pestpp-glm

May 11, 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	\
pp_hk2	pp_hk2	log	32	0	
cn_sy8	cn_sy8	log	1	0	
gr_sy4	gr_sy4	log	705	0	
gr_vka3	gr_vka3	log	705	0	
pp_rech1	pp_rech1	log	32	0	
gr_sy5	gr_sy5	log	705	0	
pp_prsity0	pp_prsity0	log	32	0	
pp_sy2	pp_sy2	log	32	0	
cn_sy7	cn_sy7	log	1	0	
pp_sy0	pp_sy0	log	32	0	
cn_prsity8	cn_prsity8	log	1	0	

gr_prsity5	gr_prsity5	log	705	0
drncond_k00	drncond_k00	log	10	0
cn_vka7	cn_vka7	log	1	0
pp_strt2	pp_strt2	log	32	0
gr_hk3	gr_hk3	log	705	0
welflux	welflux	log	2	0 to 0.176091
pp_strt0	pp_strt0	log	32	0
gr_strt5	gr_strt5	log	705	0
cn_prsity7	cn_prsity7	log	1	0
pp_sy1	pp_sy1	log	32	0
gr_strt4	gr_strt4	log	705	0
gr_ss4	gr_ss4	log	705	0
pp_vka0	pp_vka0	log	32	0
gr_ss3	gr_ss3	log	705	0
pp_hk0	pp_hk0	log	32	0
cn_hk7	cn_hk7	log	1	0
pp_ss2	pp_ss2	log	32	0
cn_ss7	cn_ss7	log	1	0
gr_rech3	gr_rech3	log	705	0
...	...	...	...	...
gr_hk5	gr_hk5	log	705	0
pp_hk1	pp_hk1	log	32	0
cn_hk8	cn_hk8	log	1	0
pp_rech0	pp_rech0	log	32	0
gr_ss5	gr_ss5	log	705	0
gr_vka5	gr_vka5	log	705	0
cn_rech5	cn_rech5	log	1	-0.39794
cn_prsity6	cn_prsity6	log	1	0
cn_rech4	cn_rech4	log	1	0
gr_rech2	gr_rech2	log	705	0
cn_strt7	cn_strt7	log	1	0
pp_strt1	pp_strt1	log	32	0
pp_prsity2	pp_prsity2	log	32	0
pp_ss0	pp_ss0	log	32	0
pp_vka2	pp_vka2	log	32	0
pp_ss1	pp_ss1	log	32	0
pp_prsity1	pp_prsity1	log	32	0
cn_strt8	cn_strt8	log	1	0
gr_hk4	gr_hk4	log	705	0
gr_sy3	gr_sy3	log	705	0
gr_vka4	gr_vka4	log	705	0
pp_vka1	pp_vka1	log	32	0
cn_ss8	cn_ss8	log	1	0
strk	strk	log	40	0
cn_vka8	cn_vka8	log	1	0
cn_vka6	cn_vka6	log	1	0
cn_hk6	cn_hk6	log	1	0
gr_prsity3	gr_prsity3	log	705	0

cn_ss6	cn_ss6	log	1	0
welflux_k02	welflux_k02	log	6	0

	upper bound	lower bound	standard deviation
pp_hk2	1	-1	0.5
cn_sy8	0.243038	-0.60206	0.211275
gr_sy4	0.243038	-0.60206	0.211275
gr_vka3	1	-1	0.5
pp_rech1	0.0413927	-0.0457575	0.0217875
gr_sy5	0.243038	-0.60206	0.211275
pp_prsity0	0.176091	-0.30103	0.11928
pp_sy2	0.243038	-0.60206	0.211275
cn_sy7	0.243038	-0.60206	0.211275
pp_sy0	0.243038	-0.60206	0.211275
cn_prsity8	0.176091	-0.30103	0.11928
gr_prsity5	0.176091	-0.30103	0.11928
drncond_k00	1	-1	0.5
cn_vka7	1	-1	0.5
pp_strt2	0.0211893	-0.0222764	0.0108664
gr_hk3	1	-1	0.5
welflux	0.176091 to 0.30103	-0.30103 to 0	0.0752575 to 0.11928
pp_strt0	0.0211893	-0.0222764	0.0108664
gr_strt5	0.0211893	-0.0222764	0.0108664
cn_prsity7	0.176091	-0.30103	0.11928
pp_sy1	0.243038	-0.60206	0.211275
gr_strt4	0.0211893	-0.0222764	0.0108664
gr_ss4	1	-1	0.5
pp_vka0	1	-1	0.5
gr_ss3	1	-1	0.5
pp_hk0	1	-1	0.5
cn_hk7	1	-1	0.5
pp_ss2	1	-1	0.5
cn_ss7	1	-1	0.5
gr_rech3	0.0413927	-0.0457575	0.0217875
...	...	...	...
gr_hk5	1	-1	0.5
pp_hk1	1	-1	0.5
cn_hk8	1	-1	0.5
pp_rech0	0.0413927	-0.0457575	0.0217875
gr_ss5	1	-1	0.5
gr_vka5	1	-1	0.5
cn_rech5	-0.09691	-1	0.225772
cn_prsity6	0.176091	-0.30103	0.11928
cn_rech4	0.0791812	-0.09691	0.0440228
gr_rech2	0.0413927	-0.0457575	0.0217875
cn_strt7	0.0211893	-0.0222764	0.0108664
pp_strt1	0.0211893	-0.0222764	0.0108664
pp_prsity2	0.176091	-0.30103	0.11928

```
pp_ss0                    1          -1          0.5
pp_vka2                   1          -1          0.5
pp_ss1                    1          -1          0.5
pp_prsity1         0.176091    -0.30103      0.11928
cn_strt8          0.0211893  -0.0222764    0.0108664
gr_hk4                    1          -1          0.5
gr_sy3             0.243038    -0.60206     0.211275
gr_vka4                   1          -1          0.5
pp_vka1                   1          -1          0.5
cn_ss8                    1          -1          0.5
strk                      2          -2            1
cn_vka8                   1          -1          0.5
cn_vka6                   1          -1          0.5
cn_hk6                    1          -1          0.5
gr_prsity3         0.176091    -0.30103      0.11928
cn_ss6                    1          -1          0.5
welflux_k02               1          -1          0.5

[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_ss6          1
cn_rech5        1
cn_strt7        1
cn_ss7          1
cn_vka6         1
cn_sy7          1
cn_ss8          1
cn_prsity8      1
cn_vka7         1
cn_sy8          1
cn_vka8         1
cn_hk6          1
cn_strt8        1
cn_hk7          1
cn_prsity7      1
flow            1
cn_strt6        1
cn_rech4        1
cn_sy6          1
cn_prsity6      1
cn_hk8          1
welflux         2
welflux_k02     6
drncond_k00    10
pp_prsity1     32
pp_rech0       32
pp_prsity2     32
pp_prsity0     32
pp_sy2         32
pp_sy0         32
pp_strt2       32
pp_strt0       32
pp_vka0        32
pp_hk0         32
pp_ss2         32
pp_hk1         32
pp_strt1       32
pp_hk2         32
```

```
pp_ss0         32
pp_vka2        32
pp_vka1        32
pp_sy1         32
pp_ss1         32
pp_rech1       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
```

