dataworth_worked

July 18, 2019

1 data worth and related assessments

In this notebook, we will use outputs from previous notebooks (in particular pestpp-glm_part1.ipynb) to undertake data worth assessments based on first-order second-moment (FOSM) techniques. "Worth" is framed here in the context of the extent to which the uncertainty surrounding a model prediction of management interest is reduced through data collection. Given that these analyses can help target and optimize data acquisition strategies, this is a concept that really resonates with decision makers.

```
In [1]: %matplotlib inline
        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 C:\Users\knowling\Dev\GW1876\activities_csiro\notebooks\flopy
In [2]: m_d = "master_glm"
In [3]: pst = pyemu.Pst(os.path.join(m_d, "freyberg_pp.pst"))
        print(pst.npar_adj)
        pst.write_par_summary_table(filename="none")
527
Out [3]:
                            type transform count initial value upper bound
        cn_hk6
                          cn_hk6
                                        log
                                                 1
                                                               0
                                                                            1
                                        log
                                                               0
                                                                            1
        cn_hk7
                          cn_hk7
        cn hk8
                          cn hk8
                                        log
                                                 1
                                                               0
        cn_prsity6
                      cn_prsity6
                                        log
                                                 1
                                                               0
                                                                    0.0791812
        cn_prsity7
                      cn_prsity7
                                        log
                                                 1
                                                                    0.0791812
```

cn_prsity8	cn_prsity8	log	1	0	0.0791812
cn_rech4	cn_rech4	log	1	0	0.0413927
cn_rech5	cn_rech5	log	1	0	0.0413927
cn_ss6	cn_ss6	log	1	0	1
cn_ss7	cn_ss7	log	1	0	1
cn_ss8	cn_ss8	log	1	0	1
cn_strt6	cn_strt6	log	1	0	0.0211893
cn_strt7	cn_strt7	log	1	0	0.0211893
cn_strt8	cn_strt8	log	1	0	0.0211893
cn_sy6	cn_sy6	log	1	0	0.243038
cn_sy7	cn_sy7	log	1	0	0.243038
cn_sy8	cn_sy8	log	1	0	0.243038
cn_vka6	cn_vka6	log	1	0	1
cn_vka7	cn_vka7	log	1	0	1
cn_vka8	cn_vka8	log	1	0	1
drncond_k00	drncond_k00	log	10	0	1
flow	flow	log	1	0	0.09691
gr_hk3	gr_hk3	fixed	705	1	10
gr_hk4	gr_hk4	fixed	705	1	10
gr_hk5	gr_hk5	fixed	705	1	10
gr_prsity3	gr_prsity3	fixed	705	1	1.2
gr_prsity4	gr_prsity4	fixed	705	1	1.2
gr_prsity5	gr_prsity5	fixed	705	1	1.2
gr_rech2	gr_rech2	fixed	705	1	1.1
gr_rech3	gr_rech3	fixed	705	1	1.1
0 -	0 =				
gr_strt5	gr_strt5	fixed	705	1	1.05
gr_sy3	gr_sy3	fixed	705	1	1.75
gr_sy4	gr_sy4	fixed	705	1	1.75
gr_sy5	gr_sy5	fixed	705	1	1.75
gr_vka3	gr_vka3	fixed	705	1	10
gr_vka4	gr_vka4	fixed	705	1	10
gr_vka5	gr_vka5	fixed	705	1	10
pp_hk0	pp_hk0	log	32	0	1
pp_hk1	pp_hk1	log	32	0	1
pp_hk2	pp_hk2	log	32	0	1
pp_prsity0	pp_prsity0	log	32	0	0.0791812
pp_prsity1	pp_prsity1	log	32	0	0.0791812
pp_prsity2	pp_prsity2	log	32	0	0.0791812
pp_rech0	pp_rech0	log	32	0	0.0413927
pp_rech1	pp_rech1	fixed	32	1	1.1
pp_ss0	pp_ss0	log	32	0	1
pp_ss1	pp_ss1	log	32	0	1
pp_ss2	pp_ss2	log	32	0	1
pp_strt0	pp_strt0	fixed	32	1	1.05
pp_strt1	pp_strt1	fixed	32	1	1.05
pp_strt2	pp_strt2	fixed	32	1	1.05
pp_sy0	pp_sy0	log	32	0	0.243038
-	•	_			

pp_sy1	pp_sy1	log	32	0	0.243038
pp_sy2	pp_sy2	log	32	0	0.243038
pp_vka0	pp_vka0	fixed	32	1	10
pp_vka1	pp_vka1	log	32	0	1
pp_vka2	pp_vka2	fixed	32	1	10
strk	strk	log	40	0	2
welflux	welflux	log	2	0	1
welflux_k02	welflux_k02	log	6	0	1

	lower	bound	standard	deviation		
cn_hk6		-1		0.5		
cn_hk7		-1		0.5		
cn_hk8	-1			0.5		
cn_prsity6	-0	.09691		0.0440228		
cn_prsity7	-0	.09691		0.0440228		
cn_prsity8	-0	.09691		0.0440228		
cn_rech4	-0.04	157575		0.0217875		
cn_rech5	-0.04	157575		0.0217875		
cn_ss6		-1		0.5		
cn_ss7		-1		0.5		
cn_ss8		-1		0.5		
cn_strt6	-0.02	222764		0.0108664		
cn_strt7	-0.02	222764		0.0108664		
cn_strt8	-0.02	222764		0.0108664		
cn_sy6	-0	.60206		0.211275		
cn_sy7	-0	.60206		0.211275		
cn_sy8	-0	.60206		0.211275		
cn_vka6	-1			0.5		
cn_vka7		-1		0.5		
cn_vka8		-1		0.5		
${\tt drncond_k00}$		-1		0.5		
flow	-0.3	124939		0.0554622		
gr_hk3		0.1		2.475		
gr_hk4		0.1		2.475		
gr_hk5		0.1		2.475		
gr_prsity3		0.8		0.1		
gr_prsity4		0.8		0.1		
gr_prsity5		0.8		0.1		
gr_rech2		0.9		0.05		
gr_rech3		0.9		0.05		
• • •				• • •		
gr_strt5		0.95		0.025		
gr_sy3		0.25		0.375		
gr_sy4		0.25		0.375		
gr_sy5		0.25		0.375		
gr_vka3	0.1			2.475		
gr_vka4		0.1		2.475		
gr_vka5		0.1		2.475		

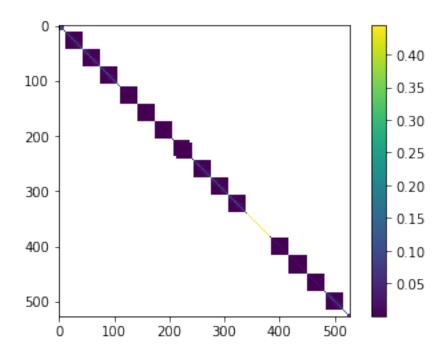
```
pp_hk0
                     -1
                                        0.5
pp_hk1
                     -1
                                        0.5
                                        0.5
pp_hk2
                     -1
pp_prsity0
               -0.09691
                                  0.0440228
               -0.09691
                                  0.0440228
pp_prsity1
pp_prsity2
               -0.09691
                                  0.0440228
pp_rech0
             -0.0457575
                                  0.0217875
                                       0.05
pp_rech1
                    0.9
                     -1
                                        0.5
pp_ss0
                     -1
                                        0.5
pp_ss1
                     -1
                                        0.5
pp_ss2
                   0.95
                                      0.025
pp_strt0
                   0.95
                                      0.025
pp_strt1
                   0.95
                                      0.025
pp_strt2
               -0.60206
                                   0.211275
pp_sy0
               -0.60206
                                   0.211275
pp_sy1
pp_sy2
               -0.60206
                                   0.211275
                                      2.475
pp_vka0
                    0.1
pp_vka1
                     -1
                                        0.5
                                      2.475
pp_vka2
                    0.1
strk
                     -2
                                          1
welflux
                     -1
                                        0.5
                     -1
                                        0.5
welflux_k02
```

[65 rows x 7 columns]

x[x<1e-7] = np.nan
c = plt.imshow(x)
plt.colorbar()</pre>

first ingredient: parameter covariance matrix (representing prior uncertainty in this instance)

Out[5]: <matplotlib.colorbar.Colorbar at 0x1b50090c470>



```
In [6]: pst.adj_par_groups
Out[6]: ['cn_hk6',
          'cn_hk7',
          'cn_hk8',
          'cn_prsity6',
          'cn_prsity7',
          'cn_prsity8',
          'cn_rech4',
          'cn_rech5',
          'cn_ss6',
          'cn_ss7',
          'cn_ss8',
          'cn_strt6',
          'cn_strt7',
          'cn_strt8',
          'cn_sy6',
          'cn_sy7',
          'cn_sy8',
          'cn_vka6',
         'cn_vka7',
          'cn_vka8',
          'drncond_k00',
          'flow',
          'pp_hk0',
          'pp_hk1',
```

```
'pp_hk2',
'pp_prsity0',
'pp_prsity1',
'pp_prsity2',
'pp_rech0',
'pp_ss0',
'pp_ss1',
'pp_ss2',
'pp_sy0',
'pp_sy1',
'pp_sy2',
'pp_vka1',
'strk',
'welflux',
'welflux_k02']
```

second ingredient: jacobian matrix

```
In [7]: jco = os.path.join(m_d, "freyberg_pp.jcb")
```

the third ingredient--the (diagonal) noise covariance matrix--populated on-the-fly using weights when constructing the Schur object below...

```
In [8]: sc = pyemu.Schur(jco=jco,parcov=cov)
In [9]: sc
Out[9]: <pyemu.sc.Schur at 0x1b50092f940>
```

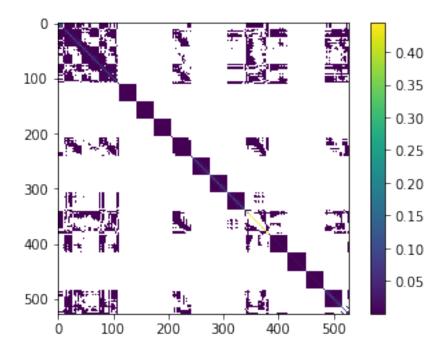
1.0.1 there we have it--all computations done and contained within sc. We will only be required to access different parts of sc below...

