pestpp-glm

May 14, 2019

1 PESTPP-GLM

In this notebook, we will run PESTPP-GLM in standard parameter estimation mode and regularization mode. In both cases, we will use the baked-in bayes-linear posterior monte carlo analysis to get posterior forecast PDFs. We will use the prior monte carlo outputs as the prior forecast PDF.

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
```

In [2]:
```
t_d = "template"
m_d = "master_glm"
```

In [3]:
```
pst = pyemu.Pst(os.path.join(t_d,"freyberg.pst"))
pst.write_par_summary_table(filename="none")
```

Out[3]:

	type	transform	count	initial value	upper bound	\
gr_sy3	gr_sy3	log	705	0	0.243038	
cn_prsity7	cn_prsity7	log	1	0	0.176091	
strk	strk	log	40	0	2	
cn_strt6	cn_strt6	log	1	0	0.0211893	
cn_strt7	cn_strt7	log	1	0	0.0211893	
pp_sy2	pp_sy2	log	32	0	0.243038	
cn_prsity6	cn_prsity6	log	1	0	0.176091	
cn_vka6	cn_vka6	log	1	0	1	
pp_prsity2	pp_prsity2	log	32	0	0.176091	
gr_vka5	gr_vka5	log	705	0	1	
pp_hk0	pp_hk0	log	32	0	1	

pp_hk2	pp_hk2	log	32	0	1
cn_ss7	cn_ss7	log	1	0	1
pp_ss0	pp_ss0	log	32	0	1
cn_ss8	cn_ss8	log	1	0	1
pp_strt2	pp_strt2	log	32	0	0.0211893
cn_vka8	cn_vka8	log	1	0	1
cn_sy7	cn_sy7	log	1	0	0.243038
cn_hk7	cn_hk7	log	1	0	1
pp_vka2	pp_vka2	log	32	0	1
pp_sy0	pp_sy0	log	32	0	0.243038
cn_prsity8	cn_prsity8	log	1	0	0.176091
gr_hk3	gr_hk3	log	705	0	1
gr_ss3	gr_ss3	log	705	0	1
gr_vka3	gr_vka3	log	705	0	1
pp_hk1	pp_hk1	log	32	0	1
gr_strt3	gr_strt3	log	705	0	0.0211893
cn_vka7	cn_vka7	log	1	0	1
gr_sy4	gr_sy4	log	705	0	0.243038
cn_rech4	cn_rech4	log	1	0	0.0791812
...	...	...	...	...	...
pp_vka1	pp_vka1	log	32	0	1
pp_strt1	pp_strt1	log	32	0	0.0211893
gr_hk5	gr_hk5	log	705	0	1
cn_strt8	cn_strt8	log	1	0	0.0211893
gr_sy5	gr_sy5	log	705	0	0.243038
flow	flow	log	1	0	0.09691
cn_sy6	cn_sy6	log	1	0	0.243038
gr_rech3	gr_rech3	log	705	0	0.0413927
pp_vka0	pp_vka0	log	32	0	1
gr_prsity5	gr_prsity5	log	705	0	0.176091
gr_strt5	gr_strt5	log	705	0	0.0211893
pp_prsity1	pp_prsity1	log	32	0	0.176091
cn_hk6	cn_hk6	log	1	0	1
welflux_k02	welflux_k02	log	6	0	1
gr_ss5	gr_ss5	log	705	0	1
pp_ss2	pp_ss2	log	32	0	1
drncond_k00	drncond_k00	log	10	0	1
pp_strt0	pp_strt0	log	32	0	0.0211893
cn_ss6	cn_ss6	log	1	0	1
gr_prsity3	gr_prsity3	log	705	0	0.176091
pp_prsity0	pp_prsity0	log	32	0	0.176091
pp_ss1	pp_ss1	log	32	0	1
gr_prsity4	gr_prsity4	log	705	0	0.176091
pp_rech1	pp_rech1	log	32	0	0.0413927
cn_hk8	cn_hk8	log	1	0	1
cn_sy8	cn_sy8	log	1	0	0.243038
pp_sy1	pp_sy1	log	32	0	0.243038
gr_ss4	gr_ss4	log	705	0	1

```
gr_strt4        gr_strt4       log    705             0   0.0211893
gr_rech2        gr_rech2       log    705             0   0.0413927

            lower bound standard deviation
gr_sy3         -0.60206           0.211275
cn_prsity7     -0.30103            0.11928
strk                 -2                  1
cn_strt6     -0.0222764          0.0108664
cn_strt7     -0.0222764          0.0108664
pp_sy2         -0.60206           0.211275
cn_prsity6     -0.30103            0.11928
cn_vka6              -1                0.5
pp_prsity2     -0.30103            0.11928
gr_vka5              -1                0.5
pp_hk0               -1                0.5
pp_hk2               -1                0.5
cn_ss7               -1                0.5
pp_ss0               -1                0.5
cn_ss8               -1                0.5
pp_strt2     -0.0222764          0.0108664
cn_vka8              -1                0.5
cn_sy7         -0.60206           0.211275
cn_hk7               -1                0.5
pp_vka2              -1                0.5
pp_sy0         -0.60206           0.211275
cn_prsity8     -0.30103            0.11928
gr_hk3               -1                0.5
gr_ss3               -1                0.5
gr_vka3              -1                0.5
pp_hk1               -1                0.5
gr_strt3     -0.0222764          0.0108664
cn_vka7              -1                0.5
gr_sy4         -0.60206           0.211275
cn_rech4       -0.09691          0.0440228
...                 ...                ...
pp_vka1              -1                0.5
pp_strt1     -0.0222764          0.0108664
gr_hk5               -1                0.5
cn_strt8     -0.0222764          0.0108664
gr_sy5         -0.60206           0.211275
flow          -0.124939          0.0554622
cn_sy6         -0.60206           0.211275
gr_rech3     -0.0457575          0.0217875
pp_vka0              -1                0.5
gr_prsity5     -0.30103            0.11928
gr_strt5     -0.0222764          0.0108664
pp_prsity1     -0.30103            0.11928
cn_hk6               -1                0.5
```

```
welflux_k02          -1                0.5
gr_ss5               -1                0.5
pp_ss2               -1                0.5
drncond_k00          -1                0.5
pp_strt0     -0.0222764          0.0108664
cn_ss6               -1                0.5
gr_prsity3    -0.30103            0.11928
pp_prsity0    -0.30103            0.11928
pp_ss1               -1                0.5
gr_prsity4    -0.30103            0.11928
pp_rech1     -0.0457575          0.0217875
cn_hk8               -1                0.5
cn_sy8        -0.60206           0.211275
pp_sy1        -0.60206           0.211275
gr_ss4               -1                0.5
gr_strt4     -0.0222764          0.0108664
gr_rech2     -0.0457575          0.0217875