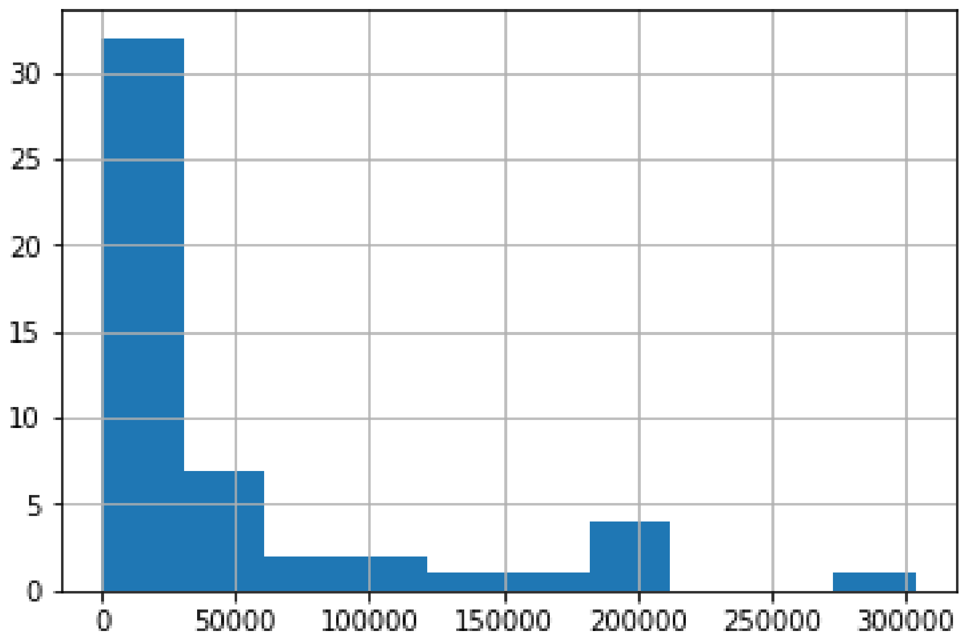
```
In [12]: pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=20,slave_ro
                                     master_dir=m_d)
```

```
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
         23      132.068613
         27      241.955380
         17      251.762763
         11      401.150874
         6       743.678567
         45      987.219988
```

```
26    1013.849110
0     1169.062995
3     1343.339505
34    1678.461764
24    1760.741891
25    2059.095743
48    3509.267647
44    3863.709179
10    3944.416014
5     5044.716191
22    5687.184751
1     6092.813002
7     6518.481483
12    6740.141680
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:

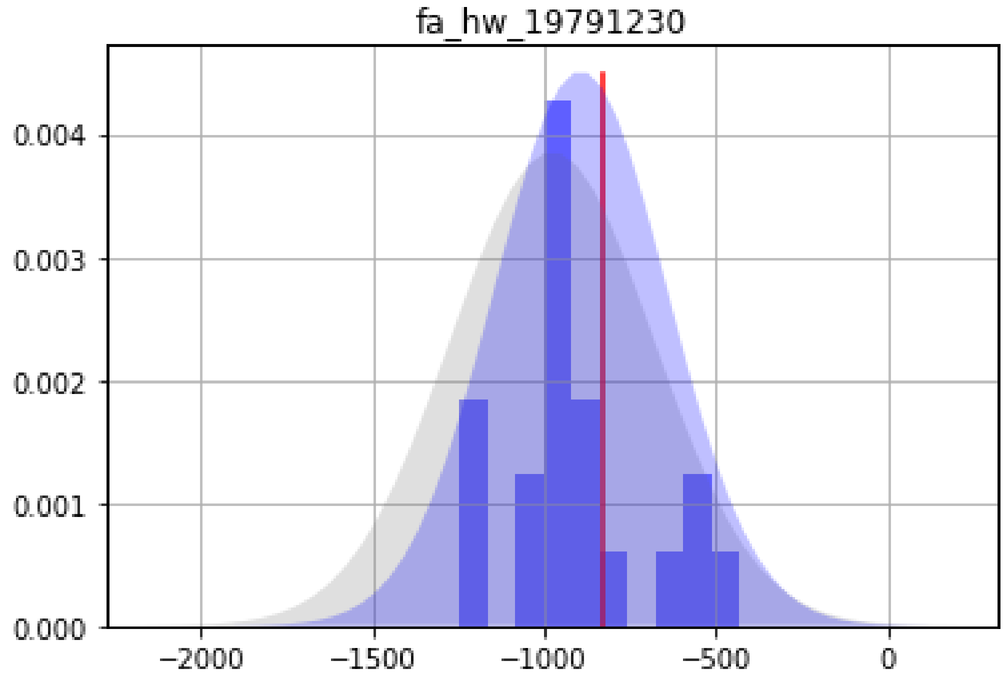
```
In [15]: oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:] #just take the 20 lowest phi
```

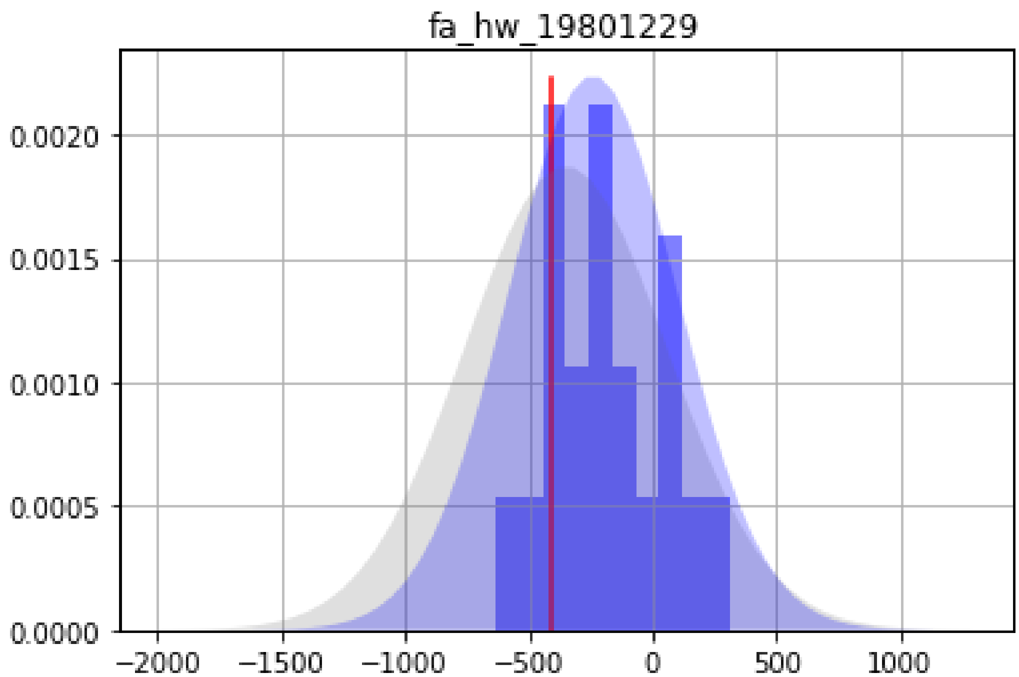
We can also load and plot the FOSM forecast results along side of the ensemble results:

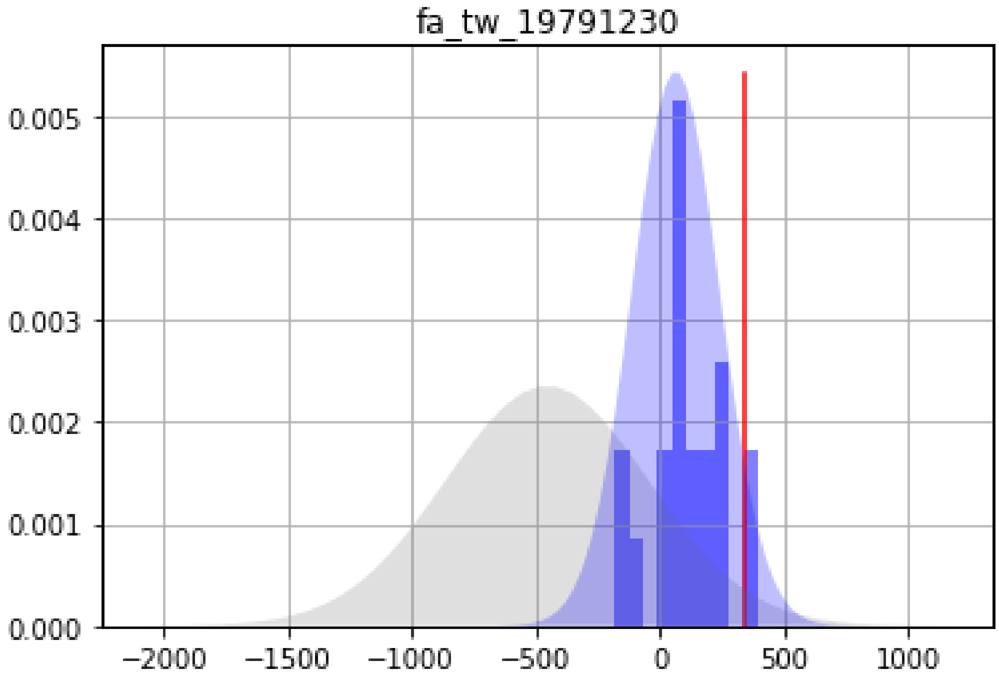
```
In [16]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