1.0.2 Parameter uncertainty

x[x<1e-7] = np.nan
c = plt.imshow(x)
plt.colorbar(c)</pre>

First let's inspect the (approx) posterior parameter covariance matrix and the reduction in parameter uncertainty through "data assimilation", before mapping to forecasts... (note that this matrix is *not* forecast-specific)

Out[11]: <matplotlib.colorbar.Colorbar at 0x1b5012ce9e8>



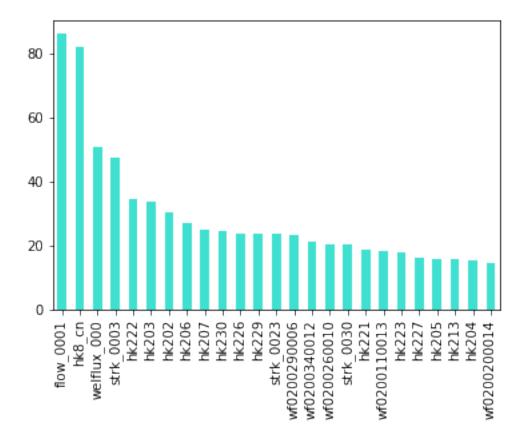
We can see the posterior variance for each parameter along the diagonal. The off-diags are symmetric.

Out[12]:		percent_reduction	post_var	<pre>prior_var</pre>
	flow_0001	8.629753e+01	0.000187	0.001367
	hk8_cn	8.216237e+01	0.019820	0.111111
	welflux_000	5.076704e+01	0.054703	0.111111
	strk_0003	4.767839e+01	0.232540	0.444444
	hk222	3.457443e+01	0.072695	0.111111
	hk203	3.372133e+01	0.073643	0.111111
	hk202	3.028185e+01	0.077465	0.111111
	hk206	2.695334e+01	0.081163	0.111111
	hk207	2.519217e+01	0.083120	0.111111
	hk230	2.464115e+01	0.083732	0.111111
	hk226	2.394589e+01	0.084505	0.111111
	hk229	2.386831e+01	0.084591	0.111111
	strk_0023	2.368509e+01	0.339177	0.444444
	wf0200290006	2.340886e+01	0.085101	0.111111
	wf0200340012	2.139508e+01	0.087339	0.111111
	wf0200260010	2.061345e+01	0.088207	0.111111
	strk_0030	2.044844e+01	0.353562	0.44444
	hk221	1.895753e+01	0.090047	0.111111

```
wf0200110013
                   1.846858e+01
                                 0.090590
                                             0.111111
hk223
                   1.796930e+01
                                 0.091145
                                             0.111111
hk227
                   1.616835e+01
                                 0.093146
                                             0.111111
hk205
                                             0.111111
                   1.602062e+01
                                 0.093310
hk213
                   1.577955e+01
                                 0.093578
                                             0.111111
hk204
                   1.551881e+01
                                 0.093868
                                             0.111111
wf0200200014
                   1.474544e+01
                                 0.094727
                                             0.111111
hk6_cn
                   1.447790e+01
                                 0.095025
                                             0.111111
hk210
                   1.440933e+01 0.095101
                                             0.111111
hk225
                   1.430781e+01 0.095214
                                             0.111111
hk220
                   1.367623e+01
                                 0.095915
                                             0.111111
wf0200090016
                   1.353431e+01 0.096073
                                             0.111111
                                       . . .
                                                  . . .
ss119
                  -2.220446e-14
                                 0.111111
                                             0.111111
rech5_cn
                  -2.220446e-14 0.000211
                                             0.000211
ss000
                  -2.220446e-14 0.111111
                                             0.111111
ss123
                  -2.220446e-14 0.111111
                                             0.111111
sy203
                  -2.220446e-14 0.019839
                                             0.019839
sy213
                  -2.220446e-14 0.019839
                                             0.019839
ss002
                  -2.220446e-14 0.111111
                                             0.111111
ss012
                  -2.220446e-14 0.111111
                                             0.111111
ss115
                  -2.220446e-14 0.111111
                                             0.111111
ss007
                  -2.220446e-14 0.111111
                                            0.111111
ss008
                  -2.220446e-14 0.111111
                                            0.111111
ss113
                  -2.220446e-14 0.111111
                                             0.111111
ss114
                  -2.220446e-14 0.111111
                                             0.111111
                  -4.440892e-14 0.019839
sy210
                                             0.019839
prsity009
                  -4.440892e-14
                                 0.000861
                                             0.000861
sy110
                  -4.440892e-14
                                 0.019839
                                             0.019839
                  -4.440892e-14
sy220
                                 0.019839
                                             0.019839
prsity209
                  -4.440892e-14 0.000861
                                             0.000861
                  -4.440892e-14
                                 0.019839
sy116
                                             0.019839
prsity025
                  -4.440892e-14
                                 0.000861
                                             0.000861
prsity215
                  -4.440892e-14 0.000861
                                             0.000861
prsity115
                  -4.440892e-14 0.000861
                                             0.000861
sy120
                  -4.440892e-14 0.019839
                                             0.019839
sy216
                  -4.440892e-14 0.019839
                                             0.019839
prsity015
                  -4.440892e-14 0.000861
                                             0.000861
prsity225
                  -4.440892e-14 0.000861
                                             0.000861
prsity125
                  -4.440892e-14 0.000861
                                             0.000861
prsity000
                  -6.661338e-14 0.000861
                                             0.000861
ss102
                  -6.661338e-14
                                 0.111111
                                             0.111111
prsity200
                  -6.661338e-14 0.000861
                                             0.000861
```

[527 rows x 3 columns]

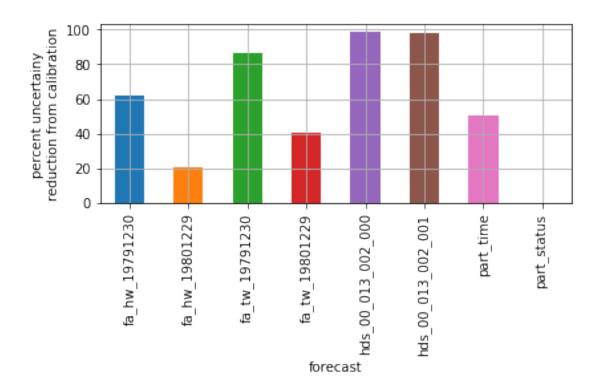
In [13]: par_sum.loc[par_sum.index[:25],"percent_reduction"].plot(kind="bar",color="turquoise"
Out[13]: <matplotlib.axes._subplots.AxesSubplot at 0x1b5006c1c18>



What have we achieved by "notionally calibrating" our model to 13 head and 1 stream flow observations? Which parameters are informed? Will they matter for the forecast of interest? Which ones are un-informed?

1.1 Forecast uncertainty

```
In [15]: forecasts = sc.pst.pestpp_options['forecasts'].split(",")
         forecasts
Out[15]: ['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']
In [16]: df = sc.get_forecast_summary()
         df
Out[16]:
                             percent_reduction
                                                     post_var
                                                                   prior_var
         fa_hw_19791230
                                     62.250126
                                                 48708.787021 129030.329448
         fa_hw_19801229
                                     20.164045 277258.059336 347284.702910
         fa_tw_19791230
                                     86.866072
                                                22609.793588 172147.988428
         fa tw 19801229
                                     40.797559 220463.794436 372389.706408
         hds_00_013_002_000
                                     98.537703
                                                     0.111608
                                                                    7.632373
         hds_00_013_002_001
                                     97.727870
                                                     0.192769
                                                                    8.484073
                                     50.756746
                                                 93226.847888 189319.023019
         part_time
         part_status
                                           NaN
                                                     0.000000
                                                                    0.000000
In [17]: # make a pretty plot
        fig = plt.figure()
         ax = plt.subplot(111)
         ax = df["percent_reduction"].plot(kind='bar',ax=ax,grid=True)
         ax.set_ylabel("percent uncertainy\nreduction from calibration")
         ax.set_xlabel("forecast")
         plt.tight_layout()
```



Surprise, surprise... Some forecasts benefit from calibration, some do not!

1.1.1 Before moving onto data worth, let's look at the contribution of different parameters to forecast uncertainty

Parameter contributions to uncertainty are quantified by "fixing" parameters (or parameter groups) and observing the uncertainty reduction as a result. This approach is of course subject to some sizable assumptions--related to parameter representativeness. But it can be very informative. Let's do by group.

```
In [18]: par_contrib = sc.get_par_group_contribution()
In [19]: par_contrib.head()
Out[19]:
                     fa_hw_19791230 fa_hw_19801229
                                                      fa_tw_19791230 fa_tw_19801229
         base
                       48708.787021
                                      277258.059336
                                                        22609.793588
                                                                       220463.794436
         cn_hk6
                       48343.538434
                                      277079.164728
                                                        22509.835083
                                                                       220406.965378
         cn_hk7
                       48708.780545
                                      277258.057052
                                                        22609.791510
                                                                       220463.730874
         cn_hk8
                       44990.748125
                                       275607.303800
                                                        21321.626080
                                                                       220162.729424
         cn_prsity6
                       48708.787021
                                      277258.059336
                                                        22609.793588
                                                                       220463.794436
                     hds_00_013_002_000 hds_00_013_002_001 part_status
                                                                               part_time
         base
                               0.111608
                                                    0.192769
                                                                      0.0
                                                                           93226.847888
         cn_hk6
                               0.110868
                                                    0.192766
                                                                      0.0
                                                                           87722.159943
                               0.111608
                                                    0.192769
                                                                      0.0 93226.236725
         cn_hk7
```

```
      cn_hk8
      0.108634
      0.187237
      0.0
      89722.098031

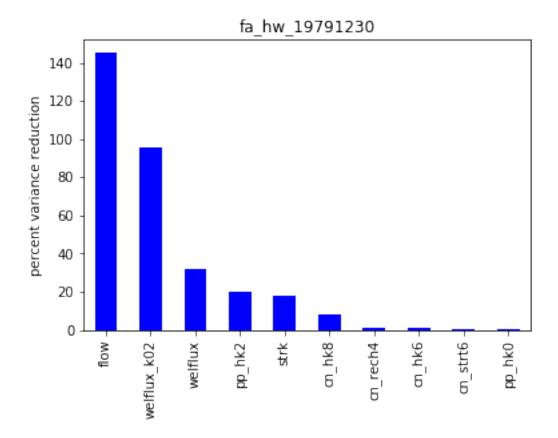
      cn_prsity6
      0.111608
      0.192769
      0.0
      93166.415889
```

