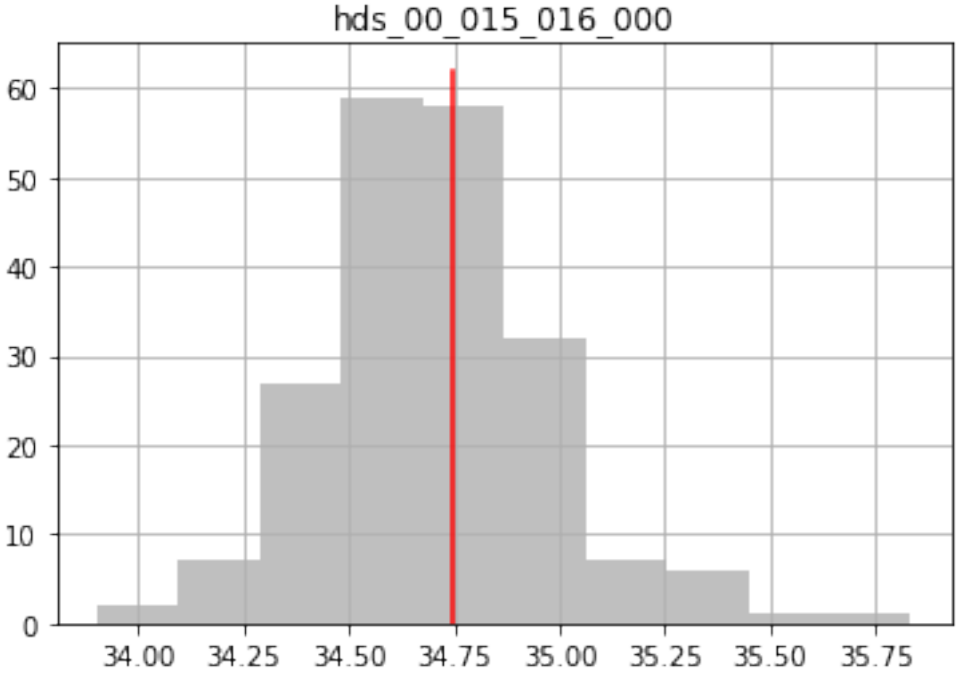
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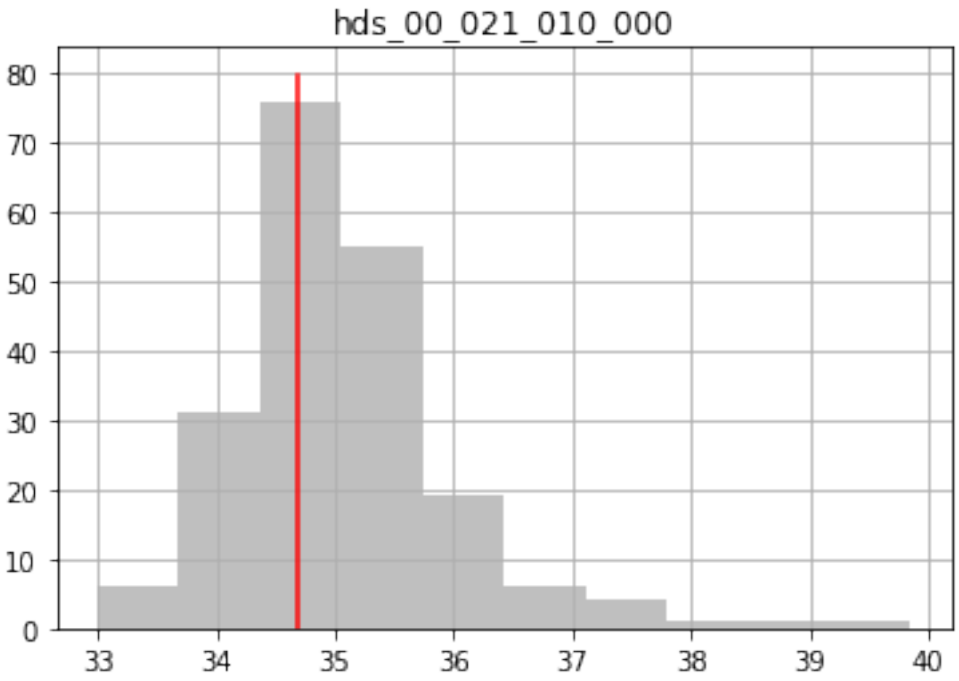
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