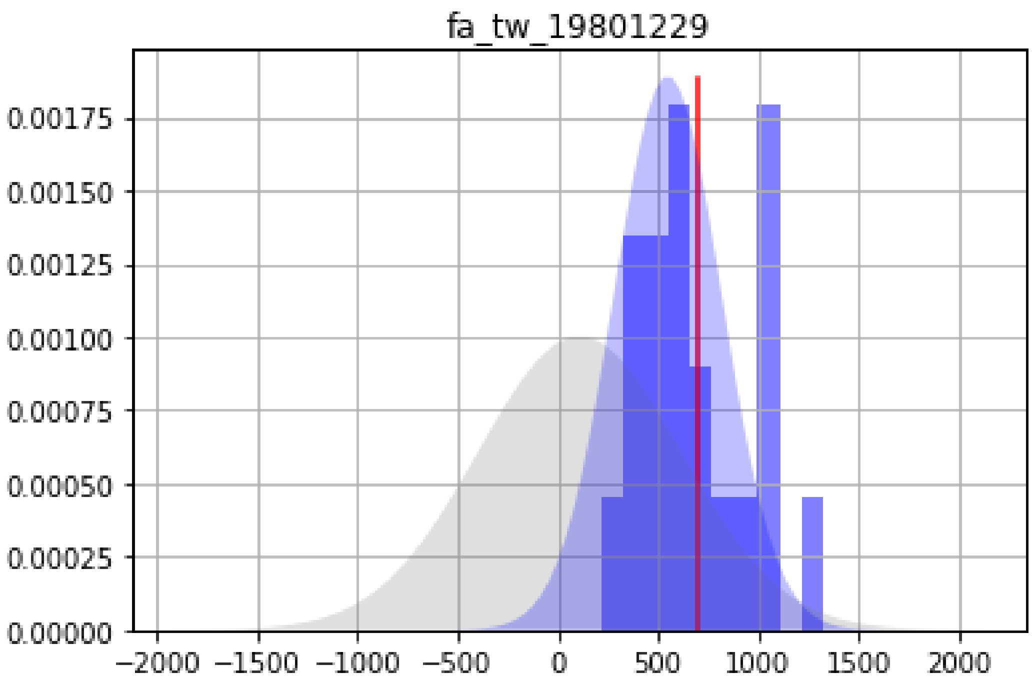
```
Out[16]:                      prior_mean  prior_stdev  prior_lower_bound  \
         name
         fa_hw_19791230        -977.2390    295.32800         -1567.8900
         fa_hw_19801229        -351.2160    409.77000         -1170.7600
         fa_tw_19791230        -453.0330    409.35100         -1271.7400
         fa_tw_19801229         108.9600    506.73200          -904.5040
         hds_00_013_002_000      39.6102      3.96314            31.6840
         hds_00_013_002_001      38.3838      4.05782            30.2681
         part_status              2.0000      0.00000             2.0000
         part_time              907.7020    570.98600          -234.2690

                              prior_upper_bound  post_mean  post_stdev  \
         name
         fa_hw_19791230               -386.5840  -893.9670  252.252000
         fa_hw_19801229                468.3240  -241.0990  342.887000
         fa_tw_19791230                365.6690    65.9087  177.081000
         fa_tw_19801229               1122.4200   549.0940  268.981000
         hds_00_013_002_000             47.5365    37.5468    0.303978
         hds_00_013_002_001             46.4994    36.2824    0.700380
         part_status                     2.0000     2.0000    0.000000
         part_time                    2049.6700   584.5470  439.730000

                              post_lower_bound  post_upper_bound
         name
         fa_hw_19791230             -1398.4700         -389.4620
         fa_hw_19801229              -926.8740          444.6750
         fa_tw_19791230              -288.2530          420.0700
         fa_tw_19801229                11.1331         1087.0600
         hds_00_013_002_000            36.9388           38.1547
         hds_00_013_002_001            34.8816           37.6831
         part_status                    2.0000            2.0000
         part_time                   -294.9140         1464.0100
```

