

pestpp-opt

May 11, 2019

1 Run PESTPP-OPT

In this notebook we will setup and solve a mgmt optimization problem around how much ground-water can be pumped while maintaining sw-gw exchange

```
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_opt"
```

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

```
Out[3]:
```

	type	transform	count	initial value \
cn_hk6	cn_hk6	log	1	0
cn_hk7	cn_hk7	log	1	0
cn_hk8	cn_hk8	log	1	0
cn_prsity6	cn_prsity6	log	1	0
cn_prsity7	cn_prsity7	log	1	0
cn_prsity8	cn_prsity8	log	1	0
cn_rech4	cn_rech4	log	1	0
cn_rech5	cn_rech5	log	1	-0.39794
cn_ss6	cn_ss6	log	1	0
cn_ss7	cn_ss7	log	1	0
cn_ss8	cn_ss8	log	1	0
cn_strt6	cn_strt6	log	1	0

cn_strt7	cn_strt7	log	1	0
cn_strt8	cn_strt8	log	1	0
cn_sy6	cn_sy6	log	1	0
cn_sy7	cn_sy7	log	1	0
cn_sy8	cn_sy8	log	1	0
cn_vka6	cn_vka6	log	1	0
cn_vka7	cn_vka7	log	1	0
cn_vka8	cn_vka8	log	1	0
drncond_k00	drncond_k00	log	10	0
flow	flow	log	1	0
gr_hk3	gr_hk3	log	705	0
gr_hk4	gr_hk4	log	705	0
gr_hk5	gr_hk5	log	705	0
gr_prsity3	gr_prsity3	log	705	0
gr_prsity4	gr_prsity4	log	705	0
gr_prsity5	gr_prsity5	log	705	0
gr_rech2	gr_rech2	log	705	0
gr_rech3	gr_rech3	log	705	0
...
gr_strt5	gr_strt5	log	705	0
gr_sy3	gr_sy3	log	705	0
gr_sy4	gr_sy4	log	705	0
gr_sy5	gr_sy5	log	705	0
gr_vka3	gr_vka3	log	705	0
gr_vka4	gr_vka4	log	705	0
gr_vka5	gr_vka5	log	705	0
pp_hk0	pp_hk0	log	32	0
pp_hk1	pp_hk1	log	32	0
pp_hk2	pp_hk2	log	32	0
pp_prsity0	pp_prsity0	log	32	0
pp_prsity1	pp_prsity1	log	32	0
pp_prsity2	pp_prsity2	log	32	0
pp_rech0	pp_rech0	log	32	0
pp_rech1	pp_rech1	log	32	0
pp_ss0	pp_ss0	log	32	0
pp_ss1	pp_ss1	log	32	0
pp_ss2	pp_ss2	log	32	0
pp_strt0	pp_strt0	log	32	0
pp_strt1	pp_strt1	log	32	0
pp_strt2	pp_strt2	log	32	0
pp_sy0	pp_sy0	log	32	0
pp_sy1	pp_sy1	log	32	0
pp_sy2	pp_sy2	log	32	0
pp_vka0	pp_vka0	log	32	0
pp_vka1	pp_vka1	log	32	0
pp_vka2	pp_vka2	log	32	0
strk	strk	log	40	0
welflux	welflux	log	2	0 to 0.176091

welflux_k02	welflux_k02	log	6	0
	upper bound	lower bound	standard deviation	
cn_hk6	1	-1	0.5	
cn_hk7	1	-1	0.5	
cn_hk8	1	-1	0.5	
cn_prsity6	0.176091	-0.30103	0.11928	
cn_prsity7	0.176091	-0.30103	0.11928	
cn_prsity8	0.176091	-0.30103	0.11928	
cn_rech4	0.0791812	-0.09691	0.0440228	
cn_rech5	-0.09691	-1	0.225772	
cn_ss6	1	-1	0.5	
cn_ss7	1	-1	0.5	
cn_ss8	1	-1	0.5	
cn_strt6	0.0211893	-0.0222764	0.0108664	
cn_strt7	0.0211893	-0.0222764	0.0108664	
cn_strt8	0.0211893	-0.0222764	0.0108664	
cn_sy6	0.243038	-0.60206	0.211275	
cn_sy7	0.243038	-0.60206	0.211275	
cn_sy8	0.243038	-0.60206	0.211275	
cn_vka6	1	-1	0.5	
cn_vka7	1	-1	0.5	
cn_vka8	1	-1	0.5	
drncond_k00	1	-1	0.5	
flow	0.09691	-0.124939	0.0554622	
gr_hk3	1	-1	0.5	
gr_hk4	1	-1	0.5	
gr_hk5	1	-1	0.5	
gr_prsity3	0.176091	-0.30103	0.11928	
gr_prsity4	0.176091	-0.30103	0.11928	
gr_prsity5	0.176091	-0.30103	0.11928	
gr_rech2	0.0413927	-0.0457575	0.0217875	
gr_rech3	0.0413927	-0.0457575	0.0217875	
...	
gr_strt5	0.0211893	-0.0222764	0.0108664	
gr_sy3	0.243038	-0.60206	0.211275	
gr_sy4	0.243038	-0.60206	0.211275	
gr_sy5	0.243038	-0.60206	0.211275	
gr_vka3	1	-1	0.5	
gr_vka4	1	-1	0.5	
gr_vka5	1	-1	0.5	
pp_hk0	1	-1	0.5	
pp_hk1	1	-1	0.5	
pp_hk2	1	-1	0.5	
pp_prsity0	0.176091	-0.30103	0.11928	
pp_prsity1	0.176091	-0.30103	0.11928	
pp_prsity2	0.176091	-0.30103	0.11928	
pp_rech0	0.0413927	-0.0457575	0.0217875	