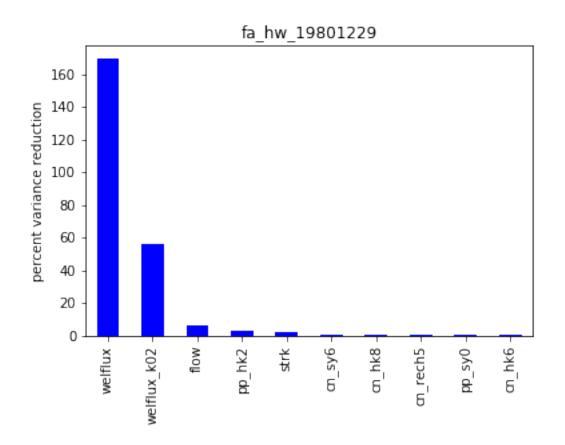
In [20]: base = par_contrib.loc["base",:]
 par_contrib = 100.0 * (base - par_contrib) / par_contrib
 par_contrib.sort_index()

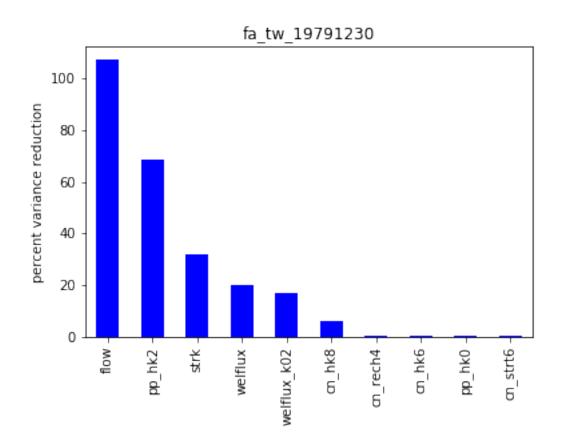
Out[20]:		fa_hw_19791230	fa_hw_19801229	fa_tw_19791230	fa_tw_19801229	\
	base	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	
	cn_hk6	7.555272e-01	6.456444e-02	4.440659e-01	2.578369e-02	
	cn_hk7	1.329528e-05	8.237482e-07	9.192837e-06	2.883103e-05	
	cn_hk8	8.264008e+00	5.989520e-01	6.041601e+00	1.367466e-01	
	cn_prsity6	-1.493767e-14	0.000000e+00	-4.827084e-14	-1.320118e-14	
	cn_prsity7	-1.493767e-14	0.000000e+00	-4.827084e-14	-1.320118e-14	
	cn_prsity8	-1.493767e-14	0.000000e+00	-4.827084e-14	-1.320118e-14	
	cn_rech4	1.328983e+00	2.071189e-03	4.946222e-01	5.626596e-02	
	cn_rech5	0.000000e+00	1.523076e-01	-6.436111e-14	1.485863e-01	
	cn_ss6	2.789907e-06	2.104129e-05	3.491816e-05	4.579829e-05	
	cn_ss7	0.000000e+00	1.341250e-05	-8.045139e-14	4.648073e-05	
	cn_ss8	4.617341e-06	1.873997e-03	1.033730e-05	3.116114e-03	
	cn_strt6	7.331869e-01	3.392103e-04	2.381097e-01	2.695676e-02	
	cn_strt7	5.529236e-06	3.978286e-09	2.567813e-06	1.265512e-07	
	cn_strt8	2.419169e-04	4.321156e-06	1.585604e-04	1.990229e-05	
	cn_sy6	6.185704e-03	6.450432e-01	6.508401e-04	7.492785e-01	
	cn_sy7	-1.493767e-14	2.099404e-14	-9.654167e-14	0.000000e+00	
	cn_sy8	-1.493767e-14	2.099404e-14	-9.654167e-14	0.000000e+00	
	cn_vka6	9.106484e-04	1.018885e-04	8.569676e-04	1.135336e-05	
	cn_vka7	5.049578e-02	4.055652e-03	9.290548e-03	7.240419e-04	
	cn_vka8	6.929210e-02	6.021175e-03	1.129875e-02	1.091725e-03	
	drncond_k00	7.415039e-04	2.742403e-06	3.318787e-03	1.220112e-05	
	flow	1.450607e+02	6.080339e+00	1.071328e+02	6.934249e-01	
	pp_hk0	4.369761e-01	5.119383e-02	4.359639e-01	2.238615e-02	
	pp_hk1	8.760160e-04	2.577004e-05	4.482011e-04	1.659310e-05	
	pp_hk2	2.033927e+01	2.805611e+00	6.856688e+01	3.596352e+00	
	pp_prsity0	0.000000e+00	4.198807e-14	0.000000e+00	1.320118e-14	
	pp_prsity1	0.000000e+00	4.198807e-14	0.000000e+00	1.320118e-14	
	pp_prsity2	0.000000e+00	4.198807e-14	0.000000e+00	1.320118e-14	
	pp_rech0	3.796292e-01	1.300183e-02	1.487279e-01	1.560503e-02	
	pp_ss0	0.000000e+00	5.870941e-08	0.000000e+00	3.408468e-06	
	pp_ss1	0.000000e+00	2.146002e-08	0.000000e+00	2.411191e-05	
	pp_ss2	8.469699e-07	4.384063e-04	8.631079e-07	9.606797e-04	
	pp_sy0	1.615596e-03	1.026042e-01	5.105185e-04	1.415935e-01	
	pp_sy1	1.493767e-14	0.000000e+00	-1.609028e-14	1.320118e-14	
	pp_sy2	1.493767e-14	0.000000e+00	-1.609028e-14	1.320118e-14	
	pp_vka1	1.641495e-02	1.580767e-03	1.411553e-02	5.243871e-04	
	strk	1.809544e+01	1.847978e+00	3.201253e+01	1.023446e+00	
	welflux	3.198862e+01	1.691162e+02	1.998213e+01	3.606368e+02	
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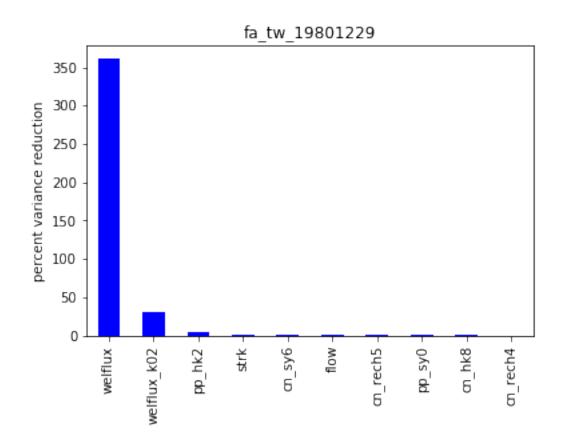
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                                          1.871559e-03
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                                                                       6.275140e+00
cn hk7
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                                          1.334577e-05
                                                                 NaN
                                                                      6.555697e-04
cn hk8
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                                          2.954897e+00
                                                                 NaN
                                                                       3.906228e+00
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                                         -1.295851e-13
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                                                                      3.857006e-04
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                                                                 NaN
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                                          1.295851e-13
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pp_ss2
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                                          1.780119e-01
                                                                 NaN
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                    5.857188e-01
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                                                                      2.361491e-01
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```

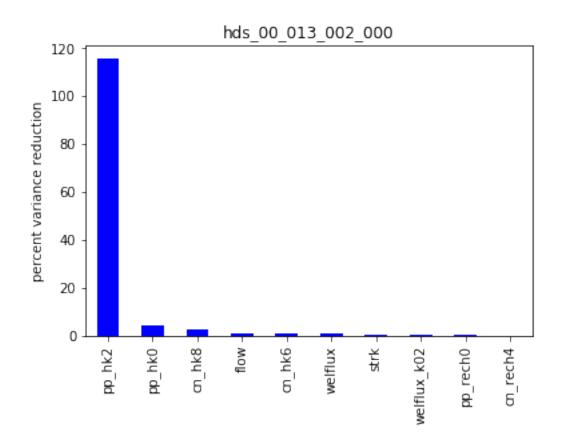
ax.set_ylabel("percent variance reduction")
plt.show()