[65 rows x 7 columns]
```

1.0.1 reduce the number of adjustable parameters

This is the painful part: we cant use 10K+ pars because we cant wait around for that many runs and then the linear algebra of factoring a 10k+ by 10K+ matrix is also difficult. So that means we need to fix a lot a parameters #frownyface

In [4]:
```
par = pst.parameter_data
```

In [5]:
```
# grid-scale pars
gr_pars = par.loc[par.pargp.apply(lambda x: "gr" in x),"parnme"]
par.loc[gr_pars,"partrans"] = "fixed"
pst.npar_adj
```

Out[5]: 719

In [6]:
```
# these are the sfr conductance parameters - Ive left all 40 adjustable
# but if you uncomment this, it will tie them into 1 parameter effectively
# strk_pars = par.loc[par.pargp=="strk","parnme"]
# p1 = strk_pars.iloc[0]
# par.loc[strk_pars.iloc[1:],"partrans"] = "tied"
# par.loc[strk_pars.iloc[1:],"partied"] = p1
pst.npar_adj
```

Out[6]: 719

In [7]:
```
par.loc[par.pargp.apply(lambda x: "pp" in x),"pargp"].unique()
```

Out[7]:
```
array(['pp_hk0', 'pp_hk1', 'pp_hk2', 'pp_prsity0', 'pp_prsity1',
       'pp_prsity2', 'pp_rech0', 'pp_rech1', 'pp_ss0', 'pp_ss1', 'pp_ss2',
       'pp_strt0', 'pp_strt1', 'pp_strt2', 'pp_sy0', 'pp_sy1', 'pp_sy2',
       'pp_vka0', 'pp_vka1', 'pp_vka2'], dtype=object)
```

Fix the storage pilot points - we still have layer-scale storage pars adjustable

In [8]:
```
#s_pars = par.loc[par.pargp.apply(lambda x: "pp" in x and ("ss" in x or "sy" in x)),"p
#par.loc[s_pars,"partrans"] = "fixed"
pst.npar_adj
```

Out[8]: 719

In [9]:
```
adj_par = par.loc[par.partrans=="log",:]
adj_par.pargp.value_counts().sort_values()
```

Out[9]:

cn_prsity7	1
cn_ss8	1
cn_strt7	1
cn_vka8	1
cn_strt6	1
cn_vka6	1
cn_prsity6	1
cn_ss6	1
cn_vka7	1
cn_hk7	1
cn_strt8	1
cn_sy7	1
cn_rech5	1
cn_hk8	1
cn_prsity8	1
cn_ss7	1
flow	1
cn_sy6	1
cn_sy8	1
cn_hk6	1
cn_rech4	1
welflux	2
welflux_k02	6
drncond_k00	10
pp_prsity0	32
pp_sy2	32
pp_ss2	32
pp_vka2	32
pp_sy0	32
pp_hk1	32
pp_ss0	32
pp_hk2	32
pp_hk0	32
pp_prsity2	32
pp_rech0	32
pp_strt1	32
pp_strt2	32
pp_sy1	32

```
pp_strt0       32
pp_rech1       32
pp_vka0        32
pp_prsity1     32
pp_ss1         32
pp_vka1        32
strk           40
Name: pargp, dtype: int64
```

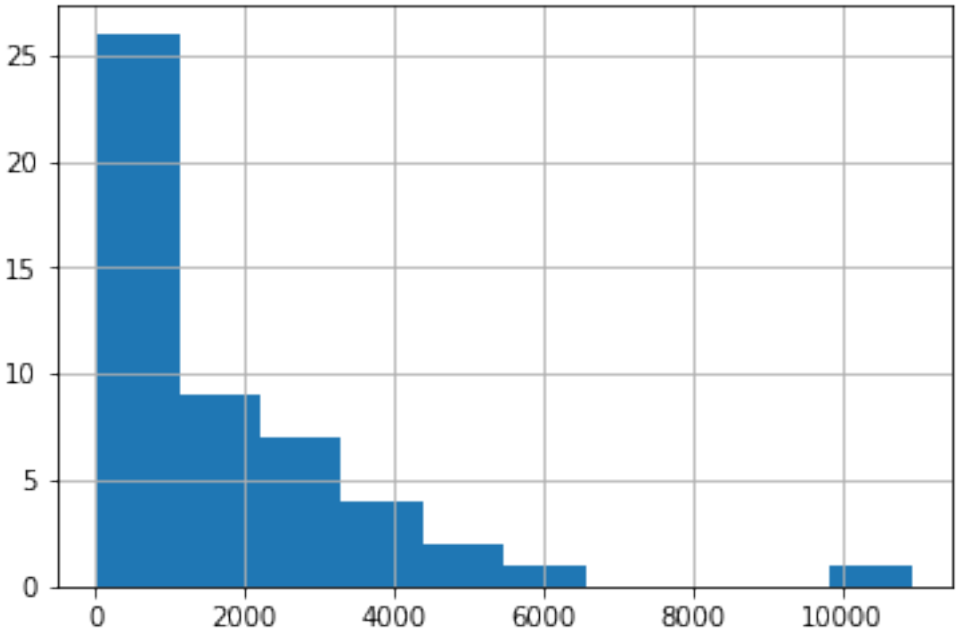
fix the future recharge pilot points, vka in layers 1 and 3 and the initial condition pilot points (we still have layer-scale pars for each of these types)

```
In [10]: fi_grps = ["pp_rech1","pp_vka0","pp_vka2","pp_strt0","pp_strt1","pp_strt2"]
         par.loc[par.pargp.apply(lambda x: x in fi_grps),"partrans"] = "fixed"
         pst.npar_adj

Out[10]: 527
```

Ok, thats better…so lets run PESTPP-GLM. We will use a single "base parameter" jacobian matrix as the basis for 6 super parameter iterations. Then we will draw 100 realizations from the FOSM posterior parameter covariance matrix and run those 100 realizations to get the psoterior forecast PDFs

```
In [11]: pst.control_data.noptmax = 3
         pst.pestpp_options["n_iter_base"] = -1
         pst.pestpp_options["n_iter_super"] = 3
         pst.pestpp_options["num_reals"] = 50 # this is how many ies uses
         pst.pestpp_options["parcov"] = "prior_cov.jcb"
         pst.write(os.path.join(t_d,"freyberg_pp.pst"))

noptmax:3, npar_adj:527, nnz_obs:14


In [12]: pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=20,slave_ro
                                      master_dir=m_d)

In [13]: df = df=pd.read_csv(os.path.join(m_d,"freyberg_pp.post.obsen.csv"),index_col=0)
         oe = pyemu.ObservationEnsemble.from_dataframe(pst=pst,df=df)

In [14]: ax = oe.phi_vector.hist()#bins=np.linspace(0,100,20))
         oe.phi_vector.sort_values().iloc[:20]

Out[14]: real_name
         16     25.142317
         48     96.610784
         47    196.376492
         30    229.606762
         44    263.271863
         22    303.080285
```

```
19     310.056487
7      333.912635
33     345.965930
41     354.876661
1      408.463563
45     534.371489
34     607.919525
39     612.149378
2      616.962285
8      809.884195
31     825.919864
36     830.734862
9      840.691128
4      867.561910
dtype: float64
```



Here we see the distribution of phi values across the 100 posterior realizations. Should we accept all of these??? The theoretical phi we should accept is number of nonzero obs (14).

To get a "posterior" ensemble, we need to throw out the realizations with large phi - lets just take the 20 best:

```
In [15]: oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:] #just take the 20 lowest phi
```

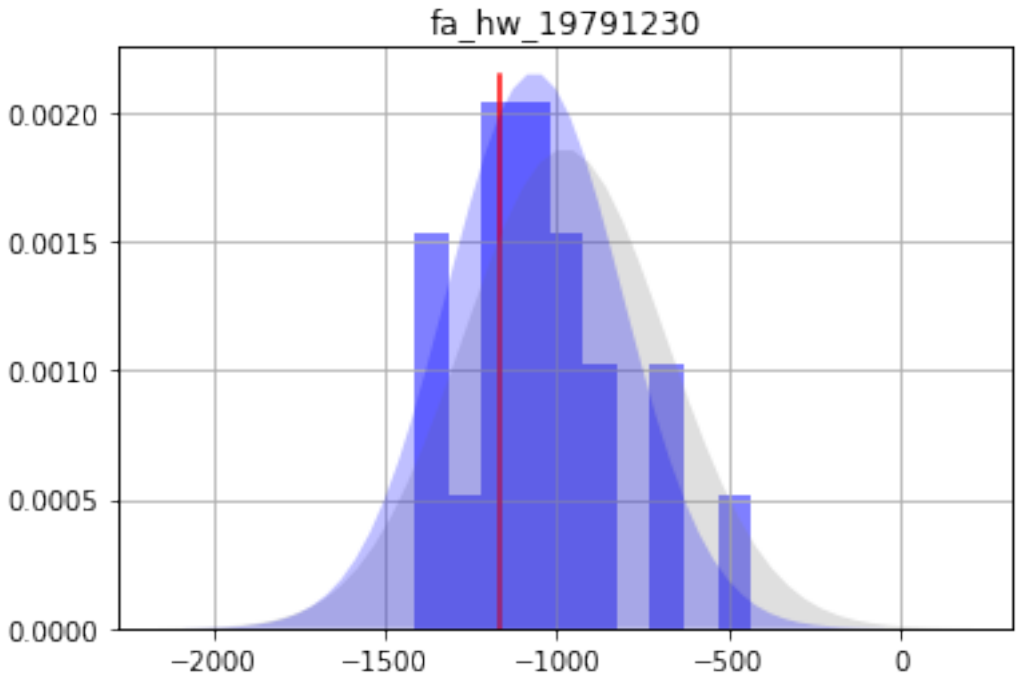
We can also load and plot the FOSM forecast results along side of the ensemble results:

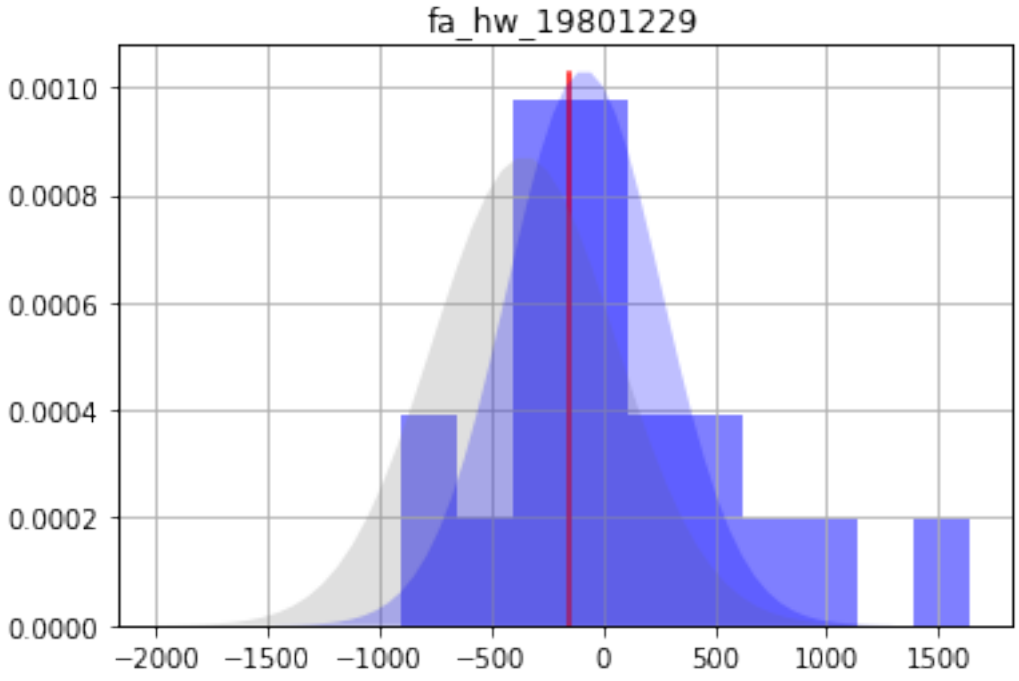
```
In [16]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

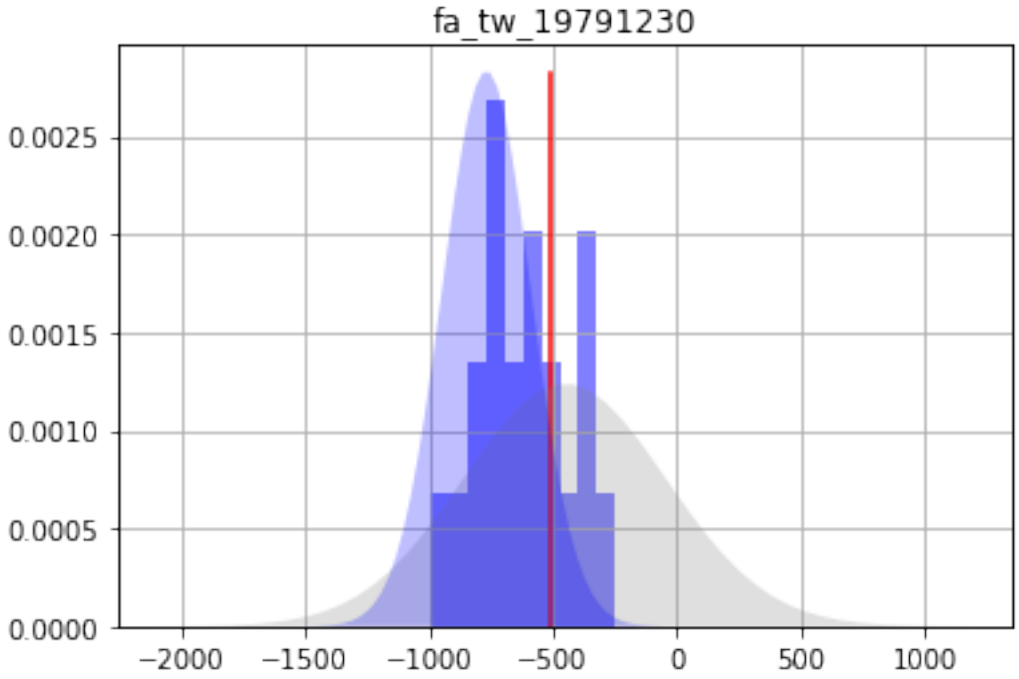
Out[16]:

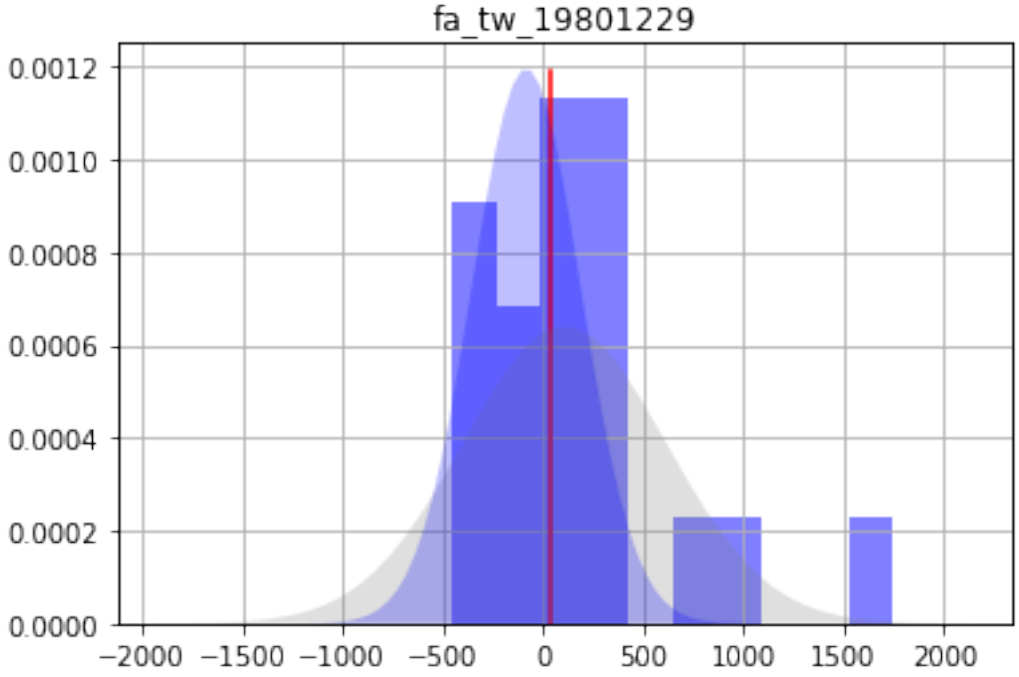
name	prior_mean	prior_stdev	prior_lower_bound	prior_upper_bound	post_mean	post_stdev	post_lower_bound	post_upper_bound
fa_hw_19791230	-977.2390	295.32800	-1567.8900	-386.5840	-1065.3500	254.734000	-1574.8100	-555.8800
fa_hw_19801229	-351.2160	409.77000	-1170.7600	468.3240	-83.0591	346.174000	-775.4080	609.2890
fa_tw_19791230	-453.0330	409.35100	-1271.7400	365.6690	-768.4280	178.717000	-1125.8600	-410.9950
fa_tw_19801229	108.9600	506.73200	-904.5040	1122.4200	-82.7267	271.393000	-625.5130	460.0600
hds_00_013_002_000	39.6102	3.96314	31.6840	47.5365	41.1798	0.318847	40.5421	41.8175
hds_00_013_002_001	38.3838	4.05782	30.2681	46.4994	39.6447	0.706586	38.2315	41.0579
part_status	2.0000	0.00000	2.0000	2.0000	2.0000	0.000000	2.0000	2.0000
part_time	907.7020	570.98600	-234.2690	2049.6700	1262.5600	440.591000	381.3790	2143.7400

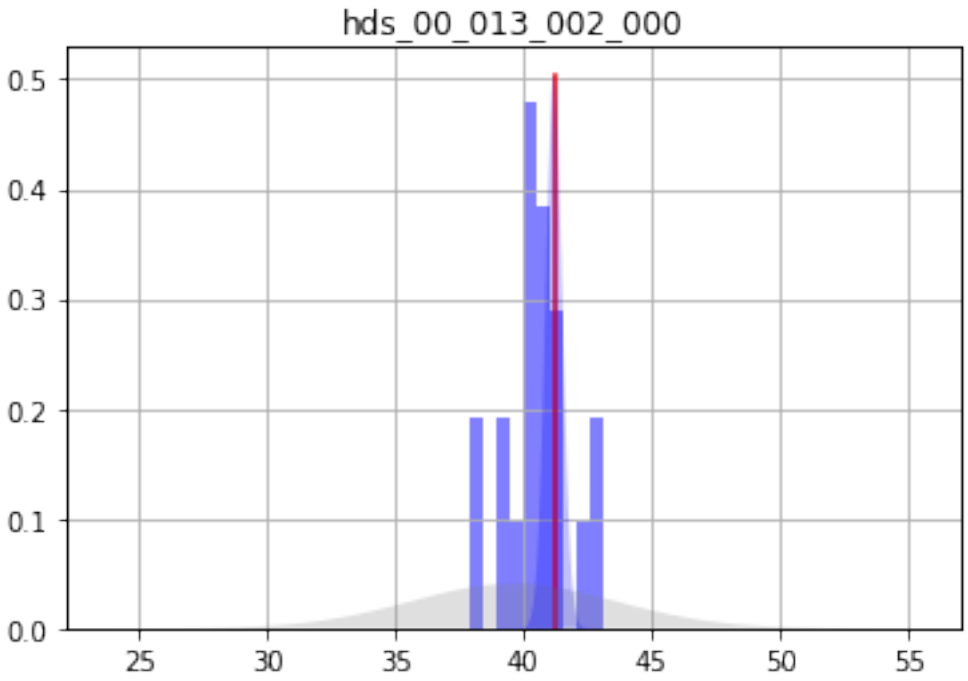
In [17]:
```
obs = pst.observation_data
fnames = pst.pestpp_options["forecasts"].split(",")
for forecast in fnames:
    ax = plt.subplot(111)
    oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
    ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
    axt = plt.twinx()
    x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"prior_mean"],f_df
    axt.fill_between(x,0,y,facecolor="0.5",alpha=0.25)
    x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"post_mean"],f_df.
    axt.fill_between(x,0,y,facecolor="b",alpha=0.25)
    axt.set_ylim(0,axt.get_ylim()[1])
    axt.set_yticks([])
    ax.set_title(forecast)
    plt.show()
```