pp_rech1	0.0413927	-0.0457575	0.0217875
pp_ss0	1	-1	0.5
pp_ss1	1	-1	0.5
pp_ss2	1	-1	0.5
pp_strt0	0.0211893	-0.0222764	0.0108664
pp_strt1	0.0211893	-0.0222764	0.0108664
pp_strt2	0.0211893	-0.0222764	0.0108664
pp_sy0	0.243038	-0.60206	0.211275
pp_sy1	0.243038	-0.60206	0.211275
pp_sy2	0.243038	-0.60206	0.211275
pp_vka0	1	-1	0.5
pp_vka1	1	-1	0.5
pp_vka2	1	-1	0.5
strk	2	-2	1
welflux	0.176091 to 0.30103	-0.30103 to 0	0.0752575 to 0.11928
welflux_k02	1	-1	0.5

[65 rows x 7 columns]

define our decision variable group and also set some ++args. Conceptually, we are going to optimize current pumping rates to make sure we meet ecological flows under both historic (current) conditions and scenario (future) conditions. Remember the scenario is an extreme 1-year drought so if we pump too much now, the system will be too low to provide critical flows if next year is an extreme drought - transient memory!

```
In [4]: pst.pestpp_options = {}
        #dvg = ["welflux_k02", "welflux"]
        dvg = ["welflux_k02"]
        pst.pestpp_options["opt_dec_var_groups"] = dvg
        pst.pestpp_options["opt_direction"] = "max"
```

For the first run, we wont use chance constraints, so just fix all non-decision-variable parameter. We also need to set some realistic bounds on the welflux multiplier decision variables. Finally, we need to specify a larger derivative increment for the decision variable group

```
In [5]: par = pst.parameter_data
        par.loc[:, "partrans"] = "fixed"

        #turn off pumping in the scenario
        par.loc["welflux_001", "parlbnd"] = 0.0
        par.loc["welflux_001", "parval1"] = 0.0
        dvg_pars = par.loc[par.pargp.apply(lambda x: x in dvg), "parnme"]
        par.loc[dvg_pars, "partrans"] = "none"
        par.loc[dvg_pars, "parlbnd"] = 0.0
        par.loc[dvg_pars, "parubnd"] = 3.0
        par.loc[dvg_pars, "parval1"] = 1.0

        pst.rectify_pgroups()
        pst.parameter_groups.loc[dvg, "inctyp"] = "absolute"
```

```
pst.parameter_groups.loc[dvg,"inctyp"] = "absolute"
pst.parameter_groups.loc[dvg,"derinc"] = 0.25
```

```
pst.parameter_groups.loc[dvg,:]
```

```
Out [5]:
```

	pargpnm	inctyp	derinc	derinclb	forcen	derincmul	\
pargpnm							
welflux_k02	welflux_k02	absolute	0.25	0.0	switch	2.0	

	dermthd	splitthresh	splitreldiff	splitaction	extra
pargpnm					
welflux_k02	parabolic	0.00001	0.5	smaller	NaN

1.0.1 define constraints

model-based and prior information constraints are identified in pestpp-opt by an obs group that starts with “less_than” or “greater_than” and a weight greater than zero. So first, we turn off all of the weights and get names for the sw-gw exchange forecasts (funny how optimization turns forecasts into constraints...)

```
In [6]: obs = pst.observation_data
obs.loc[:, "weight"] = 0.0
swgw_const = obs.loc[obs.obsnme.apply(lambda x: "fa" in x and ("hw" in x or "tw" in x))
obs.loc[swgw_const,:]
```

```
Out [6]:
```

	obsnme	obsval	weight	obgnme	extra
obsnme					
fa_hw_19791230	fa_hw_19791230	-826.11360	0.0	flaqx	NaN
fa_hw_19801229	fa_hw_19801229	-412.13960	0.0	flaqx	NaN
fa_tw_19791230	fa_tw_19791230	341.54505	0.0	flaqx	NaN
fa_tw_19801229	fa_tw_19801229	704.03419	0.0	flaqx	NaN

We need to change the obs group (obgnme) so that pestpp-opt will recognize these two model outputs as constraints. The obsval becomes the RHS of the constraint. We also need to set a lower bound constraint on the total abstraction rate (good thing we included all those list file budget components as observations!)

```
In [7]: obs.loc[swgw_const, "obgnme"] = "less_than"
obs.loc[swgw_const, "weight"] = 1.0

# we must have at least 300 m3/day of flux from gw to sw
# for historic and scenario periods
# and for both headwaters and tailwaters
obs.loc[swgw_const, "obsval"] = -300

# tot_abs_rate = ["flx_wells_19791230"]#, "flx_wells_19801229"]
# obs.loc[tot_abs_rate, "obgnme"] = "less_than"
# obs.loc[tot_abs_rate, "weight"] = 1.0
# obs.loc[tot_abs_rate, "obsval"] = -900.0
# pst.less_than_obs_constraints
```