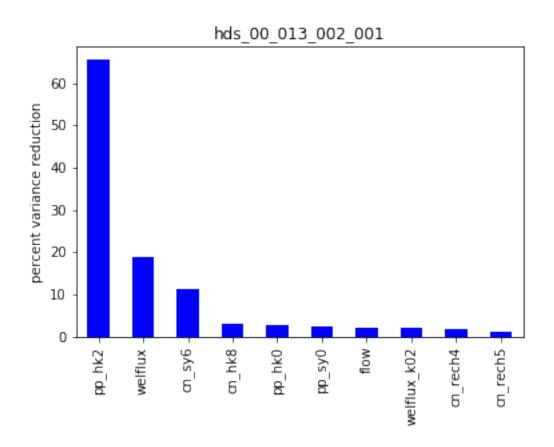


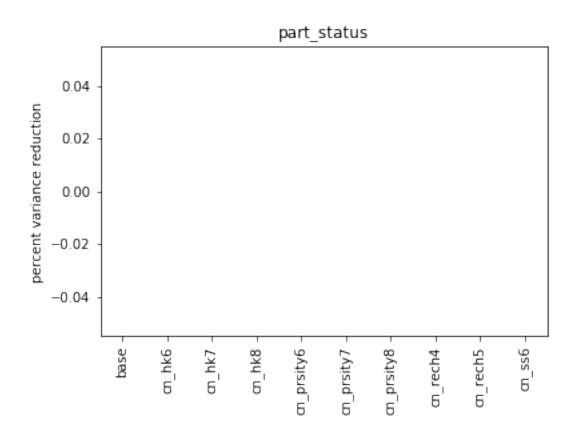


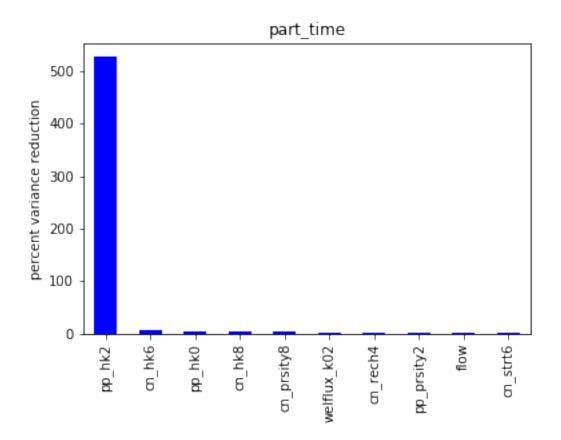












1.1.2 Data worth

1.1.3 what is the worth of existing observations?

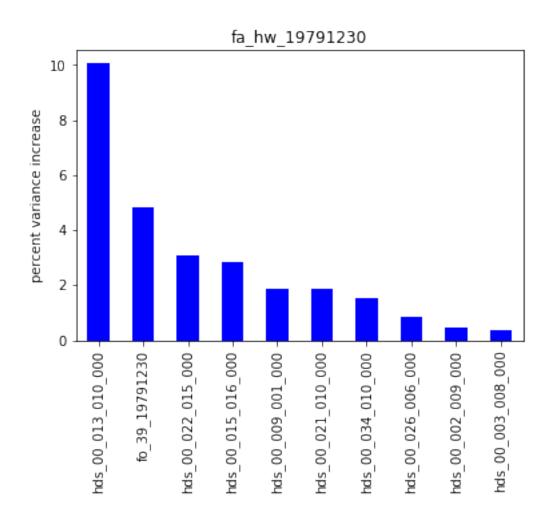
What is happening under the hood is that we are recalculating the Schur complement without some of the observations to see how the posterior forecast uncertainty increases (wrt a "base" condition in which we have all observation data available).

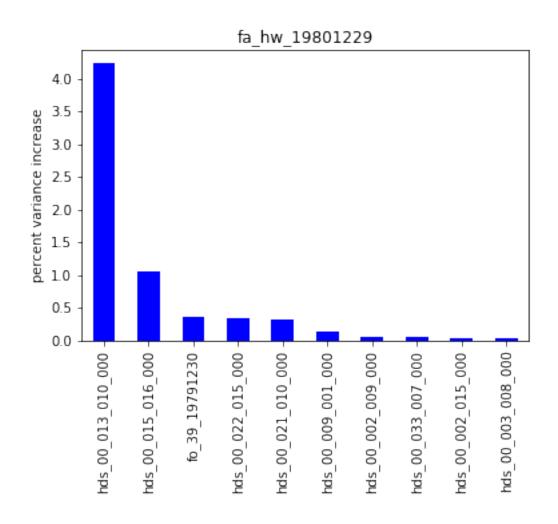
```
In [22]: dw_rm = sc.get_removed_obs_importance()
         dw_rm.head()
Out [22]:
                              fa_hw_19791230
                                              fa_hw_19801229
                                                               fa_tw_19791230
         base
                                48708.787021
                                               277258.059336
                                                                 22609.793588
         fo_39_19791230
                                51191.377140
                                               278273.504686
                                                                 23178.615771
         hds_00_002_009_000
                                48940.420250
                                               277387.232706
                                                                 22615.754525
         hds_00_002_015_000
                                48743.445105
                                               277373.413424
                                                                 22616.617273
         hds_00_003_008_000
                                48880.074463
                                               277344.626609
                                                                 22610.161149
                                              hds_00_013_002_000
                                                                   hds_00_013_002_001
                              fa_tw_19801229
         base
                               220463.794436
                                                         0.111608
                                                                              0.192769
         fo_39_19791230
                               220465.341686
                                                         0.111749
                                                                              0.193247
         hds_00_002_009_000
                               220464.858302
                                                                              0.192831
                                                         0.111696
```

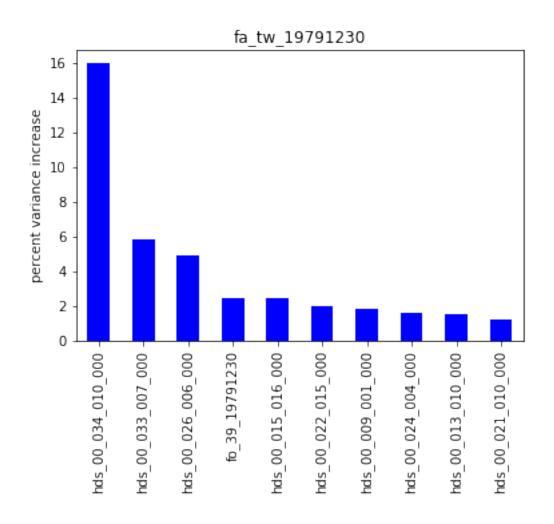
```
hds_00_002_015_000
                     220464.501038
                                              0.111613
                                                                   0.192769
hds_00_003_008_000
                                                                   0.192926
                     220463.889982
                                              0.111804
                    part_status
                                    part_time
base
                            0.0 93226.847888
fo_39_19791230
                            0.0 93298.497985
hds_00_002_009_000
                            0.0 93388.870852
hds_00_002_015_000
                            0.0 93253.399795
hds_00_003_008_000
                            0.0 94604.086151
```

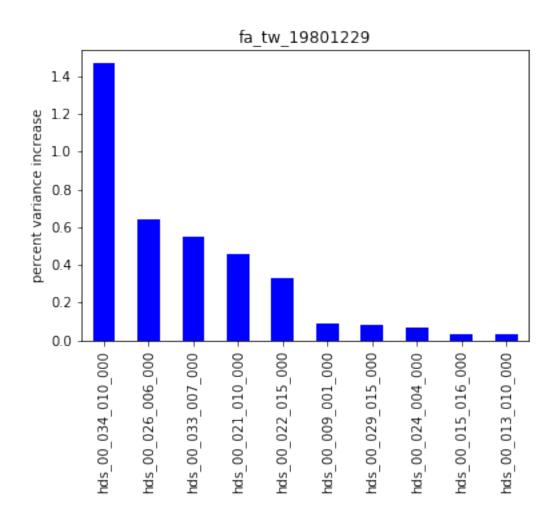
Here the base row contains the results of the Schur complement calculation (in terms of forecast uncertainty variance) using all observations.

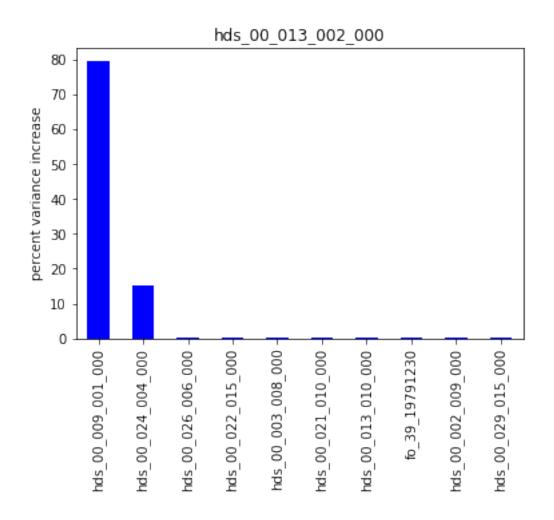
```
In [23]: # let's normalize to make more meaningful comparisons of data worth (unctainty varian
         base = dw_rm.loc["base",:]
         dw_rm = 100 * (dw_rm - base) / dw_rm
         dw_rm.head()
Out [23]:
                             fa_hw_19791230
                                              fa_hw_19801229
                                                              fa_tw_19791230 \
         base
                                   0.000000
                                                    0.000000
                                                                    0.000000
         fo_39_19791230
                                   4.849626
                                                    0.364909
                                                                    2.454082
         hds_00_002_009_000
                                   0.473296
                                                    0.046568
                                                                    0.026357
         hds_00_002_015_000
                                   0.071103
                                                    0.041588
                                                                    0.030171
         hds_00_003_008_000
                                   0.350424
                                                    0.031213
                                                                    0.001626
                             fa_tw_19801229 hds_00_013_002_000 hds_00_013_002_001 \
         base
                                   0.000000
                                                        0.000000
                                                                             0.000000
         fo 39 19791230
                                   0.000702
                                                        0.126100
                                                                             0.247304
         hds_00_002_009_000
                                   0.000483
                                                        0.078499
                                                                             0.031874
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                                                        0.004694
                                                                             0.000123
         hds_00_003_008_000
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                                                        0.175625
                                                                            0.081108
                             part_status
                                           part_time
         base
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                                      NaN
         fo_39_19791230
                                     NaN
                                            0.076797
         hds_00_002_009_000
                                      NaN
                                            0.173493
         hds_00_002_015_000
                                     NaN
                                            0.028473
         hds_00_003_008_000
                                     NaN
                                            1.455792
In [24]: for forecast in dw_rm.columns:
             fore_df = dw_rm.loc[:,forecast].copy()
             fore_df.sort_values(inplace=True, ascending=False)
             ax = fore_df.iloc[:10].plot(kind="bar",color="b")
             ax.set title(forecast)
             ax.set_ylabel("percent variance increase")
             plt.show()
```

