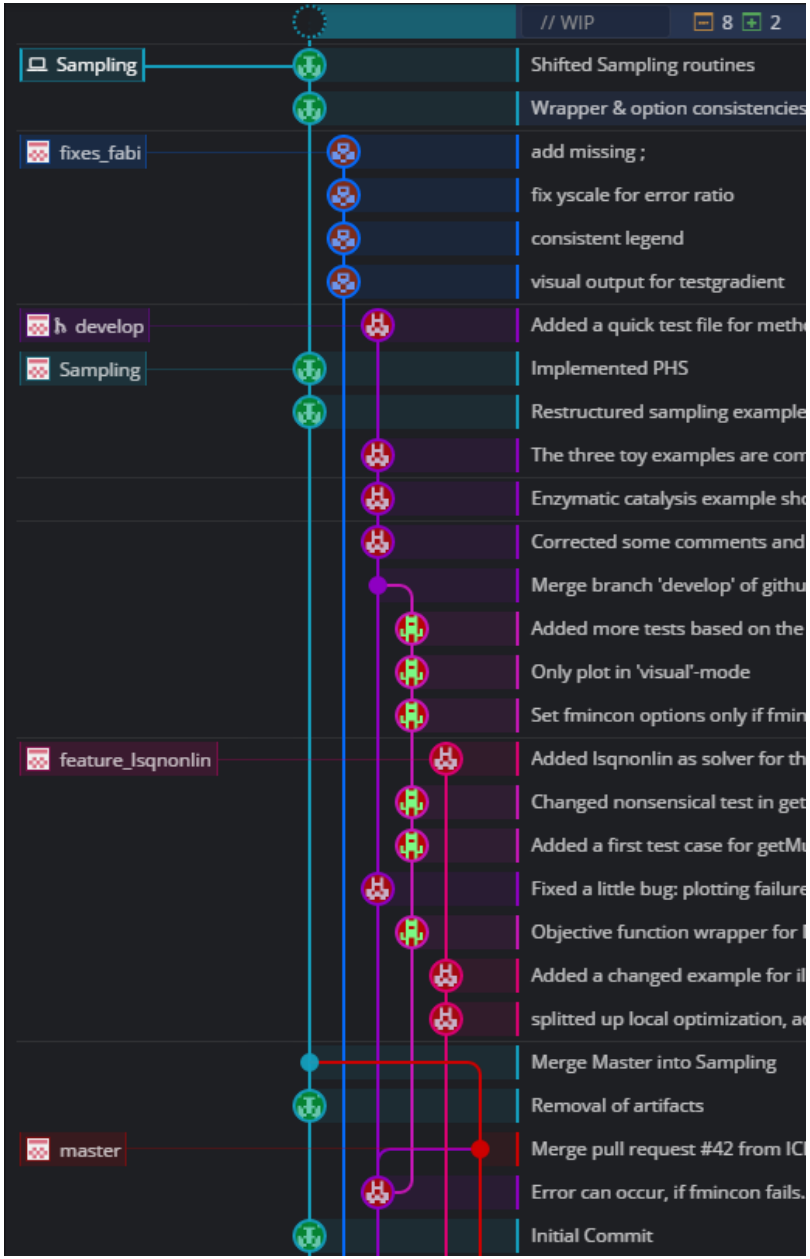
Sampling using PESTO

Application Note PESTO



- Making PESTO publically available
- Development on GitHub

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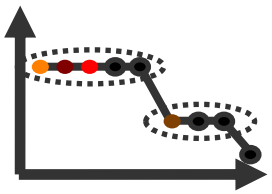
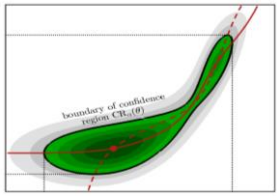
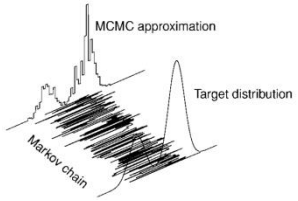