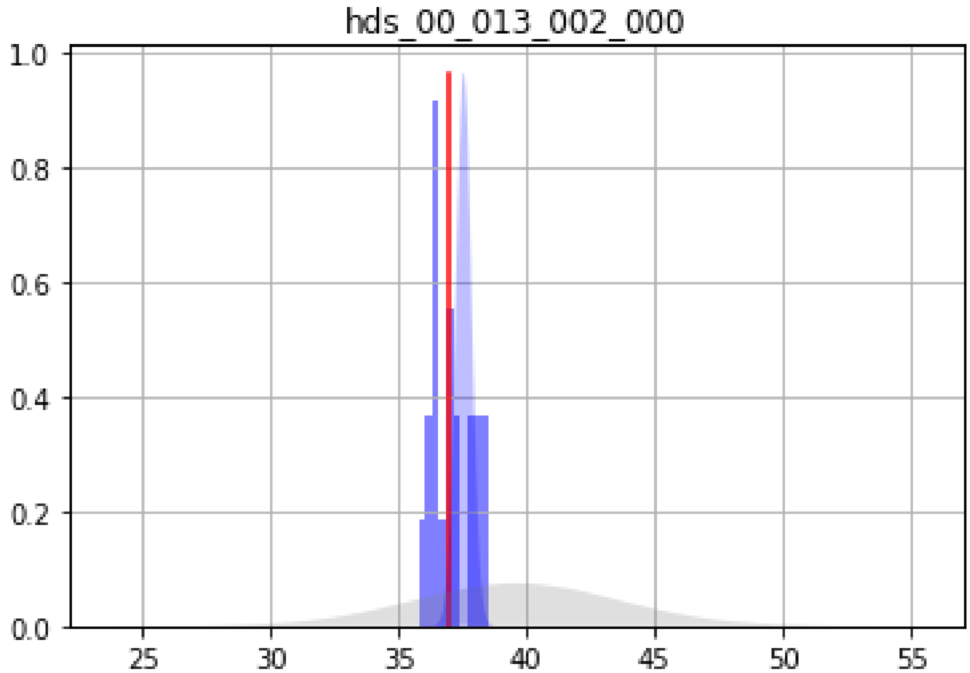
```
In [17]: obs = pst.observation_data
         fnames = pst.pestpp_options["forecasts"].split(",")
         for forecast in fnames:
             ax = plt.subplot(111)
             oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
             ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"
             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.l
             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()
```