Now we need to define a minimum total pumping rate, otherwise this opt problem might yield a solution that doesn't give enough water for the intended usage. We will do this through a prior information constraint since this just a sum of decision variable values - the required minimum value will be the sum of current pumping rates:

```
In [8]: pyemu.pst_utils.pst_config["prior_fieldnames"]
```

```
Out[8]: ['pilbl', 'equation', 'weight', 'obgnme']
```

Since all pumping wells are using the same rate, we can just use a 1.0 multiplier in front of each well flux decision variable. If that is not the case, then you need to set the multipliers to be more meaningful

```
In [9]: pi = pst.null_prior
pi.loc["pi_1", "obgnme"] = "greater_than"
pi.loc["pi_1", "pilbl"] = "pi_1"
pi.loc["pi_1", "equation"] = " + ".join(["1.0 * {}".format(d) for d in dvg_pars]) + \
    " = {}".format(par.loc[dvg_pars, "parval1"].sum())
pi.loc["pi_1", "weight"] = 1.0
pi.equation["pi_1"]
```

```
Out[9]: '1.0 * wf0200090016 + 1.0 * wf0200110013 + 1.0 * wf0200200014 + 1.0 * wf0200260010 + 1
```

```
In [10]: pst.prior_information
```

```
Out[10]:          obgnme pilbl \
          pi_1 greater_than pi_1
```

```
pi_1  1.0 * wf0200090016 + 1.0 * wf0200110013 + 1.0 * wf0200200014 + 1.0 * wf02002600
      weight
pi_1      1.0
```

```
In [11]: pst.control_data.noptmax = 1
         pst.write(os.path.join(t_d, "freyberg_opt.pst"))
         pyemu.os_utils.start_slaves(t_d, "pestpp-opt", "freyberg_opt.pst", num_slaves=10, master_
```

```
noptmax:1, npar_adj:6, nnz_obs:4
```

Let's load and inspect the response matrix

```
In [12]: jco = pyemu.Jco.from_binary(os.path.join(m_d,"freyberg_opt.1.jcb")).to_dataframe().loc
jco
```

```
Out[12]:
```

	wf0200090016	wf0200110013	wf0200200014	wf0200260010	\
fa_hw_19791230	137.57200	126.32400	46.30000	21.90800	
fa_hw_19801229	22.58400	28.65600	12.03600	12.29200	
fa_tw_19791230	6.50728	14.53516	93.28136	92.42320	

fa_tw_19801229	4.10836	7.60104	15.29948	30.88604
	wf0200290006	wf0200340012		
fa_hw_19791230	18.12000	4.8320		
fa_hw_19801229	13.12800	3.3560		
fa_tw_19791230	71.84608	82.9612		
fa_tw_19801229	34.79872	17.5232		

We see the transient effects in the nonzero value between current pumping rates (columns) and scenario sw-gw exchange (rows from 1980)

Let's also load the optimal decision variable values:

```
In [13]: par_df = pyemu.pst_utils.read_parfile(os.path.join(m_d, "freyberg_opt.1.par"))
print(par_df.loc[dvg_pars, "parval1"].sum())
par_df.loc[dvg_pars, :]
```

9.693626734842857

```
Out [13]:
```

	parnme	parval1	scale	offset
parnme				
wf0200090016	wf0200090016	3.000000	1.0	0.0
wf0200110013	wf0200110013	3.000000	1.0	0.0
wf0200200014	wf0200200014	3.000000	1.0	0.0
wf0200260010	wf0200260010	0.000000	1.0	0.0
wf0200290006	wf0200290006	0.000000	1.0	0.0
wf0200340012	wf0200340012	0.693627	1.0	0.0

The sum of these values is the optimal objective function value. However, since these are just multipliers on the pumping rate, this number isn't too meaningful. Instead, let's look at the residuals file

```
In [14]: pst = pyemu.Pst(os.path.join(m_d, "freyberg_opt.pst"), resfile=os.path.join(m_d, "freyber
pst.res.loc[pst.nnz_obs_names, :]
```

```
Out [14]:
```

	name	group	measured	modelled	residual	\
name						
fa_hw_19791230	fa_hw_19791230	less_than	-300.0	-398.5755	98.5755	
fa_hw_19801229	fa_hw_19801229	less_than	-300.0	-656.8370	356.8370	
fa_tw_19791230	fa_tw_19791230	less_than	-300.0	-414.1347	114.1347	
fa_tw_19801229	fa_tw_19801229	less_than	-300.0	-299.5820	-0.4180	
weight						
name						
fa_hw_19791230	1.0					
fa_hw_19801229	1.0					
fa_tw_19791230	1.0					
fa_tw_19801229	1.0					

Sweet as! lots of room in the optimization problem. The bounding constraint is the one closest to its RHS

1.0.2 Opt under uncertainty part 1: FOSM chance constraints

This is where the process of uncertainty quantification/history matching and mgmt optimization meet - worlds collide!