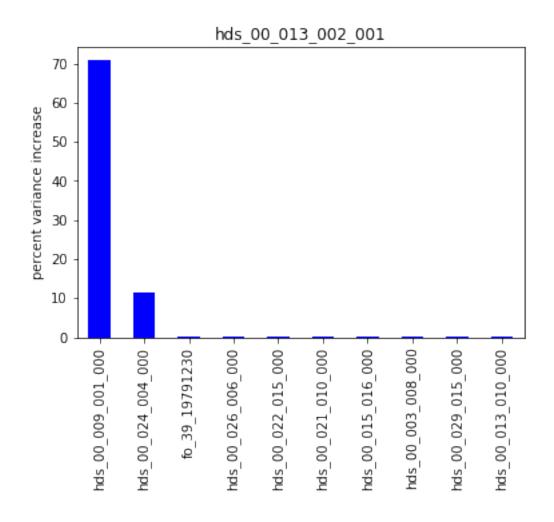


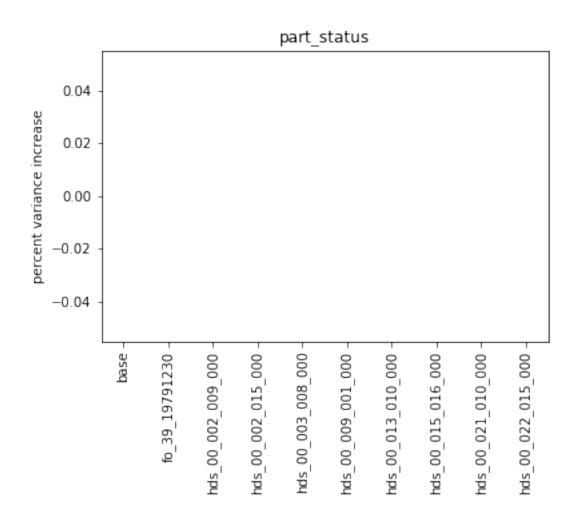


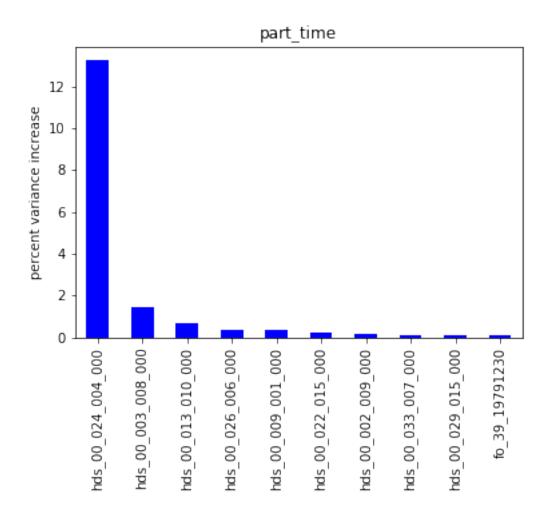






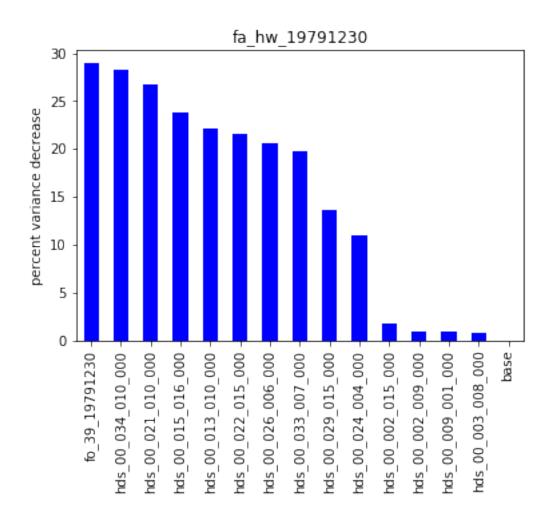


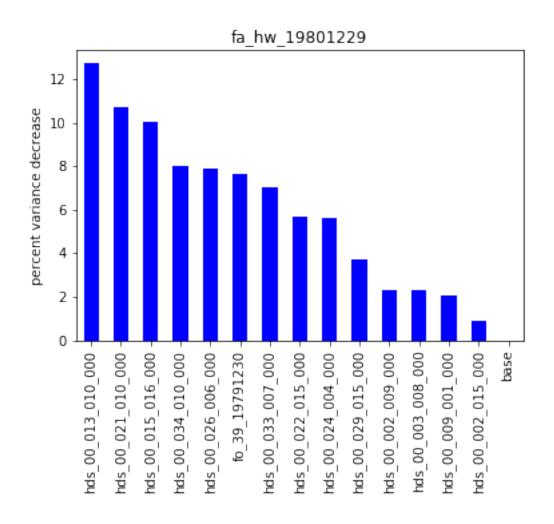


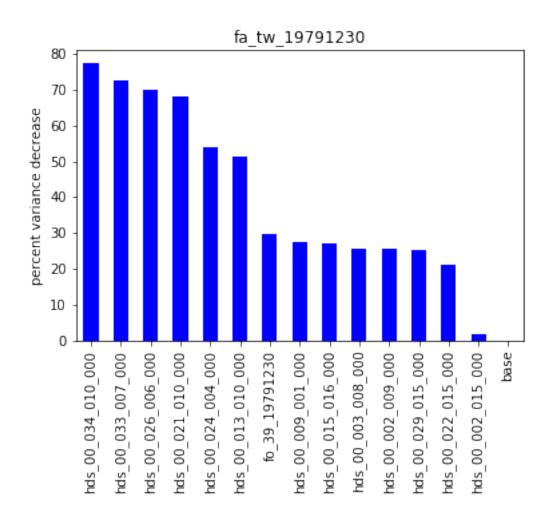


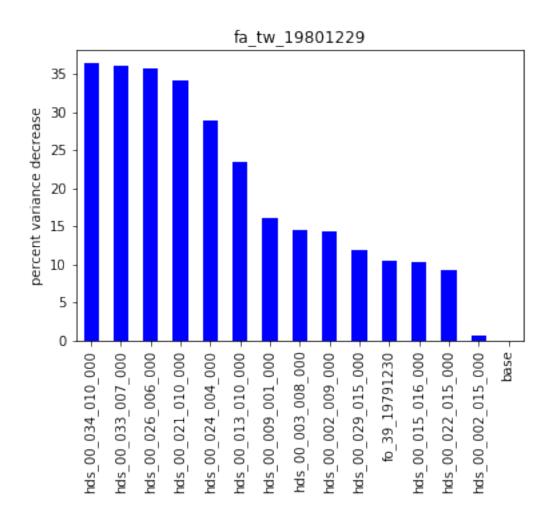
There is also an option to calculate the worth of observations by taking a "base" condition of zero observation (i.e., a priori) and calculating the reduction in uncertainty through adding observations to the dataset.

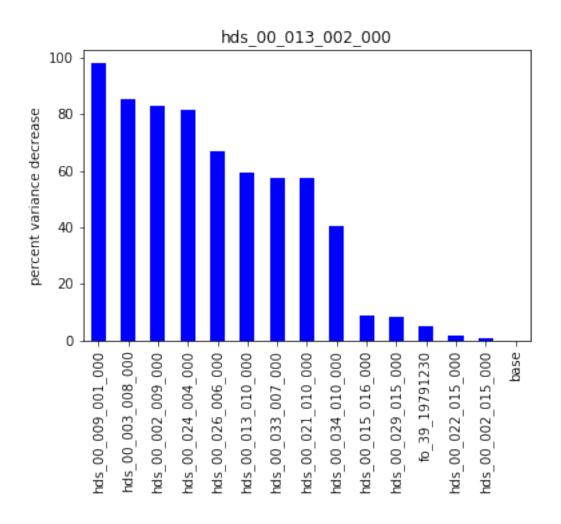
```
In [25]: dw_ad = sc.get_added_obs_importance()
    base = dw_ad.loc["base",:]
    dw_ad = 100 * (base - dw_ad) / base
    for forecast in dw_ad.columns:
        fore_df_ad = dw_ad.loc[:,forecast].copy()
        fore_df_ad.sort_values(inplace=True, ascending=False)
        ax = fore_df_ad.iloc[:20].plot(kind="bar",color="b")
        ax.set_title(forecast)
        ax.set_ylabel("percent variance decrease")
        plt.show()
```

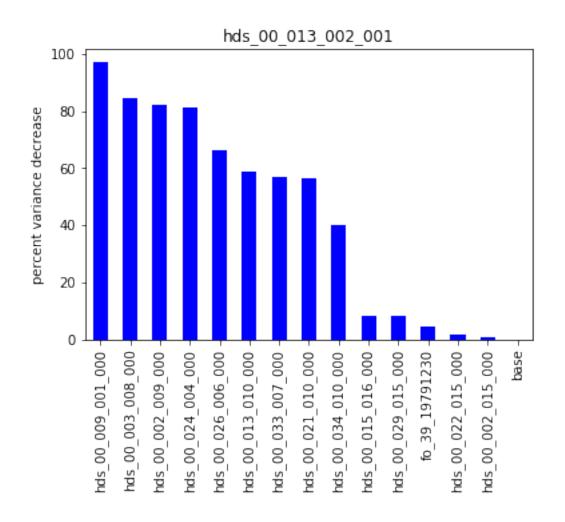


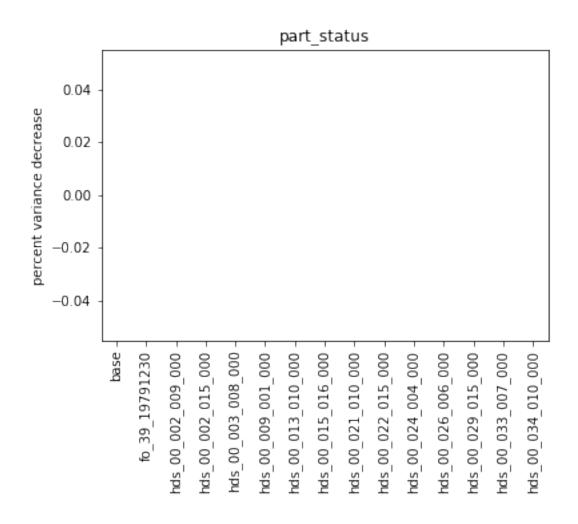


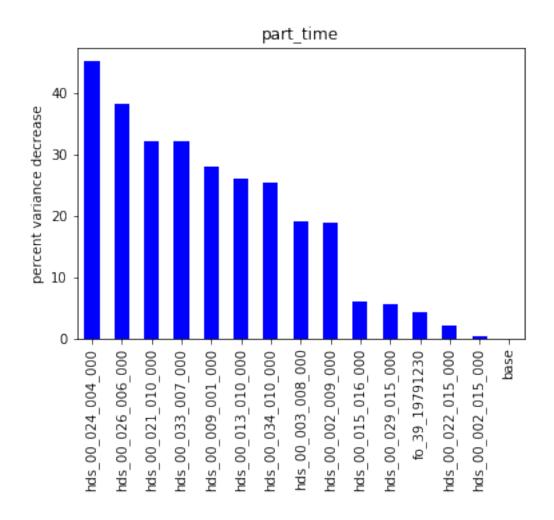












Do these two approaches give the same answer? They shouldn't.. Why? Let's discuss..