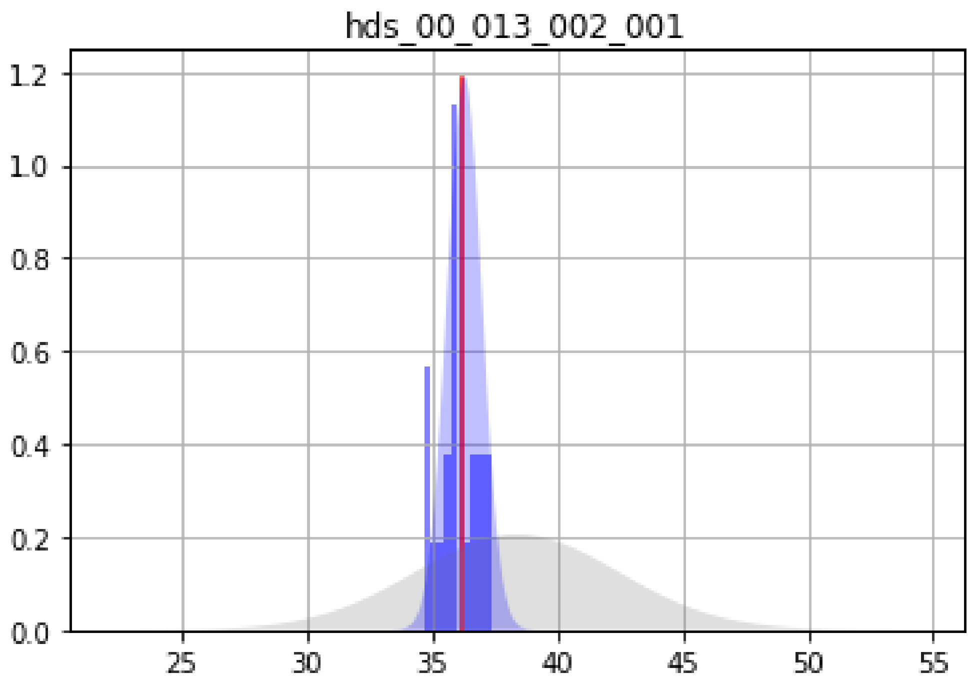

fa_hw_19791230
0.004
0.003
0.002
0.001
0.000
−2000
−1500
−1000
−500
0

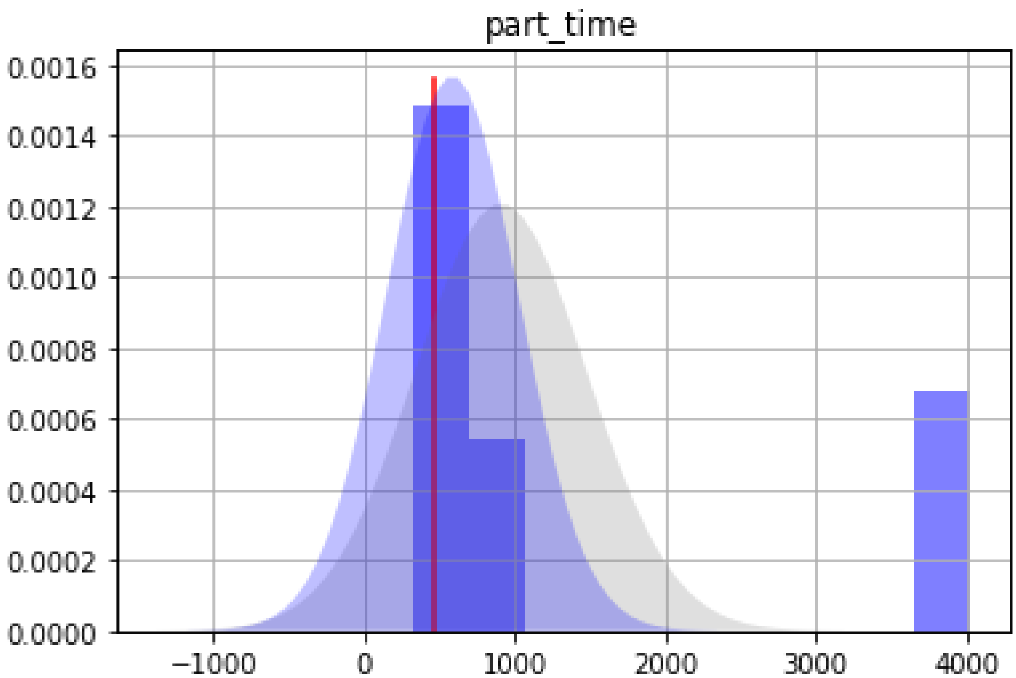

fa_hw_19801229
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000

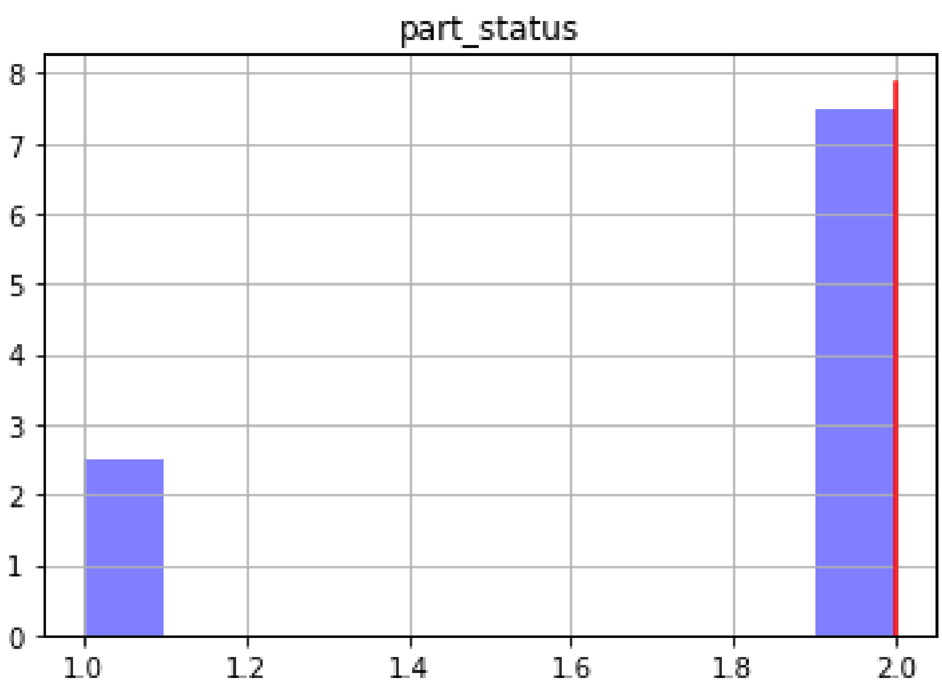

fa_tw_19791230
0.005
0.004
0.003
0.002
0.001
0.000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
−2000
−1500
−1000
−500
0
500
1000
1500
2000


hds_00_013_002_000
1.0
0.8
0.6
0.4
0.2
0.0
25
30
35
40
45
50
55


hds_00_013_002_001
1.2
1.0
0.8
0.6
0.4
0.2
0.0
25
30
35
40
45
50
55


part_time
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
−1000
0
1000
2000
3000
4000


part_status
8
7
6
5
4
3
2
1
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"))
```

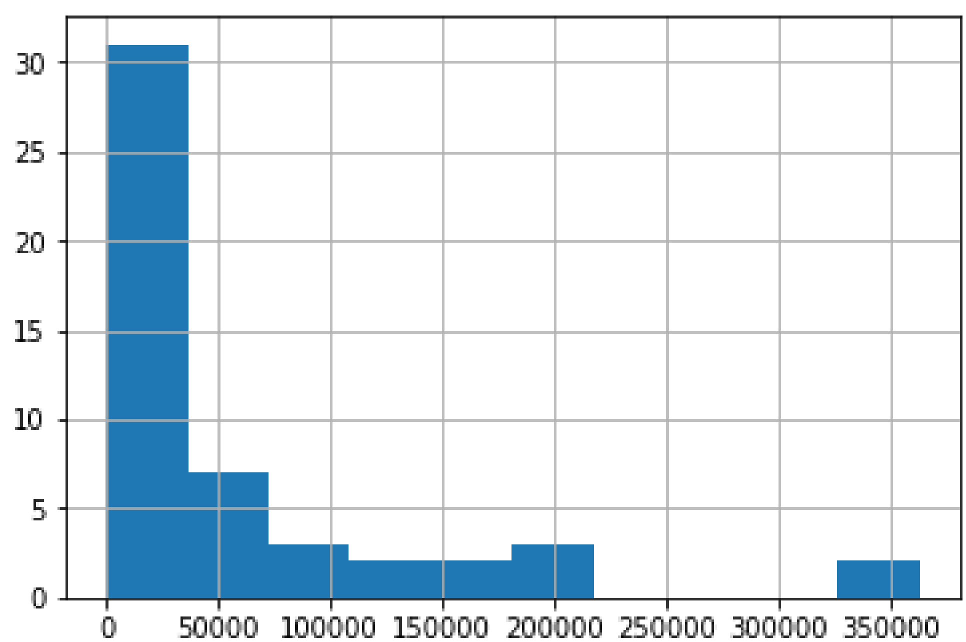
```
noptmax:3, npar_adj:527, nnz_obs:14
```

```
In [23]: pyemu.os_utils.start_slaves(t_d,"pestpp-glm","freyberg_pp.pst",num_slaves=20,slave_roo
                                     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
         12      65.129726
         44     158.777490
         34     230.349230
         26     347.112541
         1      460.694137
         8      529.199963
         30    1130.190551
         5     1500.528125
         9     1839.999806
         39    1869.307921
         24    1890.741412
         25    2670.488058
         10    3585.298670
         23    3822.347869
         48    3860.974550
         35    4367.097461
         47    5700.249613
         46    6929.476246
         17    7483.773917
         29    8384.851786
         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:

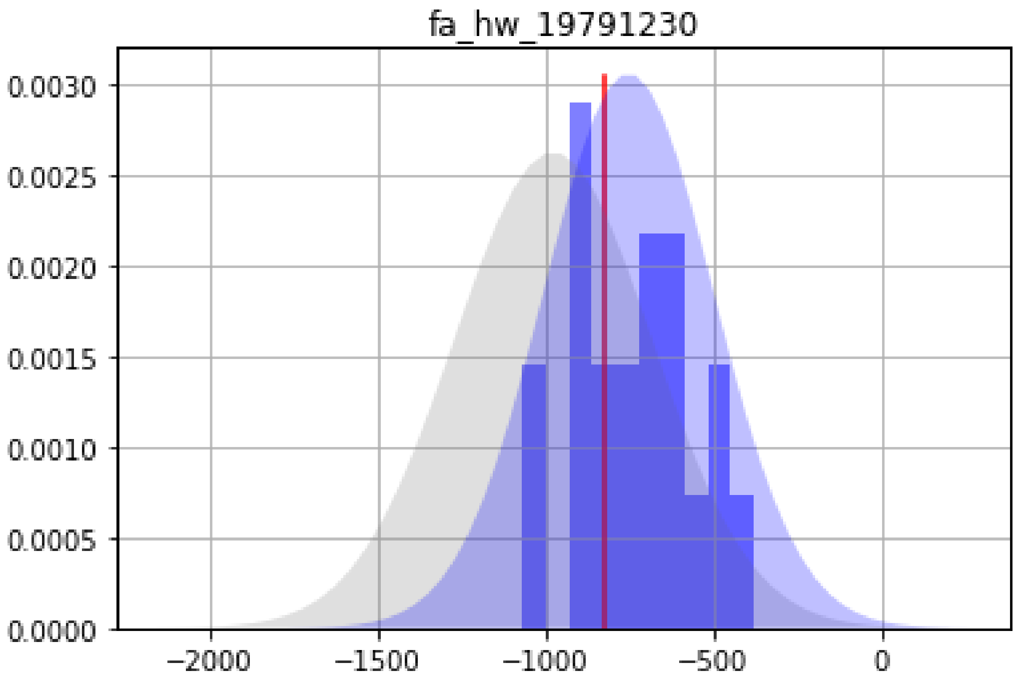
```
In [26]: oe_pt = oe.loc[oe.phi_vector.sort_values().index[:20],:]
```

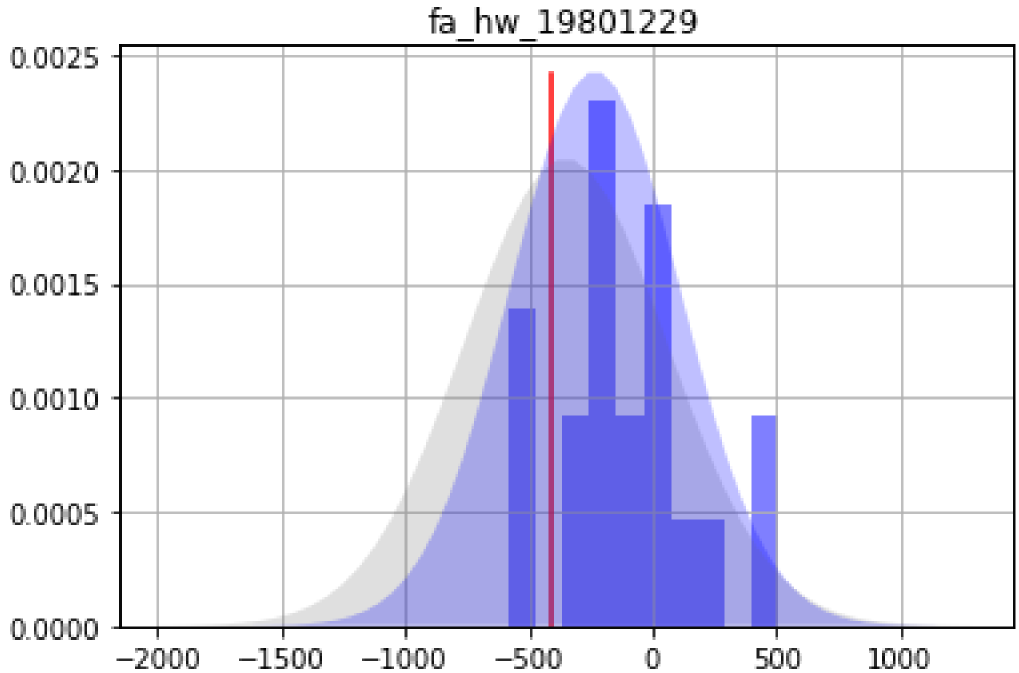
```
In [27]: f_df = pd.read_csv(os.path.join(m_d,"freyberg_pp.pred.usum.csv"),index_col=0)
         f_df.index = f_df.index.map(str.lower)
         f_df
```

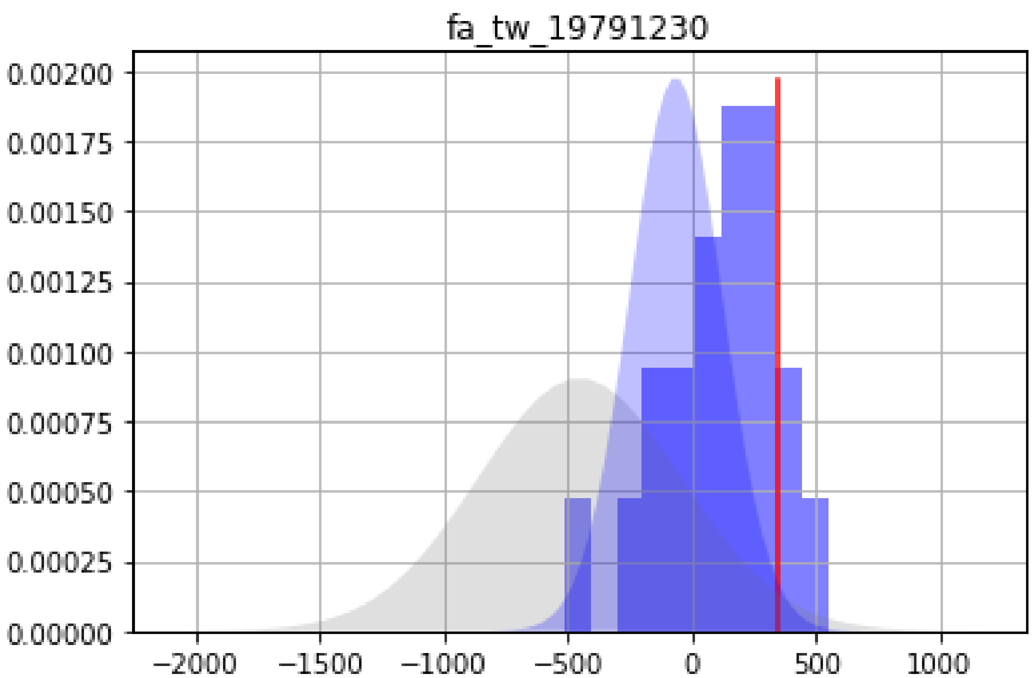
```
Out[27]:                      prior_mean  prior_stdev  prior_lower_bound  \
         name
         fa_hw_19791230        -977.2390    295.32800         -1567.8900
         fa_hw_19801229        -351.2160    409.77000         -1170.7600
         fa_tw_19791230        -453.0330    409.35100         -1271.7400
         fa_tw_19801229         108.9600    506.73200          -904.5040
         hds_00_013_002_000      39.6102      3.96314            31.6840
         hds_00_013_002_001      38.3838      4.05782            30.2681
         part_status              2.0000      0.00000             2.0000
         part_time              907.7020    570.98600          -234.2690

                              prior_upper_bound  post_mean  post_stdev  \
         name
         fa_hw_19791230               -386.5840  -752.3060  253.512000
         fa_hw_19801229                468.3240  -232.5480  345.019000
         fa_tw_19791230                365.6690   -65.1087  186.892000
         fa_tw_19801229               1122.4200   361.5050  275.230000
         hds_00_013_002_000             47.5365    37.8428    0.341048
         hds_00_013_002_001             46.4994    36.8283    0.717053
         part_status                     2.0000     1.0000    0.000000
         part_time                    2049.6700  4015.0000  441.663000

                              post_lower_bound  post_upper_bound
         name
         fa_hw_19791230             -1259.3300         -245.2820
         fa_hw_19801229              -922.5870          457.4900
         fa_tw_19791230              -438.8920          308.6740
         fa_tw_19801229              -188.9550          911.9640
         hds_00_013_002_000            37.1607           38.5249
         hds_00_013_002_001            35.3942           38.2624
         part_status                    1.0000            1.0000
         part_time                   3131.6700         4898.3300
```