Mechanically, in PESTPP-OPT, to activate the chance constraint process, we need to specify a risk $\neq 0.5$. Risk ranges from 0.001 (risk tolerant) to 0.999 (risk averse). The larger the risk value, the more confidence we have that the (uncertain) model-based constraints are truly satisfied. Here we will start with a risk tolerant stance:

```
In [15]: pst.pestpp_options["opt_risk"] = 0.4
```

For the FOSM-based chance constraints, we also need to have at least one adjustable non-dec-var parameter so that we can propagate parameter uncertainty to model-based constraints (this can also be posterior FOSM is non-constraint, non-zero-weight observations are specified). For this simple demo, let's just use the constant multiplier parameters in the prior uncertainty stance:

```
In [16]: cn_pars = par.loc[par.pargp.apply(lambda x: "cn" in x), "parname"]
         cn_pars
```

```
Out[16]: parname
hk6_cn          hk6_cn
hk7_cn          hk7_cn
hk8_cn          hk8_cn
prsity6_cn      prsity6_cn
prsity7_cn      prsity7_cn
prsity8_cn      prsity8_cn
rech4_cn        rech4_cn
rech5_cn        rech5_cn
ss6_cn          ss6_cn
ss7_cn          ss7_cn
ss8_cn          ss8_cn
strt6_cn        strt6_cn
strt7_cn        strt7_cn
strt8_cn        strt8_cn
sy6_cn          sy6_cn
sy7_cn          sy7_cn
sy8_cn          sy8_cn
vka6_cn         vka6_cn
vka7_cn         vka7_cn
vka8_cn         vka8_cn
Name: parname, dtype: object
```

```
In [17]: par = pst.parameter_data
         par.loc[cn_pars, "partrans"] = "log"
         pst.control_data.noptmax = 1
         pst.write(os.path.join(t_d, "freyberg_opt_uu1.pst"))
```

```
noptmax:1, npar_adj:26, nnz_obs:4
```


So now we need to not only fill the response matrix (between dec vars and constraints) but we also need to fill the jacobian matrix (between parameters and constraints).

```
In [18]: pyemu.os_utils.start_slaves(t_d,"pestpp-opt","freyberg_opt_uu1.pst",num_slaves=20,master=0)
```

```
In [19]: pst = pyemu.Pst(os.path.join(m_d,"freyberg_opt_uu1.pst"),resfile=os.path.join(m_d,"freyberg_opt_uu1.res"),
    pst.res.loc[pst.nnz_obs_names,:]
```

```
Out [19]:
```

	name	group	measured	modelled	residual	\
name						
fa_hw_19791230	fa_hw_19791230	less_than	-300.0	-426.6231	126.6231	
fa_hw_19801229	fa_hw_19801229	less_than	-300.0	-640.6620	340.6620	
fa_tw_19791230	fa_tw_19791230	less_than	-300.0	-223.3317	-76.6683	
fa_tw_19801229	fa_tw_19801229	less_than	-300.0	-208.3292	-91.6708	


```
weight
```

name	weight
fa_hw_19791230	1.0
fa_hw_19801229	1.0
fa_tw_19791230	1.0
fa_tw_19801229	1.0

```
In [20]: par_df = pyemu.pst_utils.read_parfile(os.path.join(m_d,"freyberg_opt_uu1.1.par"))
    print(par_df.loc[dvg_pars,"parval1"].sum())
    par_df.loc[dvg_pars,:]
```

12.500896512450069

```
Out [20]:
```

	parname	parval1	scale	offset
parname				
wf0200090016	wf0200090016	3.000000	1.0	0.0
wf0200110013	wf0200110013	3.000000	1.0	0.0
wf0200200014	wf0200200014	1.281895	1.0	0.0
wf0200260010	wf0200260010	0.000000	1.0	0.0
wf0200290006	wf0200290006	2.219002	1.0	0.0
wf0200340012	wf0200340012	3.000000	1.0	0.0

We now see how taking a risk tolerant stance allows for more pumping but that we have only a 40% chance of actually satisfying the sw-gw constraints (see how the model simulated value is actually in violation of the -300 constraint RHS. Lets check the residuals that include the FOSM-based chance constraint shift:

```
In [21]: res_df = pyemu.pst_utils.read_resfile(os.path.join(m_d,"freyberg_opt_uu1.1.sim+fosm.res"),
    res_df
```