OPTIMIZATION



PROFILING



SAMPLING

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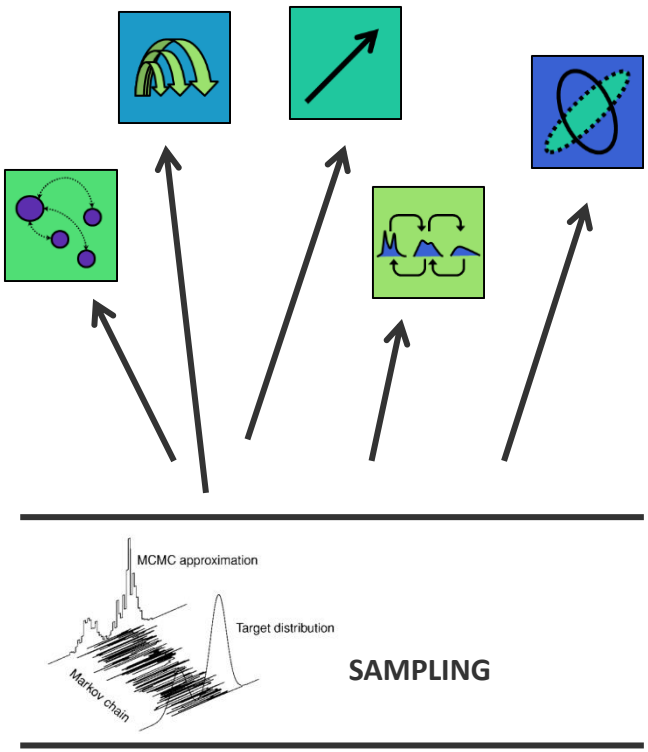
- Development on GitHub
- Main features: Interface for
  - optimization
  - profiles
  - sampling
  - Visualization

Application Note PESTO



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- Recently added validated sampling routines:
  - AM (Adaptive Metropolis)
  - DRAM (Delayed Rejection AM)
  - MALA (Metropolis-adjusted Langevin Algorithm)
  - PT (Parallel Tempering)
  - PHS (Parallel Hierarchical Sampling)

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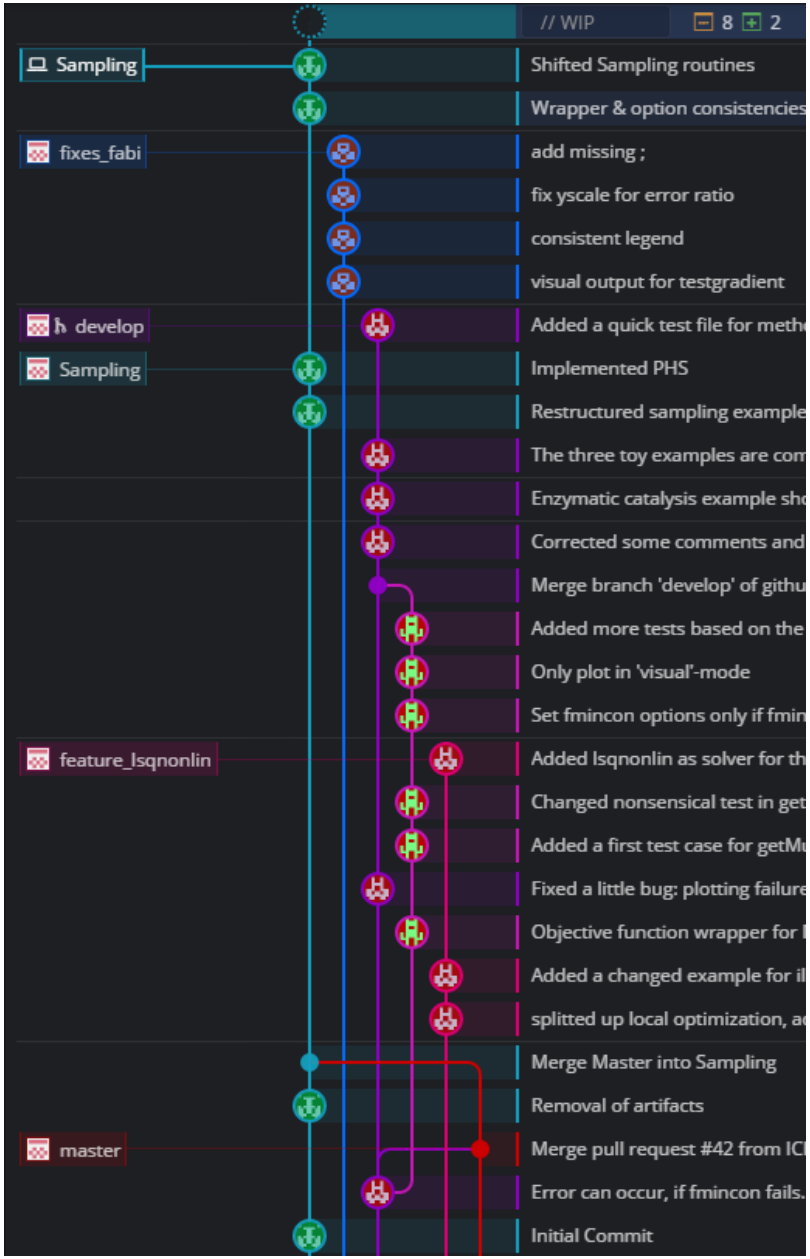