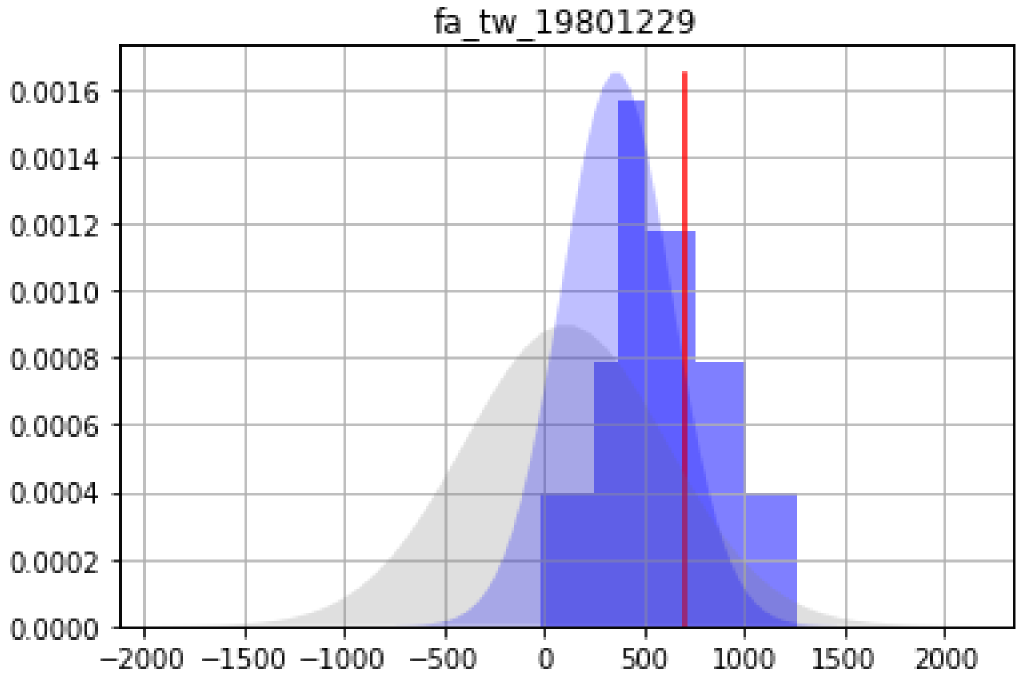
```
In [28]: obs = pst.observation_data
         fnames = pst.pestpp_options["forecasts"].split(",")
         for forecast in fnames:
             ax = plt.subplot(111)
             oe_pt.loc[:,forecast].hist(ax=ax,color="b",alpha=0.5,normed=True)
             ax.plot([obs.loc[forecast,"obsval"],obs.loc[forecast,"obsval"]],ax.get_ylim(),"r"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

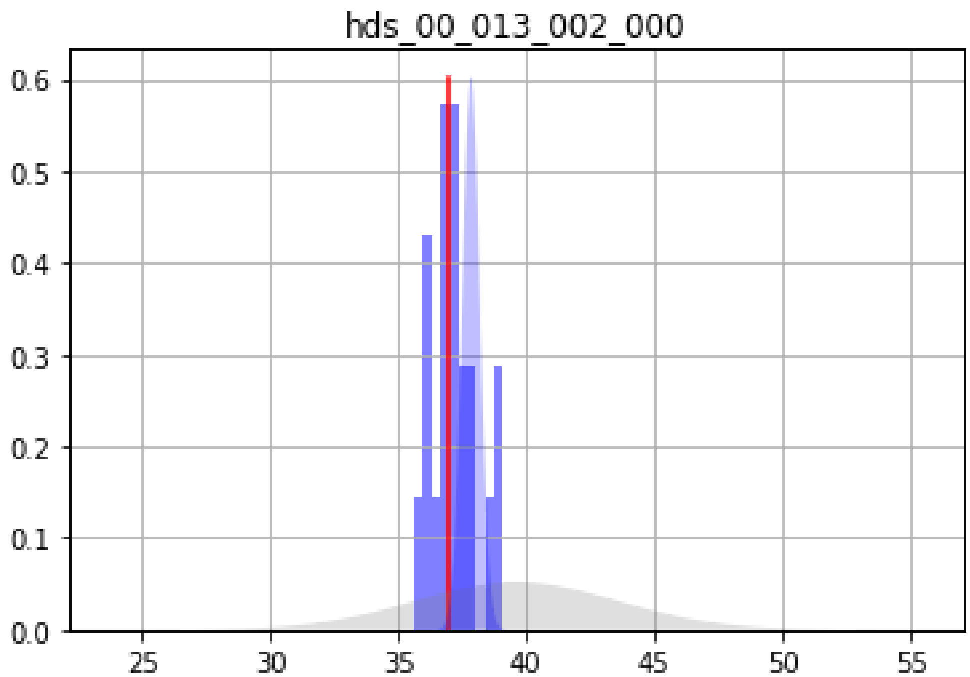
```
x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"prior_mean"],f_df
axt.fill_between(x,0,y,facecolor="0.5",alpha=0.25)
x,y = pyemu.plot_utils.gaussian_distribution(f_df.loc[forecast,"post_mean"],f_df.l
axt.fill_between(x,0,y,facecolor="b",alpha=0.25)
axt.set_ylim(0,axt.get_ylim()[1])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