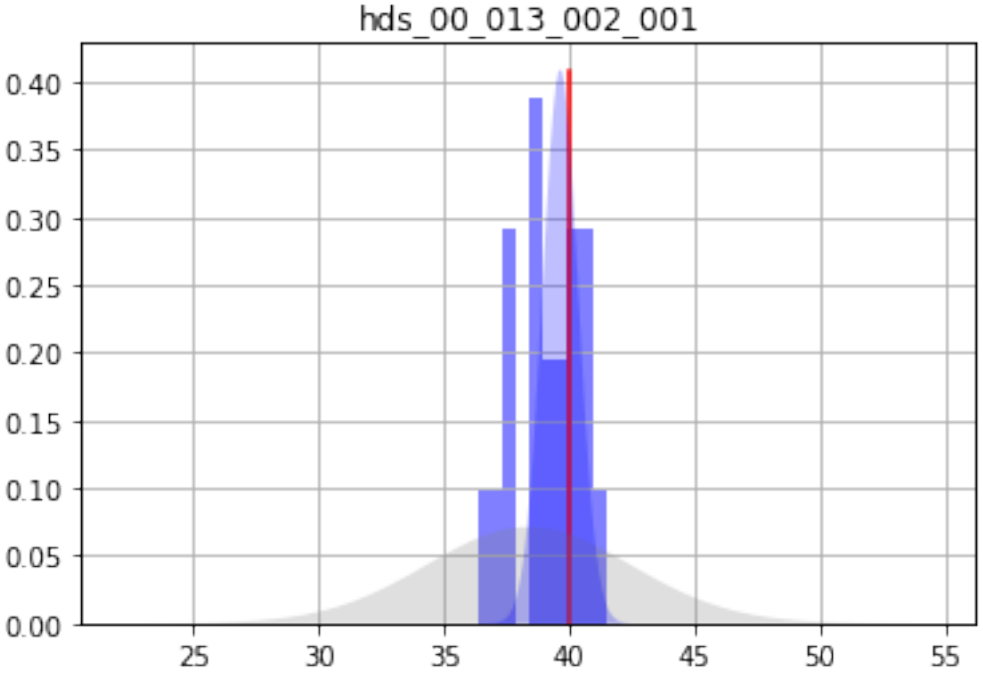

fa_hw_19791230
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0

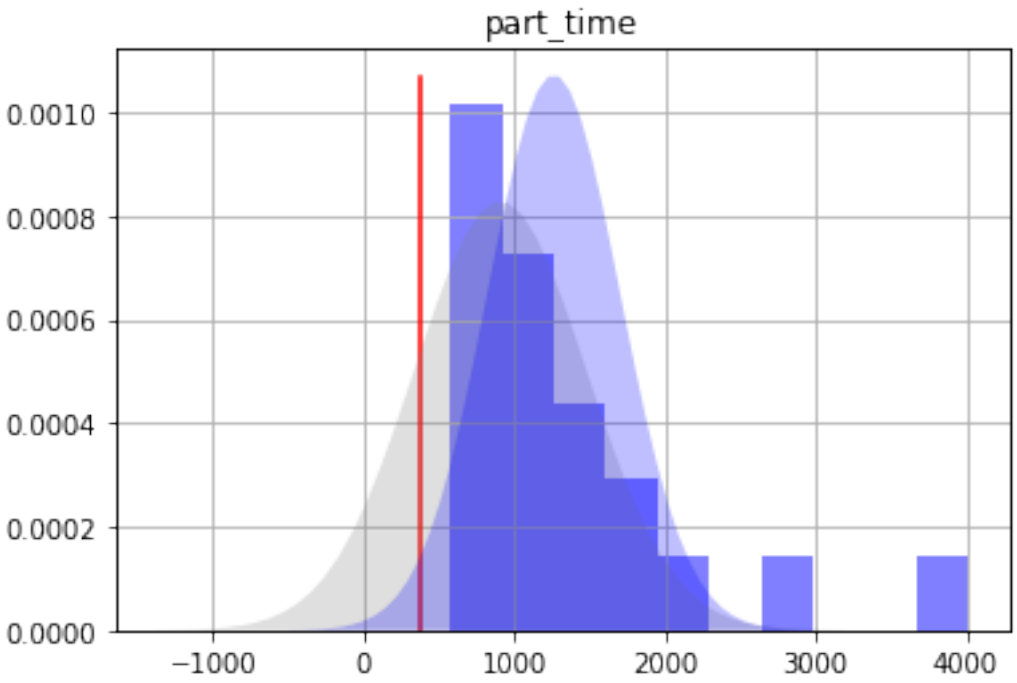

fa_hw_19801229
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000
1500

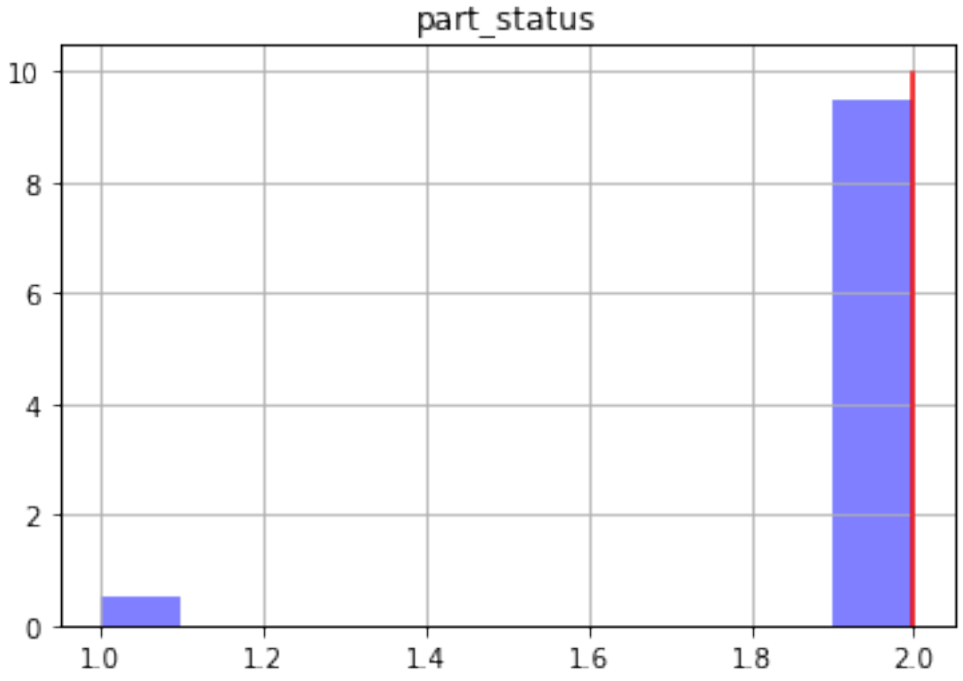

fa_tw_19791230
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000
1500
2000


hds_00_013_002_000
0.5
0.4
0.3
0.2
0.1
0.0
25
30
35
40
45
50
55


hds_00_013_002_001
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
25
30
35
40
45
50
55


part_time
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−1000
0
1000
2000
3000
4000


part_status
10
8
6
4
2
0
1.0
1.2
1.4
1.6
1.8
2.0

1.0.2 Setup of Tikhonov regularization

Now lets setup and use some formal regularization to bring the final phi up to around 14. We will use first-order regularization based on the covariance matrix we build earlier:

```
In [18]: cov = pyemu.Cov.from_binary(os.path.join(t_d,"prior_cov.jcb"))
```

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

```
In [19]: pyemu.helpers.first_order_pearson_tikhonov(pst,cov)
```

```
getting CC matrix
processing
```

```
In [20]: pst.prior_information.head()
```

```
Out[20]:                                                    equation    obgnme  \
         pilbl
         pcc_1  1.0 * log(dc0000390005) - 1.0 * log(dc0000390006) = 0.0  regul_cc
         pcc_2  1.0 * log(dc0000390005) - 1.0 * log(dc0000390007) = 0.0  regul_cc
         pcc_3  1.0 * log(dc0000390005) - 1.0 * log(dc0000390008) = 0.0  regul_cc
         pcc_4  1.0 * log(dc0000390005) - 1.0 * log(dc0000390009) = 0.0  regul_cc
         pcc_5  1.0 * log(dc0000390005) - 1.0 * log(dc0000390010) = 0.0  regul_cc

                pilbl    weight
         pilbl
         pcc_1  pcc_1  0.904837
         pcc_2  pcc_2  0.818731
         pcc_3  pcc_3  0.740818
         pcc_4  pcc_4  0.670320
         pcc_5  pcc_5  0.606531
```

```
In [21]: shutil.copy2(os.path.join(m_d,"freyberg_pp.jcb"),os.path.join(t_d,"restart_pp.jcb"))
```

```
Out[21]: 'template/restart_pp.jcb'
```