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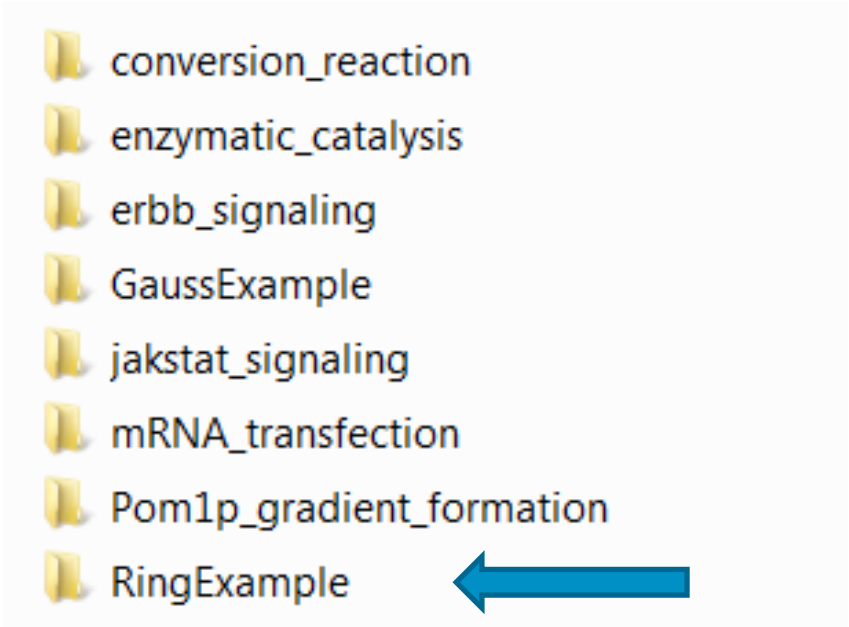
  - PT (Parallel Tempering)
  - PHS (Parallel Hierarchical Sampling)
- Reworked & modularized most of the sampling code
- Added 2 new sampling examples (no biological meaning)
- Currently: Adapting the existing examples

How to use sampling in PESTO?

Define the problem as a cost function (RingExample)

```
% Initialize example problem
path(pathdef);
addpath(genpath([pwd filesep '..' filesep '..']));
radius = 15;
sigma = 2;
logP = @(theta) simulateRingLLH(theta,radius,sigma);
ringDimension           = 2;
```



How to use sampling in PESTO?

Set general options

```
clear opt; clear par;
par.number                = ringDimension;
par.min                   = -25*ones(ringDimension,1);
par.max                   = 25*ones(ringDimension,1);
par.obj_type              = 'log-posterior';

opt.rndSeed               = 3;
opt.nIterations           = 1e5;
```

Set algorithm-specific options

```
% Using PT
opt.samplingAlgorithm     = 'PT';
opt.objOutNumber          = 1;
opt.PT.nTemps             = 3;
opt.PT.exponentT          = 4;
opt.PT.alpha              = 0.51;
opt.PT.temperatureAlpha   = 0.51;
opt.PT.memoryLength       = 1;
opt.PT.regFactor          = 1e-4;
opt.PT.temperatureAdaptionScheme =  'Lacki15'; %'Vousden16'; %
opt.theta0                = repmat([-15*ones(ringDimension,1)],1,opt.PT.nTemps);
opt.sigma0                = 1e5*diag(ones(1,ringDimension));
```

How to use sampling in PESTO?