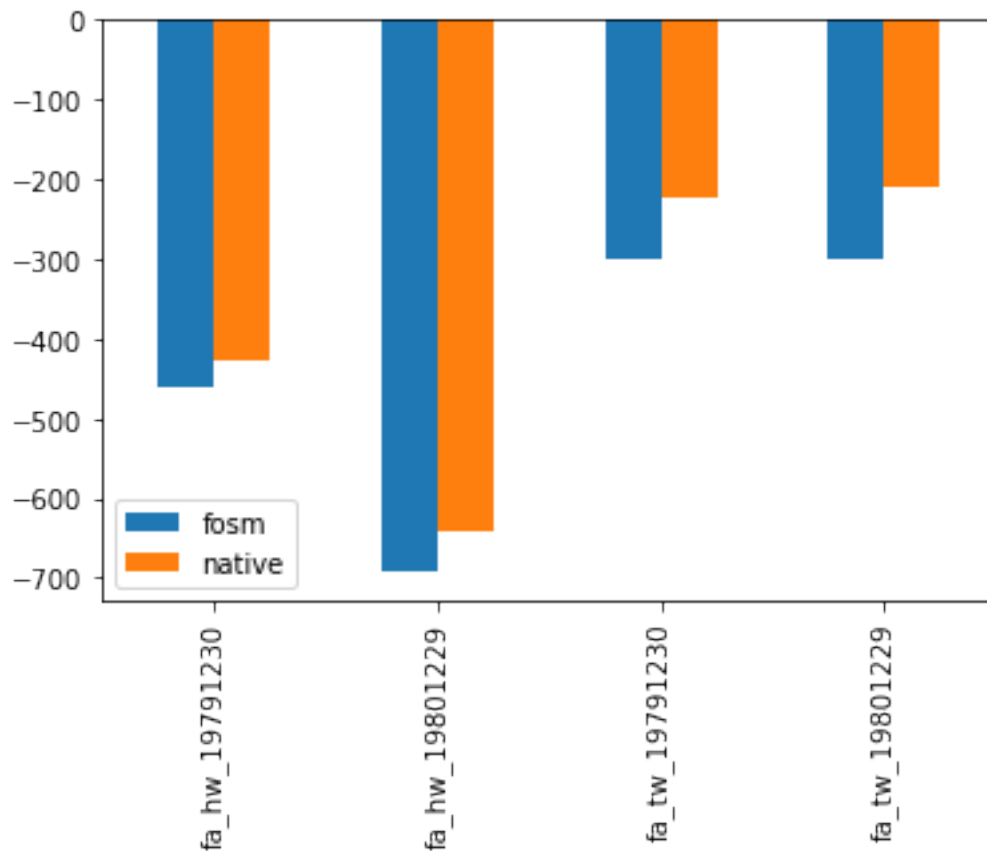
```
Out [21]:
```

	name	group	measured	modelled	residual	\
name						
fa_hw_19791230	fa_hw_19791230	less_than	-300.0	-461.842970	161.842970	

fa_hw_19801229	fa_hw_19801229	less_than	-300.0	-693.498392	393.498392
fa_tw_19791230	fa_tw_19791230	less_than	-300.0	-299.758707	-0.241293
fa_tw_19801229	fa_tw_19801229	less_than	-300.0	-299.676541	-0.323459

	weight
name	
fa_hw_19791230	1.0
fa_hw_19801229	1.0
fa_tw_19791230	1.0
fa_tw_19801229	1.0

```
In [22]: ax = pd.DataFrame({"native":pst.res.modelled,"fosl":res_df.modelled}).loc[pst.nnz_obs]
```



1.0.3 Opt under uncertainty part 2: ensemble-based chance constraints

PESTPP-OPT can also skip the FOSM calculations if users specify model-based constraint weights as standard deviations (e.g. uncertainty in the forecasts/constraints). These can be derived from existing ensembles (oh snap!)

```
In [23]: obs_df = pd.read_csv(os.path.join("master_prior_sweep", "sweep_out.csv"), index_col=0)
obs_df = obs_df.loc[obs_df.failed_flag==0,:]
```

```

In [24]: pr_std = obs_df.std().loc[pst.nnz_obs_names]
         pr_std

Out [24]: fa_hw_19791230    401.410907
         fa_hw_19801229    519.546370
         fa_tw_19791230    577.145769
         fa_tw_19801229    676.650071
         dtype: float64

In [25]: pst.observation_data.loc[pst.nnz_obs_names,"weight"] = pr_std.loc[pst.nnz_obs_names]
         pst.pestpp_options["opt_std_weights"] = True
         pst.write(os.path.join(t_d,"freyberg_opt_uu2.pst"))

noptmax:1, npar_adj:26, nnz_obs:4

In [26]: pyemu.os_utils.start_slaves(t_d,"pestpp-opt","freyberg_opt_uu2.pst",num_slaves=10,master_pid=0)

In [27]: par_df = pyemu.pst_utils.read_parfile(os.path.join(m_d,"freyberg_opt_uu2.1.par"))
         print(par_df.loc[dvg_pars,"parval1"].sum())
         par_df.loc[dvg_pars,:]

13.44184717037496

Out [27]:
```

	parnme	parval1	scale	offset
parnme				
wf0200090016	wf0200090016	3.000000	1.0	0.0
wf0200110013	wf0200110013	3.000000	1.0	0.0
wf0200200014	wf0200200014	0.000000	1.0	0.0
wf0200260010	wf0200260010	1.441847	1.0	0.0
wf0200290006	wf0200290006	3.000000	1.0	0.0
wf0200340012	wf0200340012	3.000000	1.0	0.0

Why is the objective function higher when we use the ensemble-based constraint uncertainty compared to the FOSM constraint uncertainty? remember how many more parameters were used in the ensemble analyses compared to just the hand full of constant by layer parameters???