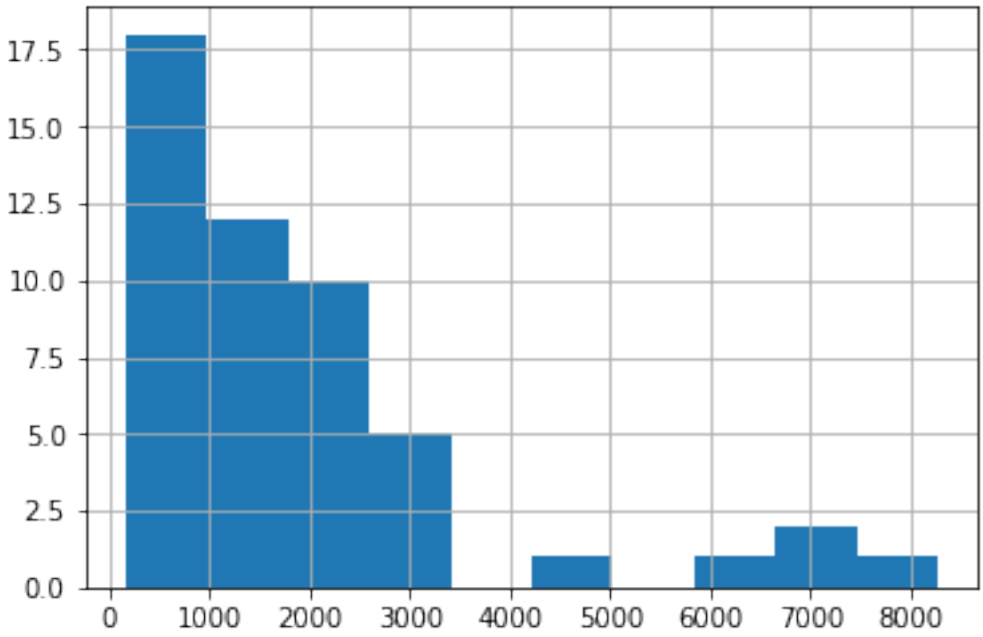
```
In [22]: pst.pestpp_options["base_jacobian"] = "restart_pp.jcb"
         pst.reg_data.phimlim = pst.nnz_obs
         pst.reg_data.phimaccept = pst.reg_data.phimlim * 1.1
         pst.write(os.path.join(t_d,"freyberg_pp.pst"))
```

```
noptmax:3, npar_adj:527, nnz_obs:14
```

```
In [23]: pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=20,slave_ro
                                    master_dir=m_d)
```

```
In [24]: df = df=pd.read_csv(os.path.join(m_d,"freyberg_pp.post.obsen.csv"),index_col=0)
         oe = pyemu.ObservationEnsemble.from_dataframe(pst=pst,df=df)
```

```
In [25]: ax = oe.phi_vector.hist()#bins=np.linspace(0,100,20))
         oe.phi_vector.sort_values().iloc[:20]

Out[25]: real_name
         16     158.641168
         48     198.054854
         19     220.581275
         45     249.971990
         7      295.967588
         46     365.560372
         30     412.222279
         44     415.910991
         38     416.580172
         47     426.089192
         41     443.122798
         2      461.704473
         8      507.139324
         1      637.120829
         17     688.400904
         29     720.689601
         22     824.461560
         9      847.839389
         12     973.938262
         18    1089.504943
         dtype: float64
```



Same as before, to get a "posterior" ensemble, we need to throw out the realizations with large phi - lets just take the 20 best:

```
In [26]: oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:]
```

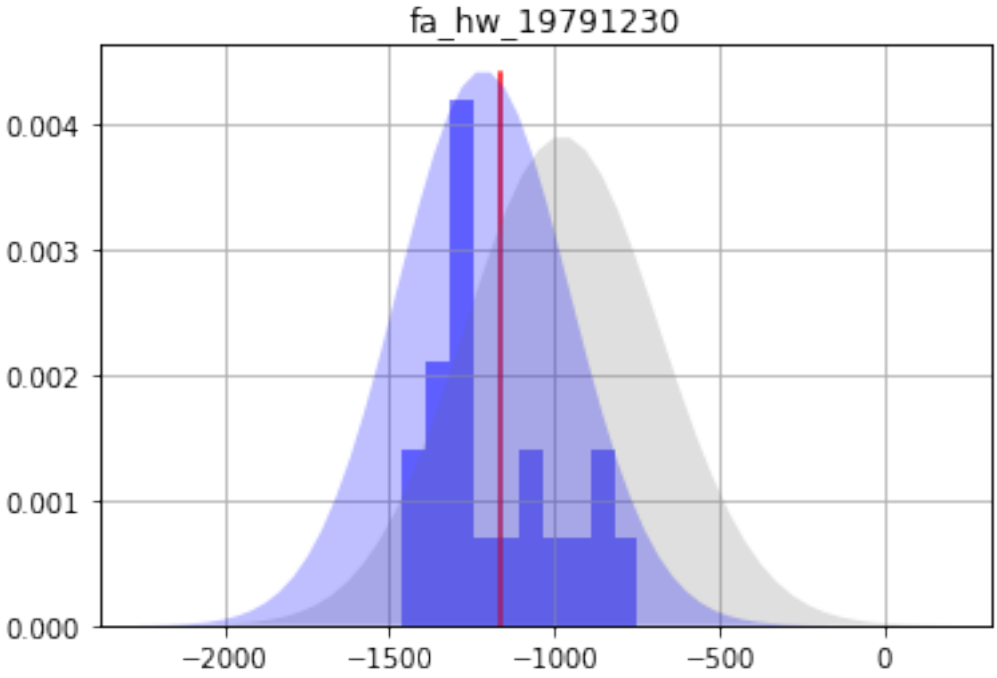
```
In [27]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

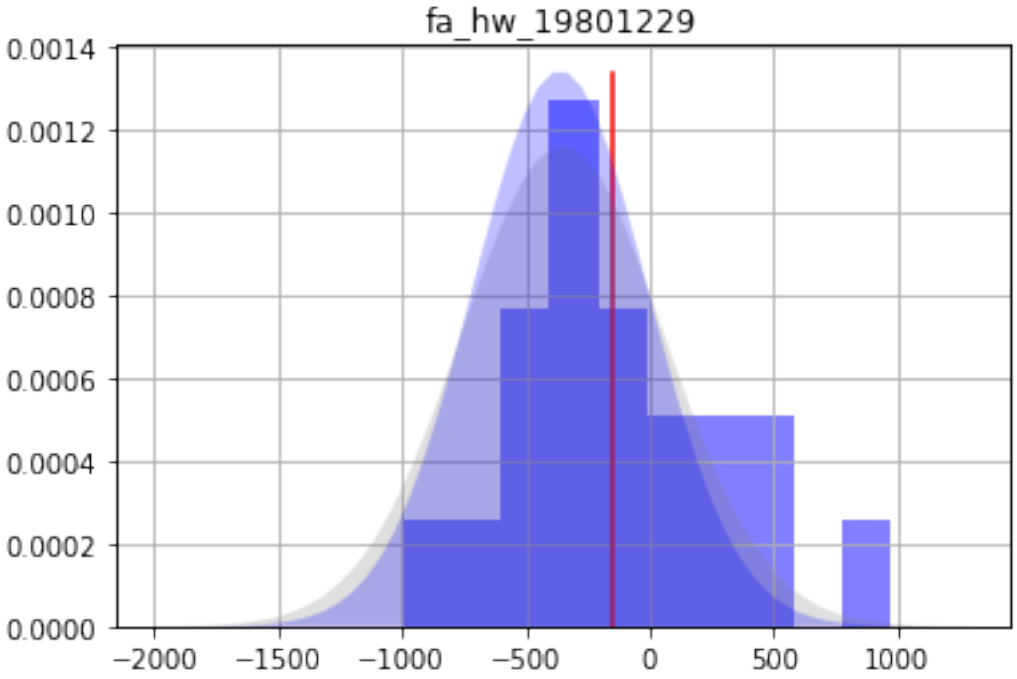
Out[27]:

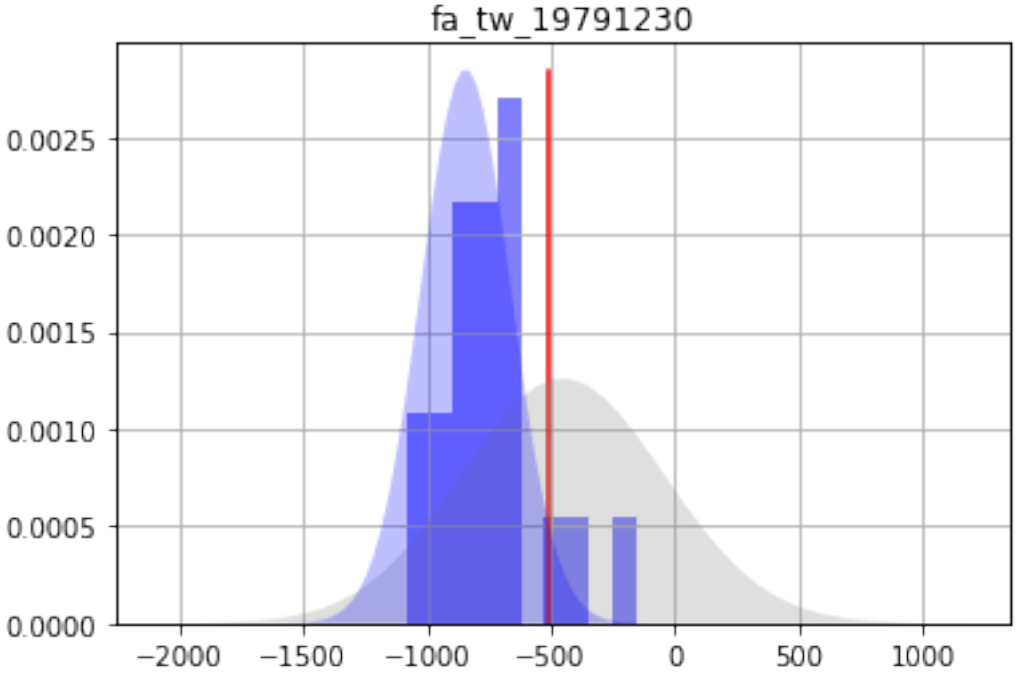
	prior_mean	prior_stdev	prior_lower_bound	prior_upper_bound	post_mean	post_stdev	post_lower_bound	post_upper_bound
name								
fa_hw_19791230	-977.2390	295.32800	-1567.8900	-386.5840	-1216.0200	260.359000	-1736.7400	-695.3070
fa_hw_19801229	-351.2160	409.77000	-1170.7600	468.3240	-361.9980	354.547000	-1071.0900	347.0970
fa_tw_19791230	-453.0330	409.35100	-1271.7400	365.6690	-844.1200	180.713000	-1205.5400	-482.6950
fa_tw_19801229	108.9600	506.73200	-904.5040	1122.4200	-123.6460	274.499000	-672.6450	425.3520
hds_00_013_002_000	39.6102	3.96314	31.6840	47.5365	41.0266	0.331155	40.3643	41.6889
hds_00_013_002_001	38.3838	4.05782	30.2681	46.4994	39.5589	0.713937	38.1311	40.9868
part_status	2.0000	0.00000	2.0000	2.0000	2.0000	0.000000	2.0000	2.0000
part_time	907.7020	570.98600	-234.2690	2049.6700	1831.8700	449.783000	932.3080	2731.4400