Set general options

```
clear opt; clear par;
par.number              = ringDimension;
par.min                 = -25*ones(ringDimension,1);
par.max                 = 25*ones(ringDimension,1);
par.obj_type            = 'log-posterior';

opt.rndSeed             = 3;
opt.nIterations         = 1e5;
```

Set algorithm-specific options

```
% Using DRAM
opt.samplingAlgorithm     = 'DRAM';
opt.objOutNumber          = 1;
opt.DRAM.nTry             = 5;
opt.DRAM.verbosityMode    = 'debug';
opt.DRAM.adaptionInterval = 1;
opt.DRAM.regFactor        = 1e-4;
opt.theta0                = -15*ones(ringDimension,1);
opt.sigma0                = 1e5*diag(ones(1,ringDimension));
```

How to use sampling in PESTO?

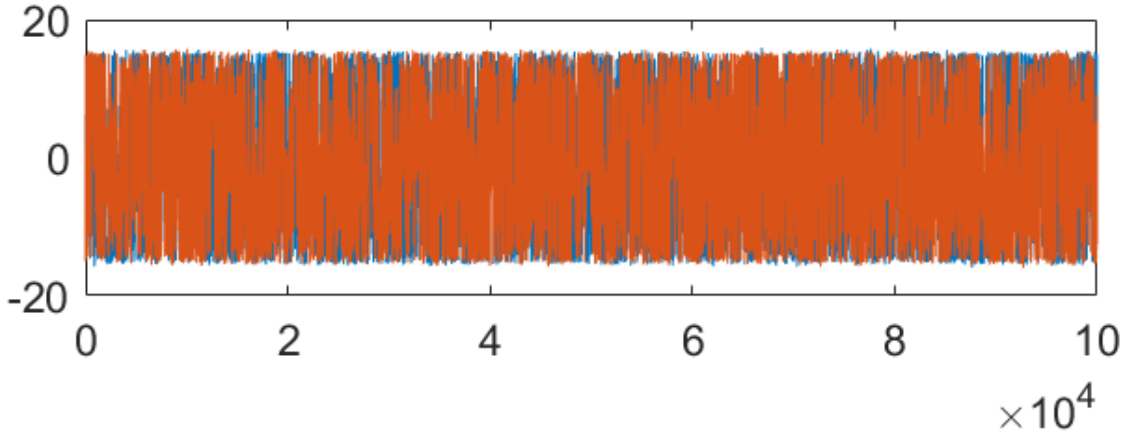
Start the sampling

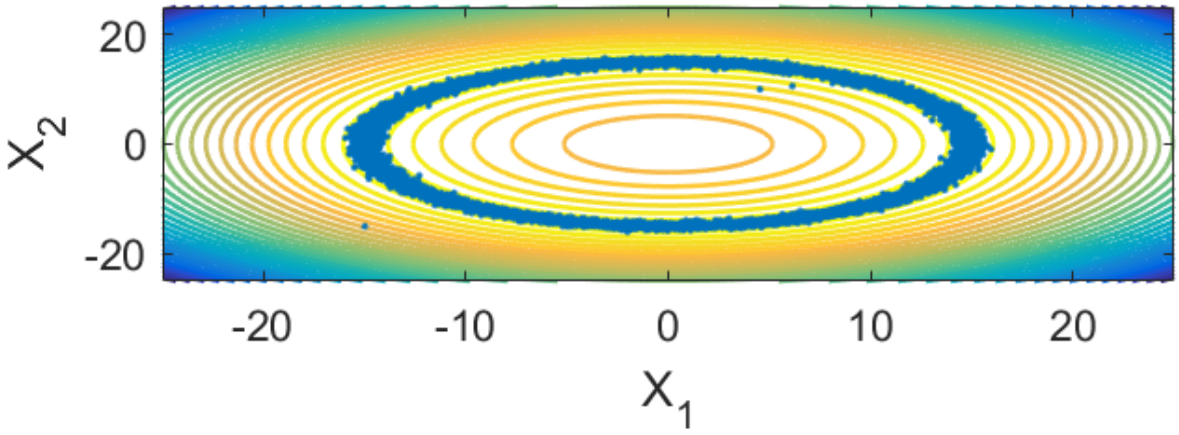
```
par = getParameterSamples(par, logP, opt);
```

How to use sampling in PESTO?