1.0.4 Super secret mode

turns out, if the opt problem is truly linear, we can reuse results of a previous PESTPP-OPT run to modify lots of the pieces of the optimization problem and resolve the optimization problem without running the model even once! WAT!? This is done by specifying some additional ++ args (and copying some files around)

```

In [28]: shutil.copy2(os.path.join(m_d,"freyberg_opt_uu2.1.jcb"),os.path.join(m_d,"restart.jcb"))
         shutil.copy2(os.path.join(m_d,"freyberg_opt_uu2.1.jcb.rei"),os.path.join(m_d,"restart.rei"))

         pst.pestpp_options["base_jacobian"] = "restart.jcb"
         pst.pestpp_options["hotstart_resfile"] = "restart.rei"
         pst.pestpp_options["opt_skip_final"] = True
         pst.write(os.path.join(m_d,"freyberg_opt_restart.pst"))

```

```
noptmax:1, npar_adj:26, nnz_obs:4
```

```
In [29]: pyemu.os_utils.run("pestpp-opt freyberg_opt_restart.pst", cwd=m_d)
```

```
In [30]: par_df = pyemu.pst_utils.read_parfile(os.path.join(m_d, "freyberg_opt_restart.1.par"))
print(par_df.loc[dvg_pars, "parval1"].sum())
par_df.loc[dvg_pars, :]
```

```
13.44184717037496
```

```
Out [30]:
```

	parnme	parval1	scale	offset
parnme				
wf0200090016	wf0200090016	3.000000	1.0	0.0
wf0200110013	wf0200110013	3.000000	1.0	0.0
wf0200200014	wf0200200014	0.000000	1.0	0.0
wf0200260010	wf0200260010	1.441847	1.0	0.0
wf0200290006	wf0200290006	3.000000	1.0	0.0
wf0200340012	wf0200340012	3.000000	1.0	0.0

Oh snap! that means we can do all sort of kewl optimization testing really really fast... we can test a (slightly) risk averse stance too:

```
In [31]: pst.pestpp_options["opt_risk"] = 0.51
pst.write(os.path.join(m_d, "freyberg_opt_restart.pst"))
pyemu.os_utils.run("pestpp-opt freyberg_opt_restart.pst", cwd=m_d)
par_df = pyemu.pst_utils.read_parfile(os.path.join(m_d, "freyberg_opt_restart.1.par"))
print(par_df.loc[dvg_pars, "parval1"].sum())
par_df.loc[dvg_pars, :]
```

```
noptmax:1, npar_adj:26, nnz_obs:4
```

```
8.685701475362208
```

```
Out [31]:
```

	parnme	parval1	scale	offset
parnme				
wf0200090016	wf0200090016	3.000000	1.0	0.0
wf0200110013	wf0200110013	3.000000	1.0	0.0
wf0200200014	wf0200200014	2.685701	1.0	0.0
wf0200260010	wf0200260010	0.000000	1.0	0.0
wf0200290006	wf0200290006	0.000000	1.0	0.0
wf0200340012	wf0200340012	0.000000	1.0	0.0

Lets use the functionality to evaluate how our OUU problem changes if we use posterior standard deviations - this is a critically important use of the uncertainty analysis from history matching:

```
In [32]: obs_df = pd.read_csv(os.path.join("master_ies", "freyberg_ies.3.obs.csv"), index_col=0)

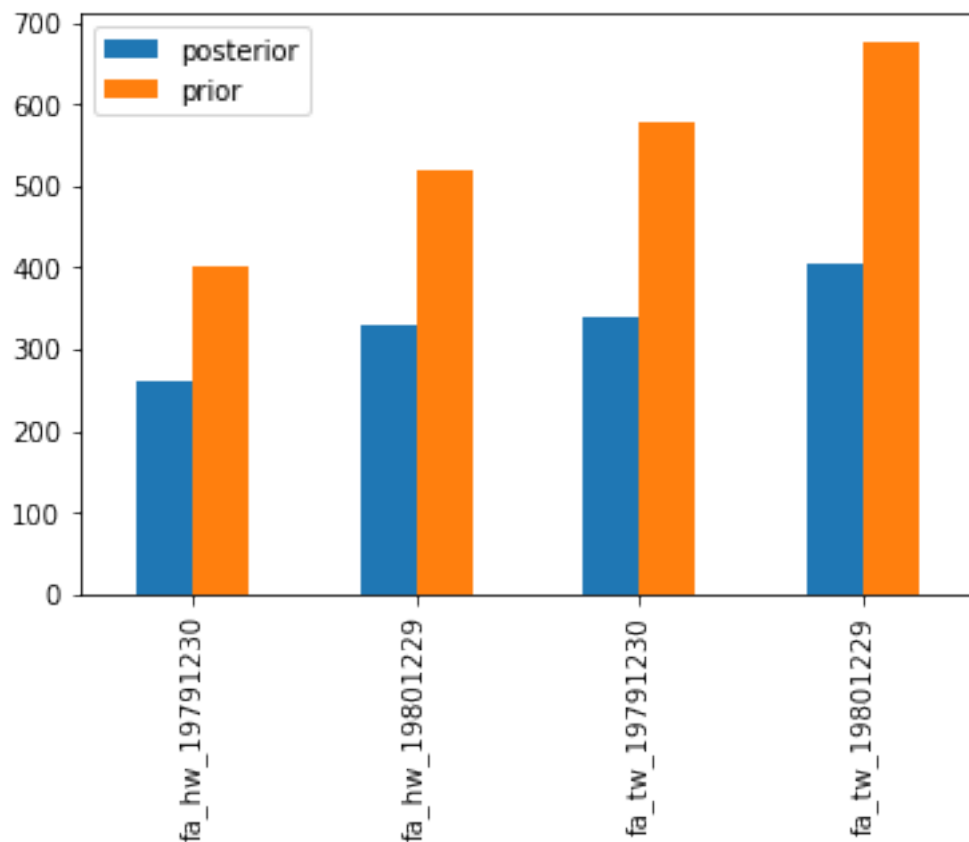
#df = df=pd.read_csv(os.path.join("master_glm", "freyberg_pp.post.obsen.csv"), index_col=0)
#obs_df = pyemu.ObservationEnsemble.from_dataframe(pst=pst, df=df)
#obs_df = obs_df.loc[obs_df.phi_vector.sort_values().index[:20],:]
pt_std = obs_df.std().loc[pst.nnz_obs_names]
obs_df.std().loc[pst.nnz_obs_names]
#obs_df.max().loc[pst.nnz_obs_names]
```

```
Out[32]: fa_hw_19791230    259.832061
fa_hw_19801229    329.911338
fa_tw_19791230    339.650343
fa_tw_19801229    404.975422
dtype: float64
```