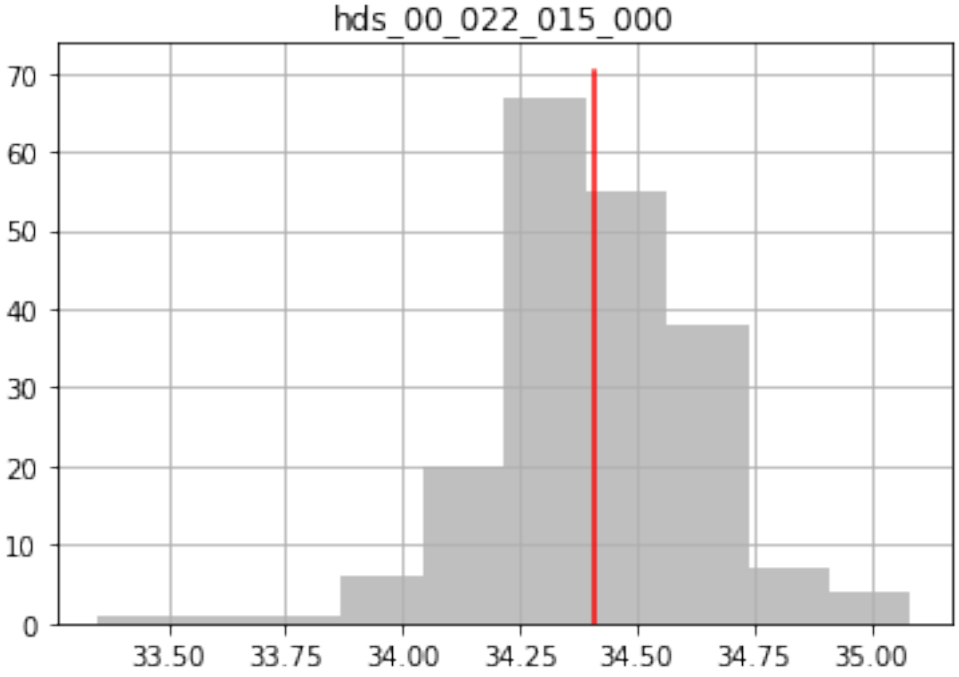
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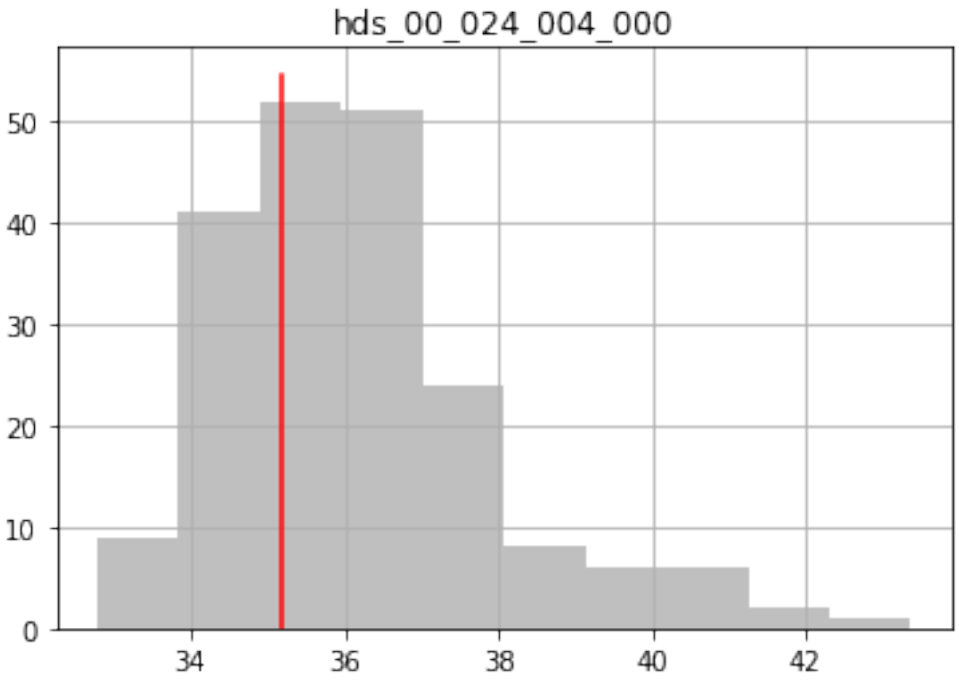
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