Visualize the results

```
% Visualize
figure
subplot(2,1,1); plot(squeeze(par.S.par(:,:,1))')
subplot(2,1,2);
plotRing(); hold all
plot(squeeze(par.S.par(1,:,1))',squeeze(par.S.par(2,:,1))','.')
```

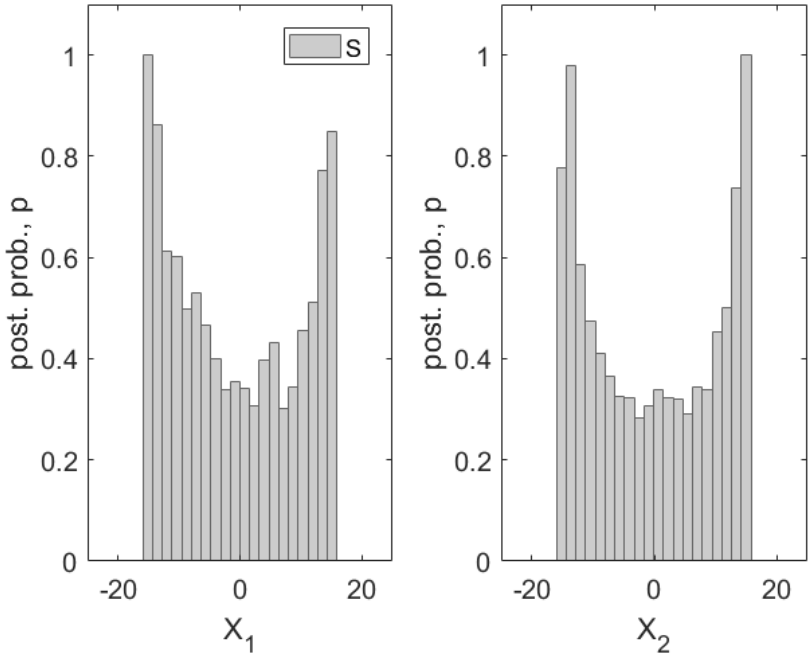


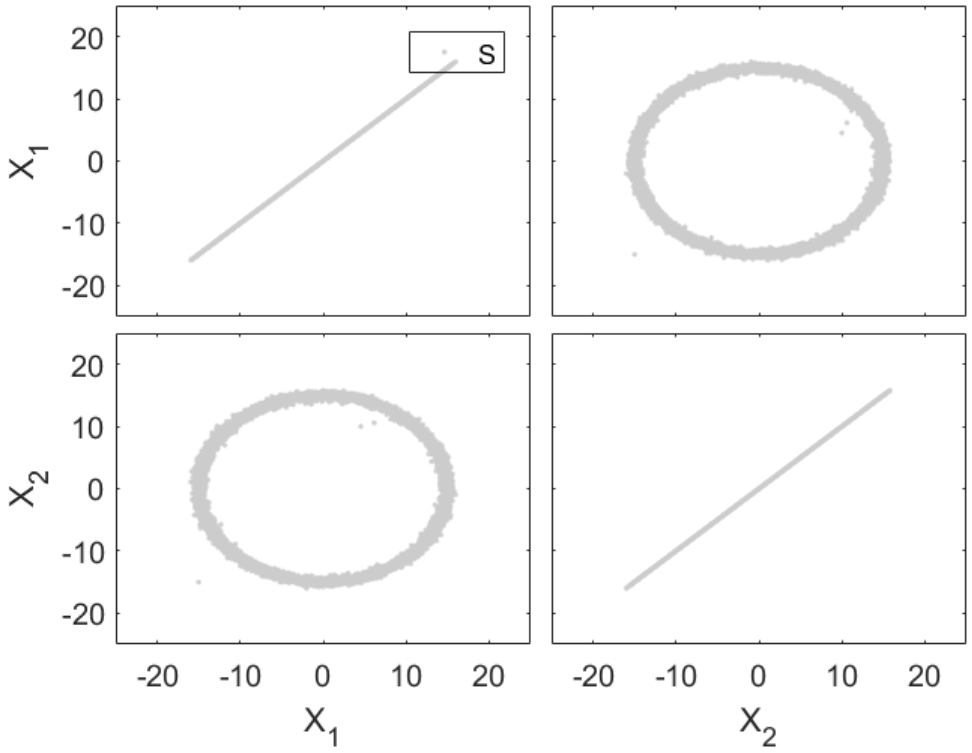


How to use sampling in PESTO?