How much lower is the posterior standard deviations are compared to the prior?

```
In [33]: pd.DataFrame({"prior":pr_std, "posterior":pt_std}).plot(kind="bar")
```

```
Out[33]: <matplotlib.axes._subplots.AxesSubplot at 0x182136ee10>
```



This implies that the chance constraints (which express the important model input uncertainty propagated to the forecast/constraints) is significantly lower, meaning uncertainty has less “value” in the optimization objective function

```
In [34]: pst.observation_data.loc[pst.nnz_obs_names,"weight"] = pt_std.loc[pst.nnz_obs_names]
         pst.observation_data.loc[pst.nnz_obs_names,"weight"]
```

```
Out [34]: obsnme
         fa_hw_19791230    259.832061
         fa_hw_19801229    329.911338
         fa_tw_19791230    339.650343
         fa_tw_19801229    404.975422
         Name: weight, dtype: float64
```

```
In [35]: pst.write(os.path.join(m_d,"freyberg_opt_restart.pst"))
         pyemu.os_utils.run("pestpp-opt freyberg_opt_restart.pst",cwd=m_d)
         par_df = pyemu.pst_utils.read_parfile(os.path.join(m_d,"freyberg_opt_restart.1.par"))
         print(par_df.loc[dvg_pars,"parval1"].sum())
         par_df.loc[dvg_pars,:]
```

```
noptmax:1, npar_adj:26, nnz_obs:4
9.11425410128325
```

```
Out [35]:
```

	parnme	parval1	scale	offset
parnme				
wf0200090016	wf0200090016	3.000000	1.0	0.0
wf0200110013	wf0200110013	3.000000	1.0	0.0
wf0200200014	wf0200200014	3.000000	1.0	0.0
wf0200260010	wf0200260010	0.000000	1.0	0.0
wf0200290006	wf0200290006	0.000000	1.0	0.0
wf0200340012	wf0200340012	0.114254	1.0	0.0

```
In [36]: pyemu.pst_utils.read_resfile(os.path.join(m_d,"freyberg_opt_restart.1.est+fosm.rei"))
```

```
Out [36]:
```

	name	group	measured	modelled	residual	\
name						
fa_hw_19791230	fa_hw_19791230	less_than	-300.0	-394.641108	94.641108	
fa_hw_19801229	fa_hw_19801229	less_than	-300.0	-651.015907	351.015907	
fa_tw_19791230	fa_tw_19791230	less_than	-300.0	-453.622516	153.622516	
fa_tw_19801229	fa_tw_19801229	less_than	-300.0	-300.000000	0.000000	
		weight				
name						
fa_hw_19791230	fa_hw_19791230	259.832061				
fa_hw_19801229	fa_hw_19801229	329.911338				
fa_tw_19791230	fa_tw_19791230	339.650343				
fa_tw_19801229	fa_tw_19801229	404.975422				

Again we see that scenarion tail water flux is the binding constraint. So! Lets reformulate the problem to be constrained by the total sw-gw flux across all reaches instead of splitting into headwaters and tailwaters. Good thing we have added the list file budget components to the control file!

```
In [37]: pst = pyemu.Pst(os.path.join(m_d,"freyberg_opt_restart.pst"))
        obs = pst.observation_data
        obs.loc[pst.nnz_obs_names,"obgnme"] = "sw-gw"
        obs.loc[pst.nnz_obs_names,"weight"] = 0.0
```

```
In [38]: tot_swgw = obs.loc[obs.obgnme=="flx_stream_", "obsnme"]
```

```
In [39]: obs.loc[tot_swgw,"obgnme"] = "less_than"
        obs.loc[tot_swgw,"weight"] = 1.0
        obs.loc[tot_swgw,"weight"] = obs_df.std().loc[pst.nnz_obs_names]
        obs.loc[tot_swgw,"obsval"] = -600
```