1.1.4 what is the worth of potential observations? what data should we collect?

Recall we are "carrying" cell-by-cell heads, reach-based sfr flows, etc..

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```

We can therefore repeat above analysis for the observations that currently have zero weight by turning those observations "on".

Beware: calculating the Schur complement for all potential observation types and locations could take some time!! So we will sample to speed things up. You may need to further reduce the number of potential obs - you can do this by adding [0::2] to take every second element for example.

```
df_worth_new = sc.get_added_obs_importance(obslist_dict=new_obs, base_obslist=sc.pst.:
        print("took:",datetime.now() - start)
took: 0:02:46.098102
In [29]: df_worth_new.head()
Out [29]:
                            fa_hw_19791230 fa_hw_19801229 fa_tw_19791230 \
        base
                              48708.787021 277258.059336
                                                              22609.793588
        hds_00_000_000_000
                              48680.325274
                                             277236.472932
                                                              22609.717448
        hds_00_000_000_001
                              48676.577443 275221.256112
                                                              22608.768505
        hds_00_000_001_000
                              48681.561424 277236.427929
                                                              22609.645559
                                             275165.006823
        hds_00_000_001_001
                              48678.434575
                                                              22608.968020
                            fa_tw_19801229 hds_00_013_002_000 hds_00_013_002_001 \
                             220463.794436
                                                      0.111608
                                                                          0.192769
        base
        hds_00_000_000_000
                             220463.630209
                                                      0.111602
                                                                          0.192745
        hds_00_000_000_001
                             218435.629344
                                                      0.111608
                                                                          0.191419
        hds_00_000_001_000
                             220463.643286
                                                      0.111598
                                                                          0.192738
        hds_00_000_001_001
                             218391.377944
                                                      0.111607
                                                                          0.191471
                            part_status
                                            part_time
        base
                                    0.0 93226.847888
        hds_00_000_000_000
                                    0.0 91552.821262
        hds_00_000_000_001
                                    0.0 91946.009838
        hds_00_000_001_000
                                    0.0 91612.117694
        hds_00_000_001_001
                                    0.0 91987.119582
```

1.1.5 nice! now let's process a little bit and make some plots of (potential) data worth

```
In [30]: def worth_plot_prep(df):
    # some processing
    df_new_base = df.loc["base",:].copy() # "base" row
    df_new_imax = df.apply(lambda x: df_new_base - x, axis=1).idxmax() # obs with la
    df_new_worth = 100.0 * (df.apply(lambda x: df_new_base - x, axis=1) / df_new_base

# plot prep
    df_new_worth_plot = df_new_worth[df_new_worth.index != 'base'].copy()
    df_new_worth_plot.loc[:,'names'] = df_new_worth_plot.index
    names = df_new_worth_plot.names
    df_new_worth_plot.loc[:,"i"] = names.apply(lambda x: int(x[8:10]))
    df_new_worth_plot.loc[:,"j"] = names.apply(lambda x: int(x[11:14]))
    df_new_worth_plot.loc[:,'kper'] = names.apply(lambda x: int(x[-3:]))
    #df_new_worth_plot.head()

    return df_new_worth_plot, df_new_imax
In [31]: df_worth_new_plot, df_worth_new_imax = worth_plot_prep(df_worth_new)
```

```
Out [32]:
                                              fa_hw_19801229 fa_tw_19791230
                              fa_hw_19791230
         hds_00_000_000_000
                                                                     0.000337
                                    0.058432
                                                     0.007786
         hds_00_000_000_001
                                    0.066127
                                                     0.734624
                                                                     0.004534
         hds_00_000_001_000
                                    0.055895
                                                     0.007802
                                                                     0.000655
         hds_00_000_001_001
                                    0.062314
                                                     0.754911
                                                                     0.003651
         hds_00_000_002_000
                                    0.055161
                                                     0.007937
                                                                     0.000654
                                              hds_00_013_002_000 hds_00_013_002_001
                              fa_tw_19801229
         hds_00_000_000_000
                                                         0.005094
                                    0.000074
                                                                              0.012494
         hds 00 000 000 001
                                                         0.000115
                                                                              0.700256
                                    0.919954
         hds_00_000_001_000
                                    0.000069
                                                         0.009101
                                                                              0.016127
         hds_00_000_001_001
                                    0.940026
                                                         0.001312
                                                                              0.673578
         hds_00_000_002_000
                                    0.000066
                                                         0.018307
                                                                              0.022293
                              part_status
                                           part_time
                                                                               j
                                                                                  kper
                                                                    names
         hds_00_000_000_000
                                      NaN
                                            1.795649
                                                       hds_00_000_000_000
                                                                           0
                                                                               0
                                                                                     0
         hds_00_000_000_001
                                                       hds_00_000_000_001
                                            1.373894
                                                                            0
                                                                               0
                                                                                     1
                                      \mathtt{NaN}
         hds_00_000_001_000
                                            1.732044
                                                       hds_00_000_001_000
                                                                                     0
                                      NaN
         hds_00_000_001_001
                                      NaN
                                            1.329798
                                                       hds_00_000_001_001
                                                                            0
                                                                               1
                                                                                     1
         hds_00_000_002_000
                                      NaN
                                            1.577571
                                                       hds_00_000_002_000
                                                                                     0
In [33]: df_worth_new_imax # which obs causes largest unc var reduction?
Out[33]: fa_hw_19791230
                                hds_00_009_016_001
         fa_hw_19801229
                                hds_00_011_013_001
                                hds_00_020_014_001
         fa_tw_19791230
         fa_tw_19801229
                                hds_00_026_010_001
         hds_00_013_002_000
                                hds_00_016_001_001
         hds_00_013_002_001
                                hds_00_017_002_001
         part_status
                                              base
                                hds_00_017_002_001
         part_time
         dtype: object
In [34]: df_worth_new_plot.drop(axis=1,labels=["part_status"],inplace=True) # drop "part_statu
         df worth new plot.head()
Out [34]:
                              fa_hw_19791230
                                              fa_hw_19801229
                                                              fa_tw_19791230
         hds_00_000_000_000
                                    0.058432
                                                     0.007786
                                                                     0.000337
         hds_00_000_000_001
                                    0.066127
                                                     0.734624
                                                                     0.004534
         hds_00_000_001_000
                                    0.055895
                                                     0.007802
                                                                     0.000655
         hds_00_000_001_001
                                    0.062314
                                                     0.754911
                                                                     0.003651
         hds_00_000_002_000
                                    0.055161
                                                     0.007937
                                                                     0.000654
                                              hds_00_013_002_000 hds_00_013_002_001
                              fa_tw_19801229
         hds_00_000_000_000
                                    0.000074
                                                         0.005094
                                                                              0.012494
         hds_00_000_000_001
                                    0.919954
                                                         0.000115
                                                                              0.700256
         hds_00_000_001_000
                                    0.000069
                                                         0.009101
                                                                              0.016127
```

In [32]: df_worth_new_plot.head()

```
0.000066
                                                       0.018307
                                                                           0.022293
        hds_00_000_002_000
                             part_time
                                                     names i j
                                                                  kper
                              1.795649 hds 00 000 000 000 0
        hds 00 000 000 000
                                                              0
                                                                     0
                              1.373894 hds 00 000 000 001 0
        hds_00_000_000_001
        hds 00 000 001 000
                              1.732044 hds 00 000 001 000 0 1
                                                                     0
        hds_00_000_001_001
                              1.329798 hds_00_000_001_001 0 1
                                                                     1
                              1.577571 hds 00 000 002 000 0 2
        hds_00_000_002_000
1.1.6 plotting
In [35]: m = flopy.modflow.Modflow.load("freyberg.nam", model_ws=os.path.join(m_d))
In [36]: def plot_added importance(df_worth_plot, ml, forecast_name=None,
                                   newlox=None,):
             vmax = df worth plot[forecast name].max()
             fig, axs = plt.subplots(1,2)
             if newlox:
                 currx = []
                 curry = []
                 for i,clox in enumerate(newlox):
                     crow = int(clox[8:10])
                     ccol = int(clox[11:14])
                     currx.append(ml.sr.xcentergrid[crow,ccol])
                     curry.append(ml.sr.ycentergrid[crow,ccol])
             for sp,ax in enumerate(axs): # by kpers
                 unc_array = np.zeros_like(ml.upw.hk[0].array) - 1
                 df_worth_csp = df_worth_plot.groupby('kper').get_group(sp)
                 for i,j,unc in zip(df_worth_csp.i,df_worth_csp.j,
                                    df_worth_csp[forecast_name]):
                     unc_array[i,j] = unc
                 unc_array[unc_array == -1] = np.NaN
                 cb = ax.imshow(unc_array,interpolation="nearest",
                                alpha=0.5, extent=ml.sr.get_extent(),
                                vmin=0, vmax=vmax)
                 if sp==1:
                     plt.colorbar(cb,label="percent uncertainty reduction")
                 # plot sfr
                 sfr_data = ml.sfr.stress_period_data[0]
                 sfr_x = ml.sr.xcentergrid[sfr_data["i"],sfr_data["j"]]
                 sfr_y = ml.sr.ycentergrid[sfr_data["i"],sfr_data["j"]]
                 for (x,y) in zip(sfr_x,sfr_y):
                     ax.scatter([x],[y],marker="s",color="g",s=26)
```