Visualize the results

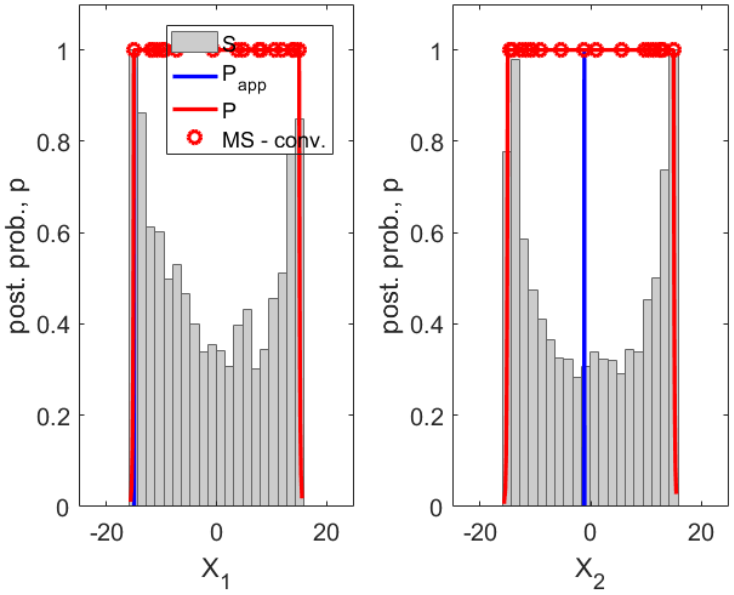
```
plotParameterSamples(par,'1D',[],[],samplingPlottingOpt)

plotParameterSamples(par,'2D',[],[],samplingPlottingOpt)
```

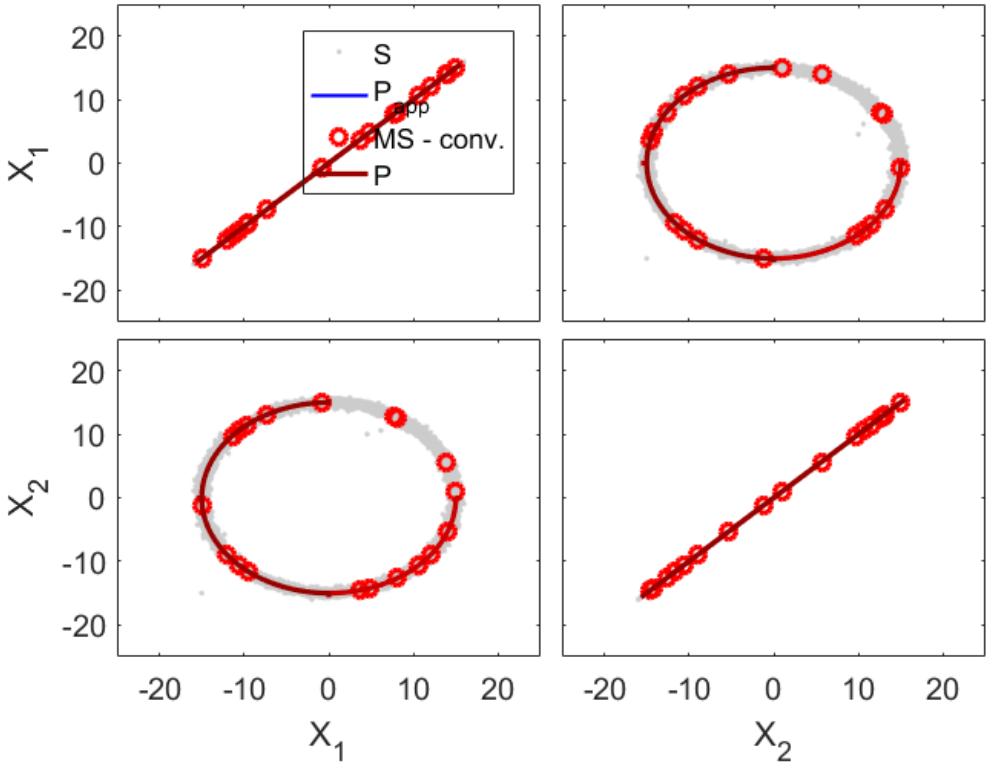




How to use sampling in PESTO?

Combine Sampling with optimization & profiling





Questions?