Since we want to find the most risk averse stance that is still feasible we will run a sweep of risk values:

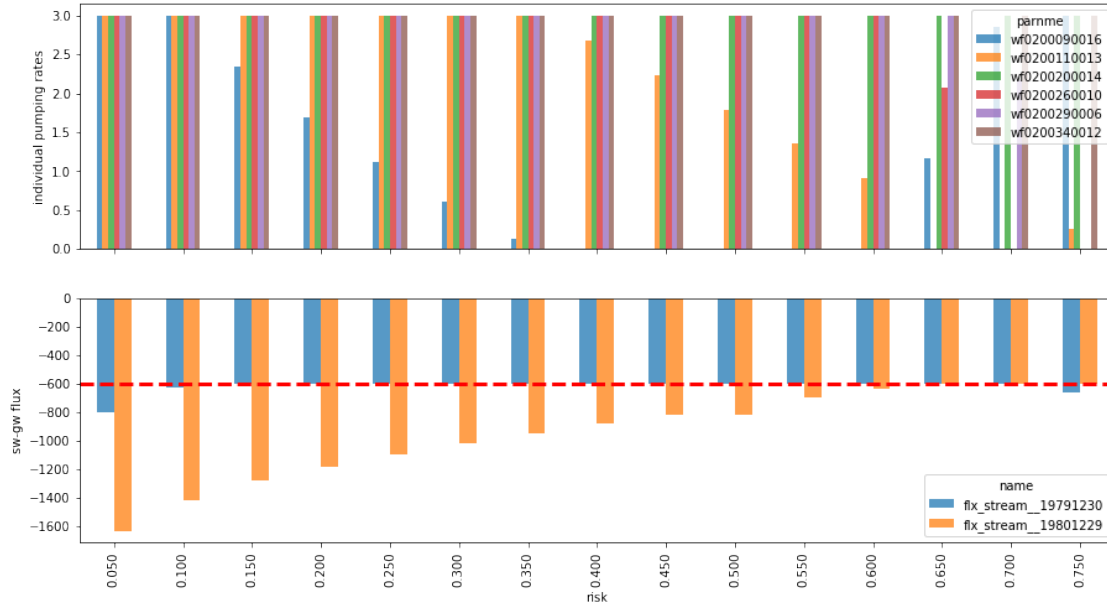
```
In [40]: par_dfs = []
        res_dfs = []
        risk_vals = np.arange(0.05,1.0,0.05)
        for risk in risk_vals:
            #try:
            #    os.remove(os.path.join(m_d,"freyberg_opt_restart.1.est+fosm.rei"))
            #except:
            #    pass
            if risk > 0.8:#par_df.parval1.sum() < 6.0:
                print("infeasible at risk",risk)
                break
            pst.pestpp_options["opt_risk"] = risk
            pst.write(os.path.join(m_d,"freyberg_opt_restart.pst"))
            pyemu.os_utils.run("pestpp-opt freyberg_opt_restart.pst",cwd=m_d)
            par_df = pyemu.pst_utils.read_parfile(os.path.join(m_d,"freyberg_opt_restart.1.par"))
            par_df = par_df.loc[dvg_pars,:]
            #when the solution is infeasible, pestpp-opt writes extreme negative values
            # to the par file:
            if par_df.parval1.sum() < 6.0:
                print("infeasible at risk",risk)
                break
            res_df = pyemu.pst_utils.read_resfile(os.path.join(m_d,"freyberg_opt_restart.1.est"))
            res_df = res_df.loc[pst.nnz_obs_names,:]
            res_dfs.append(res_df.modelled)
            par_dfs.append(par_df.parval1)

        # process the dec var and constraint dataframes for plotting
        risk_vals = risk_vals[:len(par_dfs)]
        par_df = pd.concat(par_dfs,axis=1).T
```

[illegible]

```
In [41]: fig, axes = plt.subplots(2,1,figsize=(15,8))
par_df.plot(kind="bar",ax=axes[0],alpha=0.75)
axes[0].set_ylabel("individual pumping rates")
axes[0].set_xticklabels([])
res_df.plot(kind="bar",ax=axes[1],alpha=0.75)
axes[1].plot(axes[1].get_xlim(),[-600,-600],"r--",lw=3)
axes[1].set_ylabel("sw-gw flux")
axes[1].set_xlabel("risk")
```

16



That is a world-class figure!!!

How slick was that! no more model runs needed and yet we transformed the OUU problem (by swapping constraints) and solved for a much more risk averse stance!

2 FINALLY!!!

We now see the reason for high-dimensional uncertainty quantification and history matching: to define and then reduce (through data assimilation) the uncertainty in the model-based constraints (e.g. sw-gw forecasts) so that we can find a more risk-averse management solution - we can use to model to identify an optimal pumping scheme to provide the volume of water needed for supply/ag but also provide assurances (at the given confidence) that ecological flows will be maintained under both current conditions and in the event of an extreme 1-year drought. BOOM!