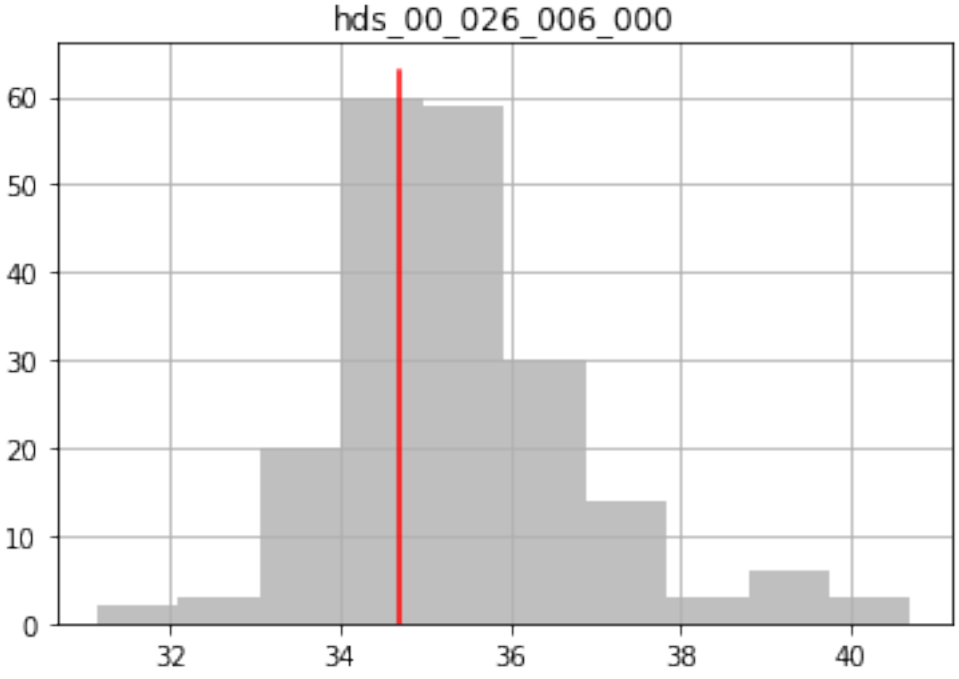
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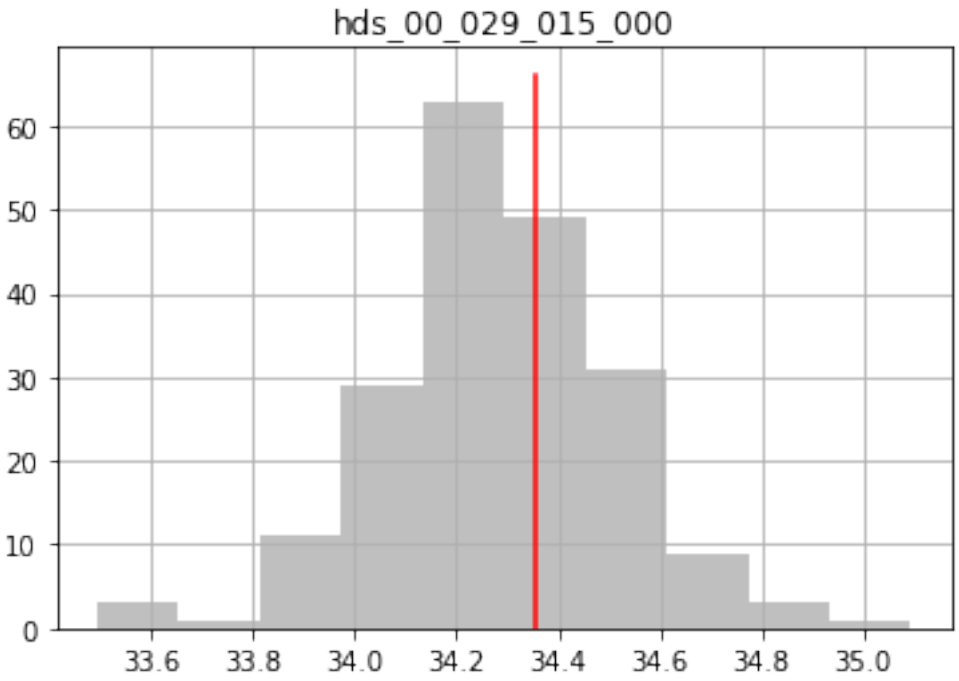
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