0.940026

0.001312

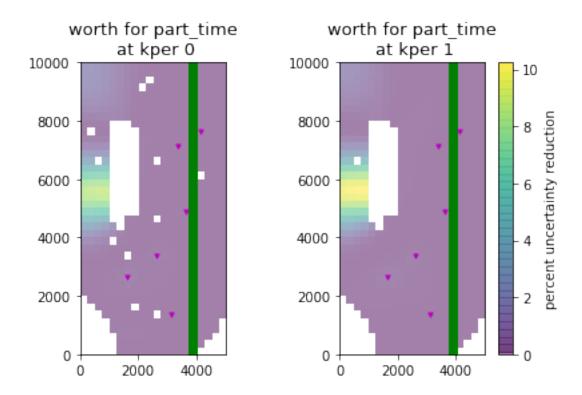
0.673578

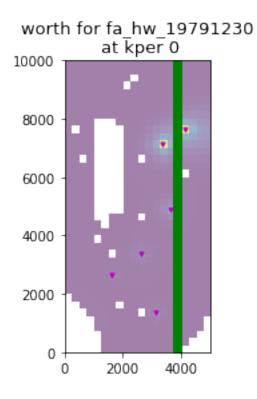
hds_00_000_001_001

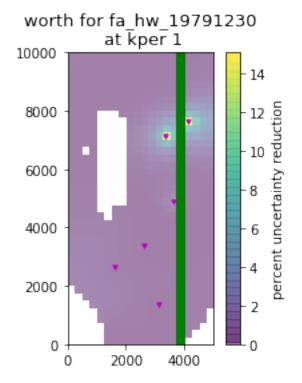
```
wel_x = ml.sr.xcentergrid[wel_data["i"], wel_data["j"]]
                 wel_y = ml.sr.ycentergrid[wel_data["i"],wel_data["j"]]
                 for w,(x,y) in enumerate(zip(wel_x,wel_y)):
                     ax.scatter([x],[y],marker="v",color="m",s=10)
                 if newlox:
                     for nl,(cx,cy,cobs) in enumerate(zip(currx, curry, newlox)):
                         csp = int(cobs[-1])
                         if csp == sp:
                             ax.plot(cx, cy, 'rd', mfc=None, ms=10, alpha=0.8)
                             ax.text(cx-50,cy-50, nl, size=10)
                 # plot the location of the forecast if possible
                 if forecast_name.startswith('hds'):
                     i = int(forecast_name[8:10])
                     j = int(forecast_name[11:14])
                     forecast_x = ml.sr.xcentergrid[i,j]
                     forecast_y = ml.sr.ycentergrid[i,j]
                     ax.scatter(forecast_x, forecast_y, marker='o', s=600, alpha=0.5)
                 ax.set_title("worth for {0}\n at kper {1}".format(forecast_name,sp), fontsize:
                 plt.tight_layout()
             return fig
In [37]: fig = plot_added_importance(df_worth_plot=df_worth_new_plot, ml=m,forecast_name="part")
```

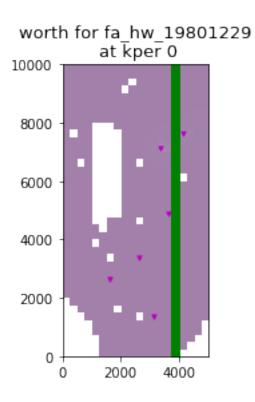
plot the pumping wells

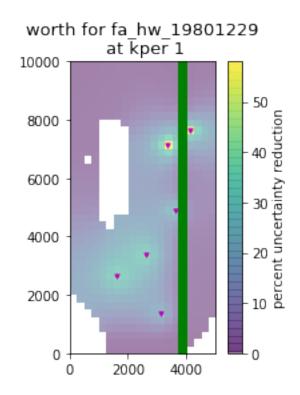
wel_data = ml.wel.stress_period_data[0]

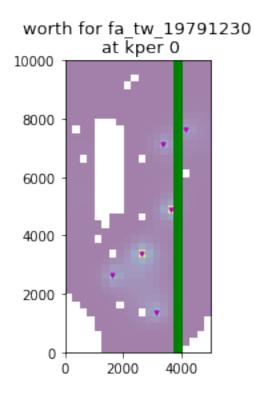


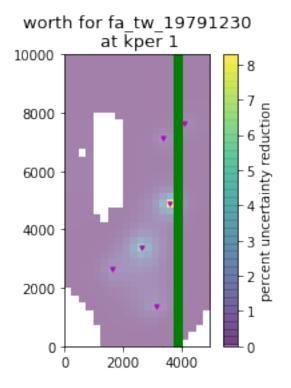


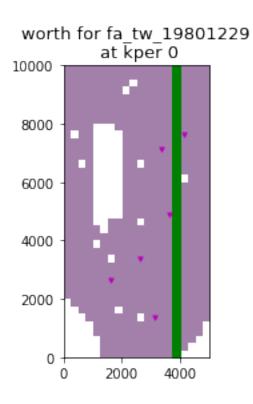


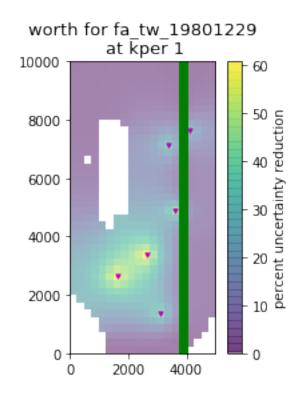


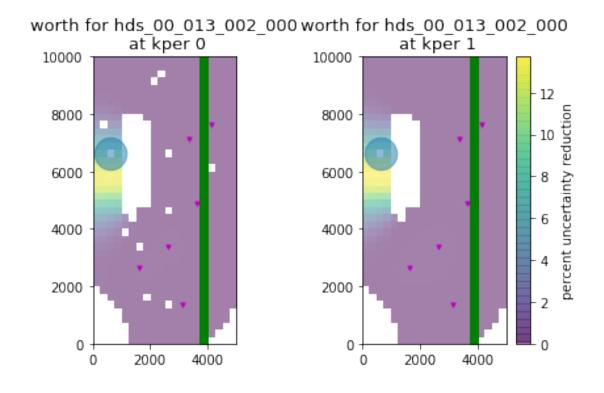


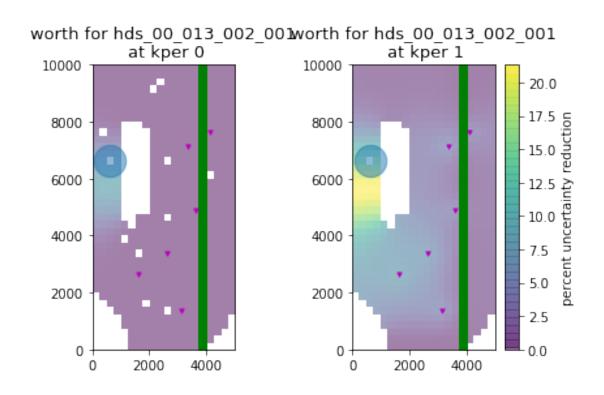


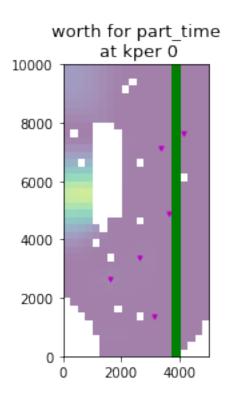


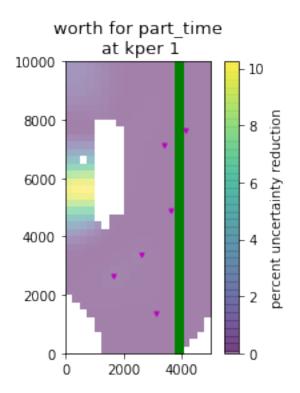












1.2 the "next best" observation

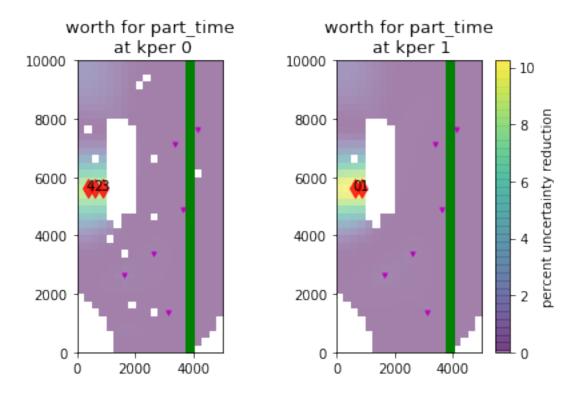
This is what we would ultimately like to know... Takes into account what we already know through incrementally making additional observations. For example, consider making an observation in the middle of the zone of highest worth. Where should we subsequently collect data?

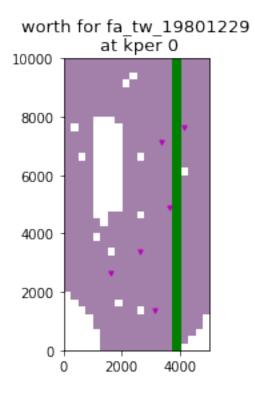
Let's just use the same potential observation list for now (the head in every top-layer cell) and evaluate which ones to collect, if we only had the budget for 5, in the context of the particle travel time prediction.