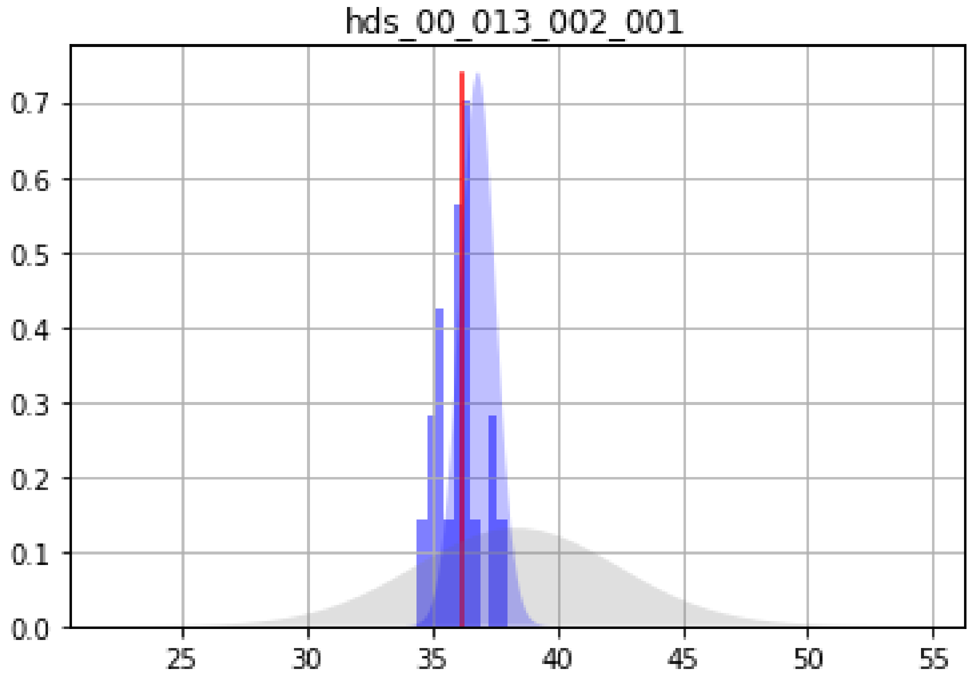


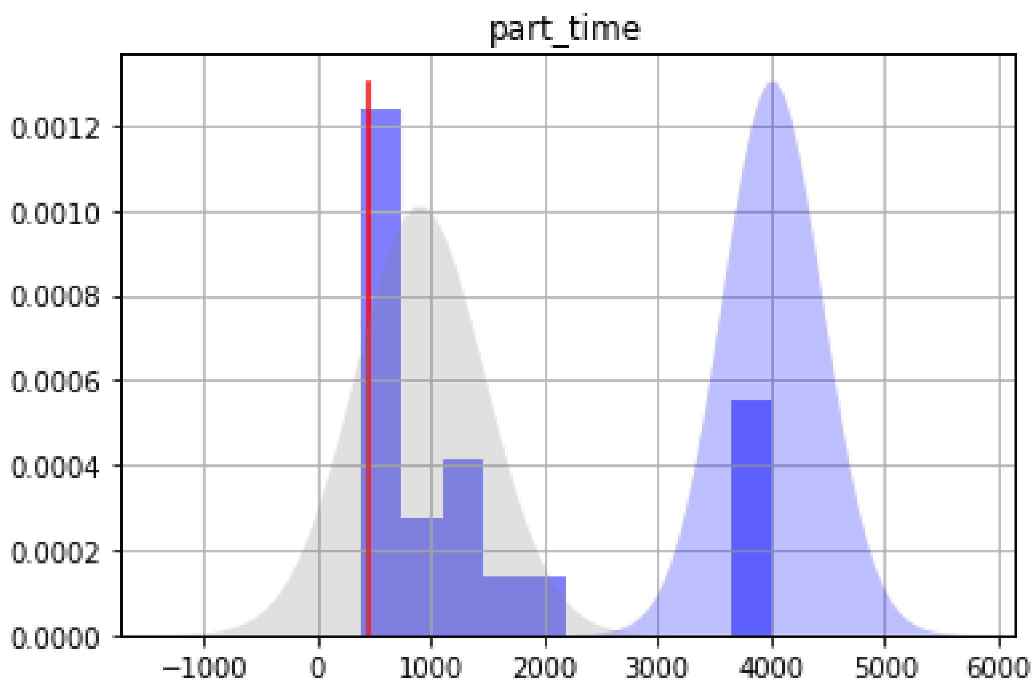

fa_hw_19801229
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−2000
−1500
−1000
−500
0
500
1000

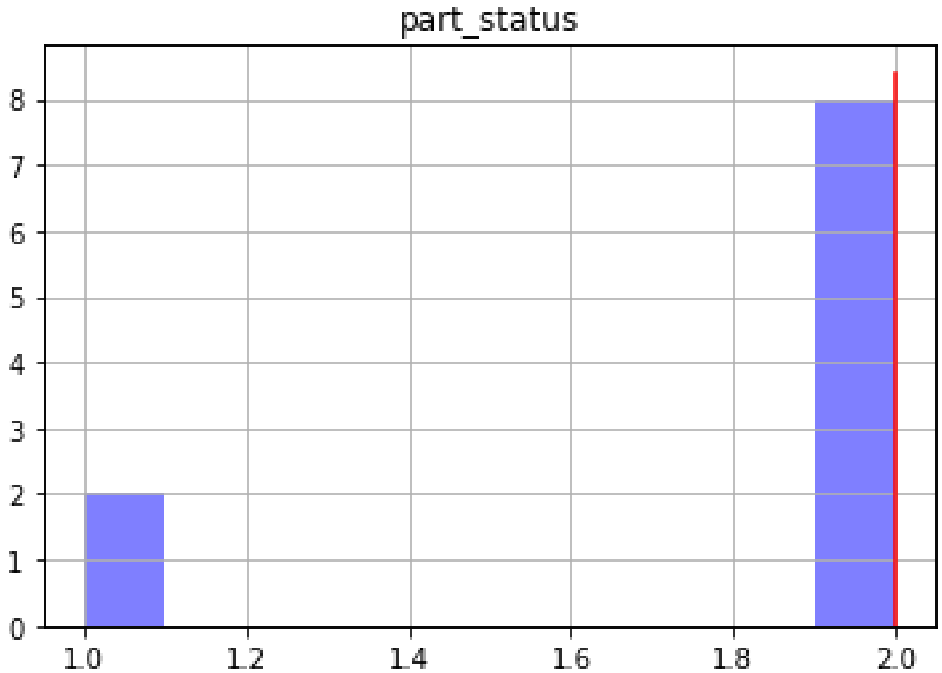

fa_tw_19791230
0.00200
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
−2000
−1500
−1000
−500
0
500
1000


fa_tw_19801229
0.0016
0.0014
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
0.6
0.5
0.4
0.3
0.2
0.1
0.0
25
30
35
40
45
50
55


hds_00_013_002_001
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
25
30
35
40
45
50
55


part_time
0.0000
0.0002
0.0004
0.0006
0.0008
0.0010
0.0012
−1000
0
1000
2000
3000
4000
5000
6000


part_status
0
1
2
3
4
5
6
7
8
1.0
1.2
1.4
1.6
1.8
2.0