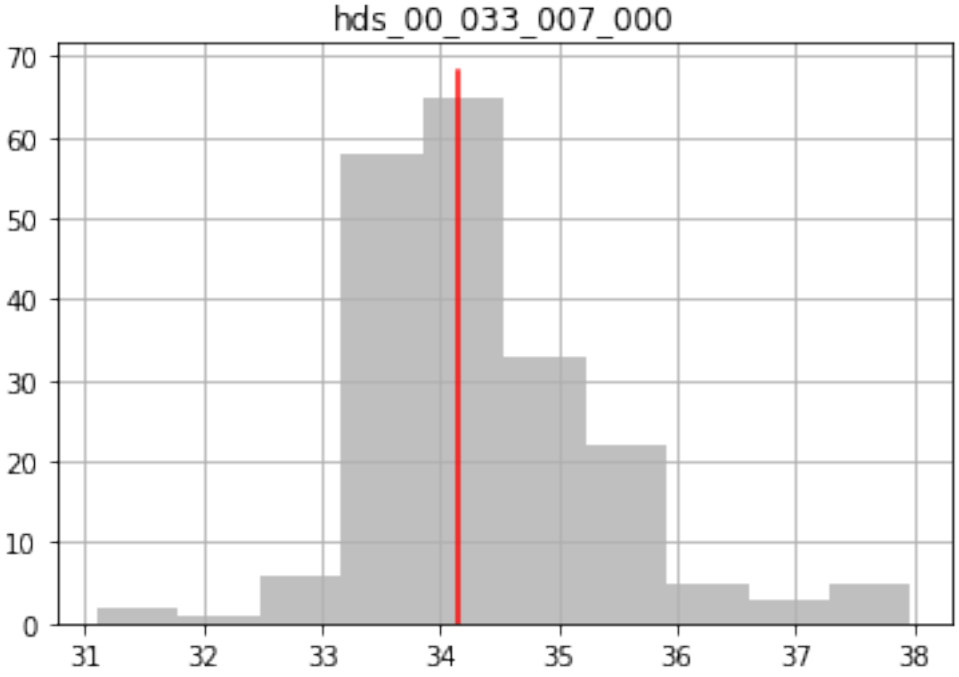
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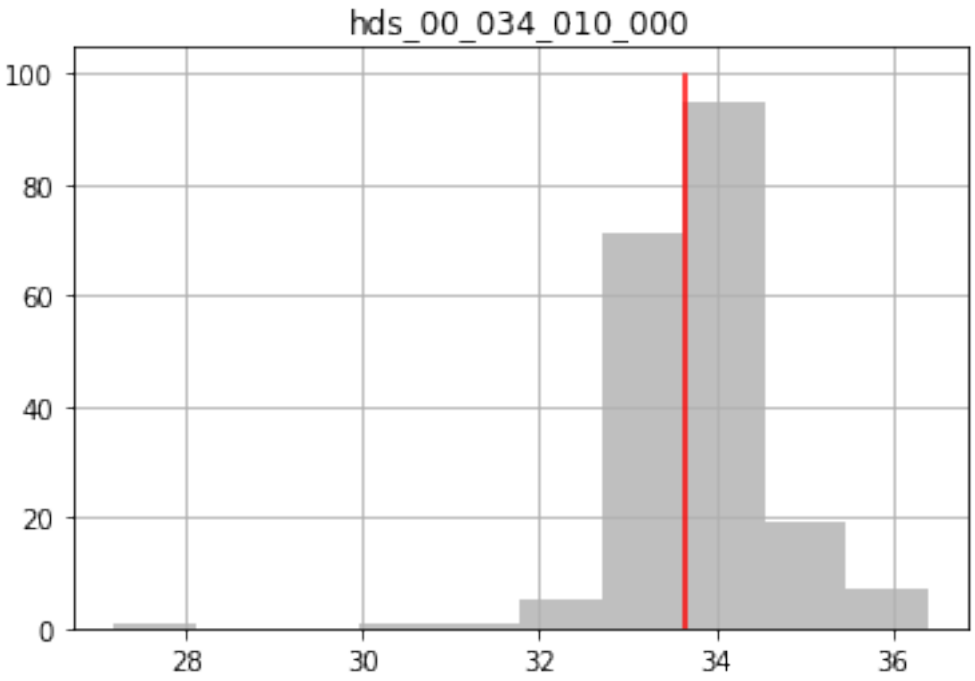
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