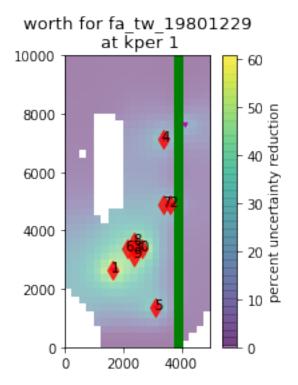
```
In [39]: start = datetime.now()
         next_most_df = sc.next_most_important_added_obs(forecast='part_time',niter=5,obslist_
                                                          base_obslist=sc.pst.nnz_obs_names,res
         print("took:",datetime.now() - start)
took: 0:11:08.660878
In [40]: next_most_df
Out [40]:
                                       best_obs
                                                 part_time_variance
         hds_00_017_002_001 hds_00_017_002_001
                                                        83678.784373
         hds_00_017_003_001
                             hds_00_017_003_001
                                                        78000.012459
         hds_00_017_002_000
                             hds_00_017_002_000
                                                        73651.906388
         hds_00_017_003_000 hds_00_017_003_000
                                                        70311.969583
```

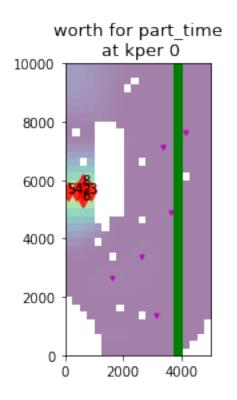
hds 00 017 001 000	hds 00 017 001 000	67685.623078

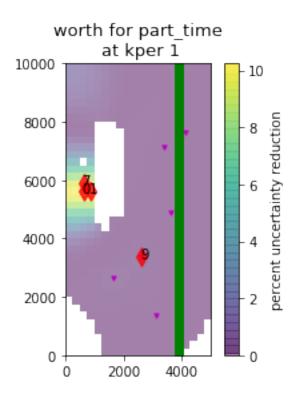
	unc_reduce_iter_base	unc_reduce_initial_base
hds_00_017_002_001	10.241753	10.241753
hds_00_017_003_001	6.786394	16.333101
hds_00_017_002_000	5.574494	20.997108
hds_00_017_003_000	4.534759	24.579699
hds_00_017_001_000	3.735277	27.396856









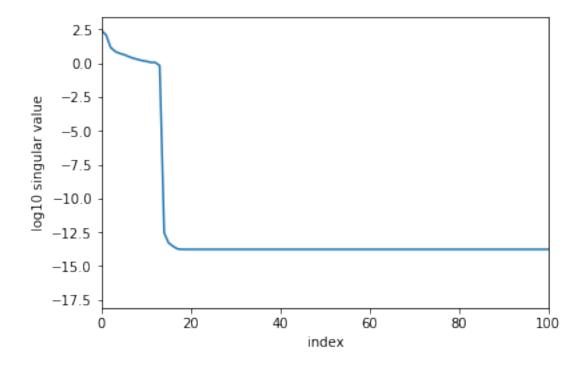


1.2.1 Note: an important assumption underpinning the above is that the model is able to fit observations to a level that is commensurate with measurement noise... Are we comfortable with this assumption? We will discuss this more in pestpp-glm_part2.ipynb

```
In [43]: # recall...
         pst.observation_data.loc[pst.nnz_obs_names,:]
Out [43]:
                                         obsnme
                                                        obsval weight
                                                                         obgnme extra
         obsnme
         fo_39_19791230
                                 fo 39 19791230
                                                                  0.01 calflux
                                                 11979.405235
                                                                                   NaN
         hds_00_002_009_000
                             hds_00_002_009_000
                                                    37.485633
                                                                  4.00 calhead
                                                                                   NaN
         hds_00_002_015_000
                             hds_00_002_015_000
                                                                  4.00 calhead
                                                                                   NaN
                                                    35.439932
         hds_00_003_008_000
                             hds_00_003_008_000
                                                                  4.00 calhead
                                                    38.297646
                                                                                   NaN
                                                                  4.00 calhead
         hds_00_009_001_000
                             hds_00_009_001_000
                                                    41.398610
                                                                                   NaN
         hds_00_013_010_000
                             hds_00_013_010_000
                                                    35.670433
                                                                  4.00 calhead
                                                                                   NaN
                                                                  4.00 calhead
         hds_00_015_016_000
                             hds_00_015_016_000
                                                    35.184689
                                                                                   NaN
         hds_00_021_010_000
                             hds_00_021_010_000
                                                                  4.00 calhead
                                                    35.792243
                                                                                   NaN
                                                                  4.00 calhead
         hds_00_022_015_000
                             hds_00_022_015_000
                                                    34.595529
                                                                                   NaN
                                                                  4.00 calhead
         hds 00 024 004 000
                             hds 00 024 004 000
                                                                                   NaN
                                                    37.360729
         hds 00 026 006 000
                             hds_00_026_006_000
                                                    36.482048
                                                                  4.00 calhead
                                                                                   NaN
                                                                  4.00 calhead
         hds_00_029_015_000
                             hds 00 029 015 000
                                                    34.903695
                                                                                   NaN
         hds_00_033_007_000
                             hds_00_033_007_000
                                                                  4.00 calhead
                                                                                   NaN
                                                    35.583158
         hds_00_034_010_000
                             hds_00_034_010_000
                                                                  4.00 calhead
                                                                                   NaN
                                                    34.610165
```

1.2.2 an "extra" if we have time: parameter identifiability

```
In [44]: la = pyemu.ErrVar(jco=jco)
In [45]: s = la.qhalfx.s # singular spectrum
         s.x[:10]
Out [45]: array([[258.05273352],
                [121.52704432],
                [ 14.808986 ],
                   7.51386804],
                5.34060963],
                   4.31992965],
                  3.13423815],
                   2.35873769],
                   1.90481097],
                  1.56222005]])
In [46]: figure = plt.figure()
         ax = plt.subplot(111)
         ax.plot(np.log10(s.x))
         ax.set_ylabel("log10 singular value")
         ax.set_xlabel("index")
         ax.set_xlim(0,100)
         plt.show()
```



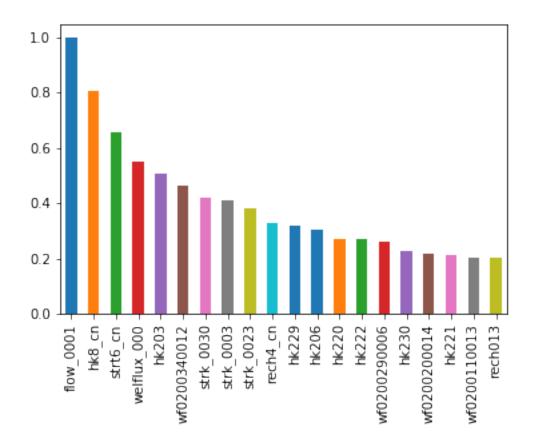
As expected, singluar spectrum decays rapidly.

Out[47]: 14

This means that, on the basis of the 14 (non-zero) weighted observations, there are 14 unique

Now let's compute the identifiability of actual model parameters based on these singular vectors. Identifiability ranges from 0 (not identified by the data) to 1 (full identified by the data).

```
In [49]: ident_df = la.get_identifiability_dataframe() # sing val trunc defaults to pst.nnz_o
In [50]: ident_df.sort_values(by="ident",ascending=False).iloc[0:20].loc[:,"ident"].plot(kind=
Out[50]: <matplotlib.axes._subplots.AxesSubplot at 0x1b50bc41518>
```



Note similarity with some of the earlier parameter contribution to forecast uncertainty results

Out[51]:		pest_css	hill_css
	dc0000390005	0.000357	0.0
	dc0000390006	0.000357	0.0
	dc0000390007	0.000437	0.0
	dc0000390008	0.000437	0.0
	dc0000390009	0.000437	0.0

In [52]: css.sort_values(by="pest_css",ascending=False)

Out[52]:		pest_css	hill_css
	flow_0001	16.373237	0.0
	strt6_cn	9.475158	0.0
	rech4_cn	6.472873	0.0
	hk8_cn	3.219146	0.0
	welflux_000	1.546175	0.0
	hk6_cn	0.596127	0.0
	rech008	0.473190	0.0

wf0200290006	0.441978	0.0
rech004	0.436865	0.0
rech000	0.409430	0.0
rech011	0.409349	0.0
rech001	0.373742	0.0
rech014	0.350733	0.0
hk202	0.343158	0.0
rech017	0.342363	0.0
wf0200260010	0.324295	0.0
rech021	0.322725	0.0
rech005	0.311130	0.0
rech002	0.310894	0.0
hk229	0.301903	0.0
hk203	0.297866	0.0
rech025	0.285918	0.0
hk206	0.284214	0.0
rech022	0.283196	0.0
hk230	0.251524	0.0
rech029	0.251069	0.0
rech018	0.248949	0.0
rech026	0.246733	0.0
wf0200340012	0.246151	0.0
rech006	0.240714	0.0
• • •		
ss128	0.000000	0.0
ss126	0.000000	0.0
ss224	0.000000	0.0
ss125	0.000000	0.0
ss124	0.000000	0.0
ss123	0.000000	0.0
ss122	0.000000	0.0
ss121	0.000000	0.0
ss120	0.000000	0.0
ss119	0.000000	0.0
ss203	0.000000	0.0
ss204	0.000000	0.0
ss205	0.000000	0.0
ss206	0.000000	0.0
ss223	0.000000	0.0
ss222	0.000000	0.0
ss221	0.000000	0.0
ss220	0.000000	0.0
ss219	0.000000	0.0
ss218	0.000000	0.0
ss217	0.000000	0.0
ss216	0.000000	0.0
ss215	0.000000	0.0
ss214	0.000000	0.0
-		- • •

ss213	0.000000	0.0
ss212	0.000000	0.0
ss210	0.000000	0.0
ss209	0.000000	0.0
ss207	0.000000	0.0
ss020	0.000000	0.0

[527 rows x 2 columns]