```
In [28]: obs = pst.observation_data
         fnames = pst.pestpp_options["forecasts"].split(",")
         for forecast in fnames:
             ax = plt.subplot(111)
             oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
             ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
             axt = plt.twinx()
```

```
x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"prior_mean"],f_df
axt.fill_between(x,0,y,facecolor="0.5",alpha=0.25)
x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"post_mean"],f_df.
axt.fill_between(x,0,y,facecolor="b",alpha=0.25)
axt.set_ylim(0,axt.get_ylim()[1])
axt.set_yticks([])
ax.set_title(forecast)
plt.show()
```




fa_hw_19801229
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19791230
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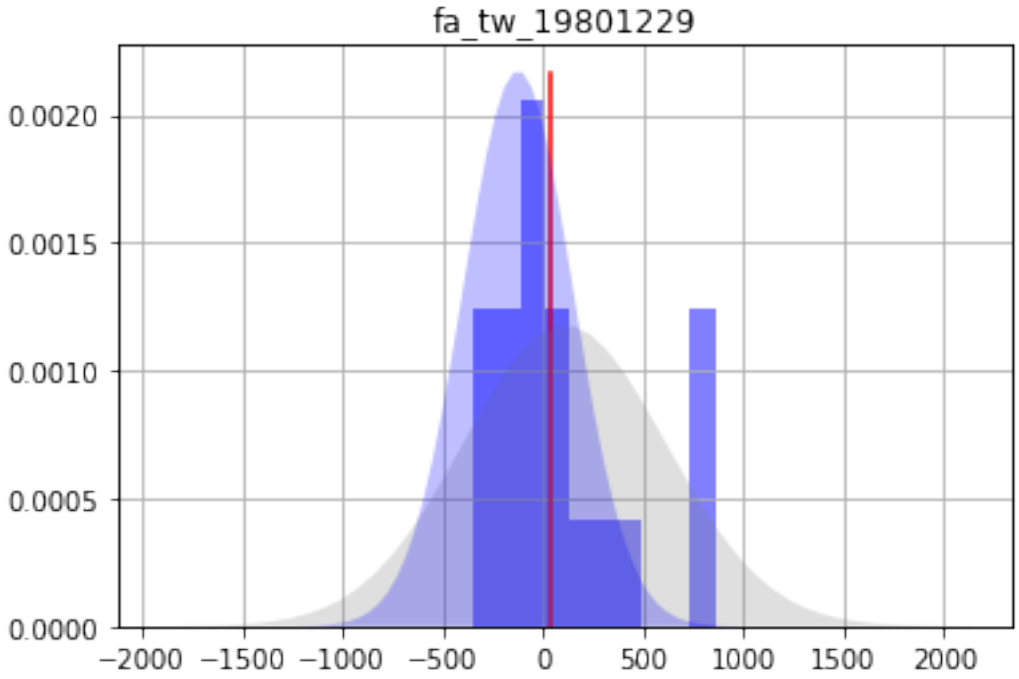
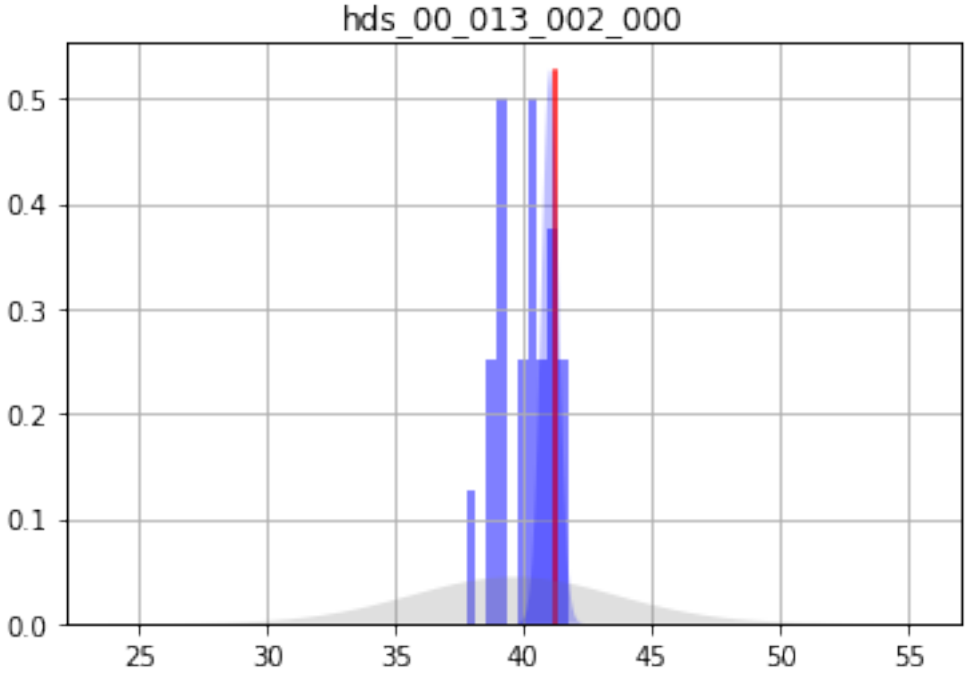
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000
1500
2000


hds_00_013_002_000
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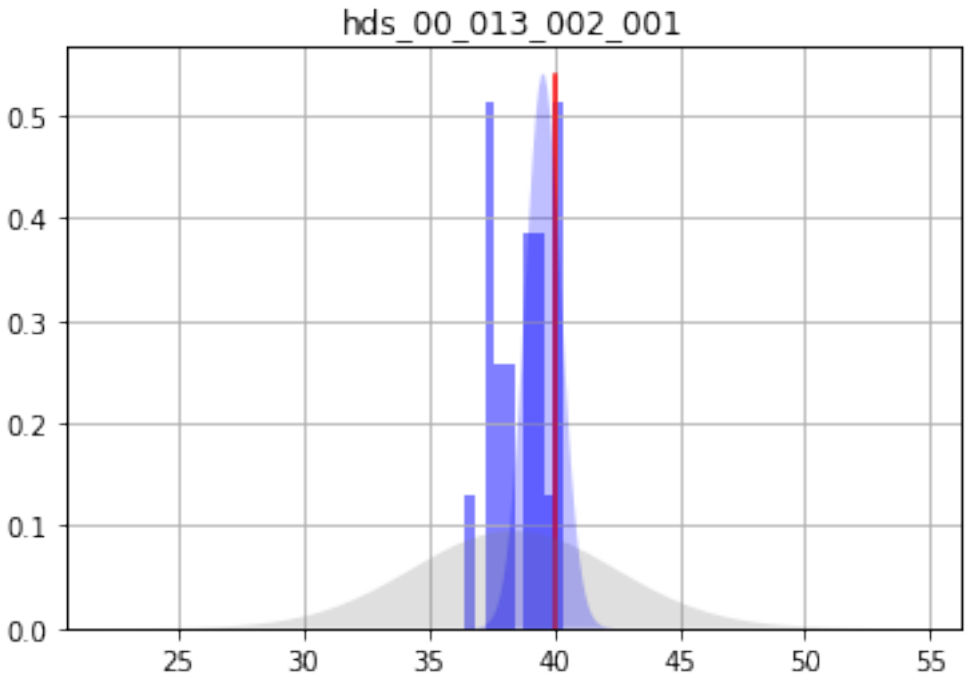
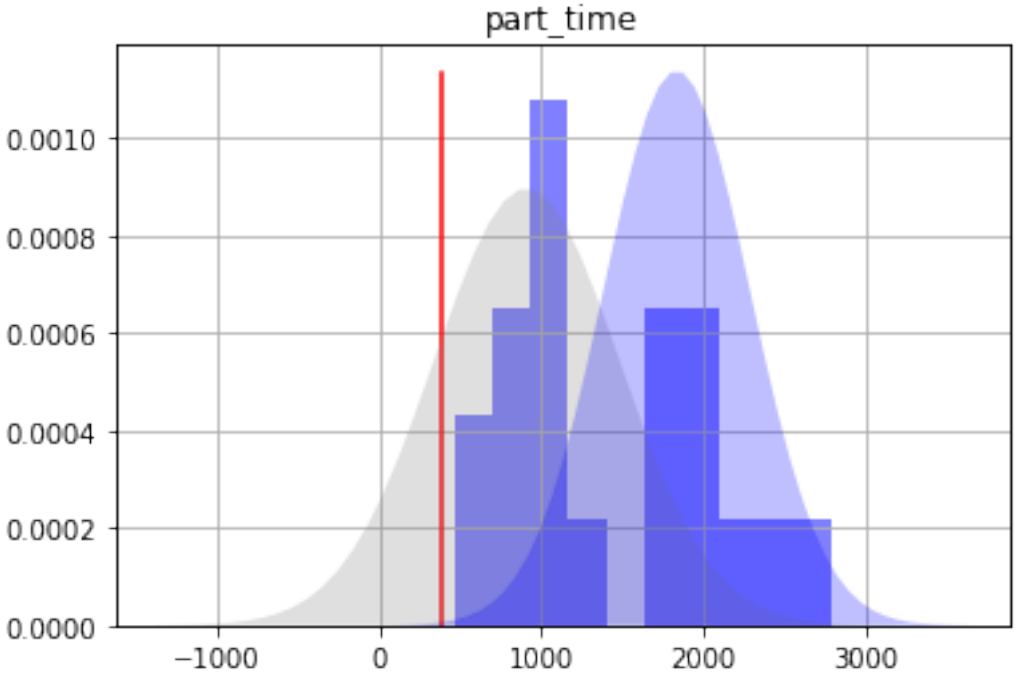
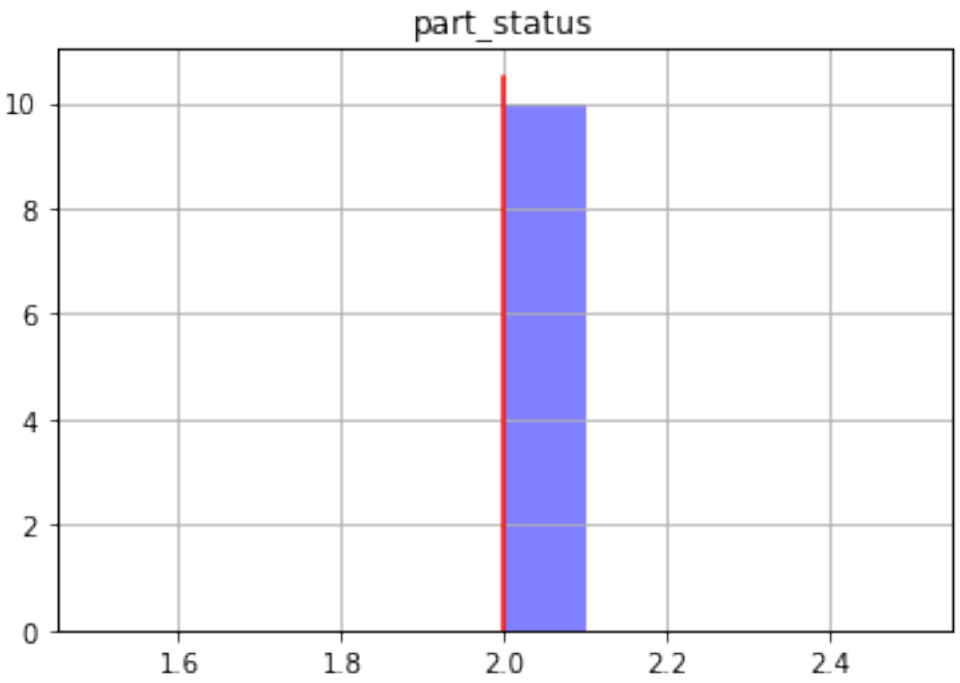
0.4
0.3
0.2
0.1
0.0
25
30
35
40
45
50
55


hds_00_013_002_001
0.5
0.4
0.3
0.2
0.1
0.0
25
30
35
40
45
50
55


part_time
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−1000
0
1000
2000
3000


part_status
10
8
6
4
2
0
1.6
1.8
2.0
2.2
2.4