Benchmark of RAT Bayes Calculation

Start with a direct calculation of the posteriors for a simple problem. We use a simple reflectivity from D2O, and fit only two parameters - Roughness and background.

The task is to calculate chi-squared on a 2D grid, with one axis representing roughness and the other background. For each pair of values, the likelihood is given by

$$P \propto \exp\left(-\frac{\chi^2}{2}\right) .$$

We calculate this on a grid, and this then gives the benchmark posterior distributions which can then be used to validate the two Bayes algorithms included in RAT.

1. **Calculation of 2D posterior.**

Start by setting up the problemDef and controlsDef input classes. We do this by converting from a RasCAL1 project.

```
[problem,controls] = r1ToProblemDef('defaultProject.mat')
```

```
problem =
  problemDef with properties:

         experimentType: 'standard'
     experimentGeometry: 'air/substrate'
                nParams: 1
                 params: 4.8444
             paramNames: {'Substrate Roughness'}
            paramConstr: {[3 8]}
          paramFitYesNo: 1
           nBackgrounds: 1
            backgrounds: 3.0690e-06
        backgroundNames: {'Background 1'}
       backgroundConstr: {[5.0000e-08 7.0000e-06]}
     backgroundFitYesNo: 1
          nScalefactors: 1
           scalefactors: 0.1014
       scalefactorNames: {'Scalefactor 1'}
      scalefactorConstr: {[0.0100 0.3000]}
    scalefactorFitYesNo: 1
              nQzshifts: 1
               qzshifts: 0
           qzshiftNames: {'Qz Shifts 1'}
          qzshiftConstr: {[-0.0300 0.0300]}
        qzshiftFitYesNo: 0
          nbairFitYesNo: 0
                nNbsubs: 1
                 nbsubs: 6.3500e-06
             nbsubNames: {'D2O'}
            nbsubConstr: {[6.3000e-06 6.4000e-06]}
          nbsubFitYesNo: 0
      numberOfContrasts: 1
           nResolutions: 1
            resolutions: 0.0300
       resolutionNames: {'Resolution 1'}
      resolutionConstr: {[0.0100 0.0500]}
```

```
     resolutionFitYesNo: 0
                allData: {[53×3 double]}
            dataPresent: 1
               resample: 0
             dataLimits: {[0.0489 0.6117]}
              simLimits: {[0.0489 0.6117]}
          contrastBacks: {[1 1]}
         contrastShifts: 1
         contrastScales: 1
           contrastNbas: 1
           contrastNbss: 1
            contrastRes: 1
     contrastRepeatSLDs: {[0 1]}
              modelType: 'layers'
         numberOfLayers: 0
          layersDetails: {0×1 cell}
         contrastLayers: {[]}
controls =
  controlsDef with properties:

            parallel: 'single'
           procedure: 'calculate'
    calcSldDuringFit: 'no'
```

Now we need to set up ranges for the parameters, and set up the calculation grid..

```
%Use a 30 x 30 grid.
%Make an array for the results...
gridSize = 30;
probArray = zeros(gridSize, gridSize);

%Make a vector of roughness values..
minRough = problem.paramConstr{1}(1);
maxRough = problem.paramConstr{1}(2);
roughVector = linspace(minRough, maxRough, gridSize);

%Also background...
minBack = problem.backgroundConstr{1}(1);
maxBack = problem.backgroundConstr{1}(2);
backsVector = linspace(minBack, maxBack, gridSize);
```

Now calculate the likelihood at all points on the grid

```
%Now for the calculation.
counter = 1;
totalGrid = gridSize^2;
controls.procedure = 'calculate';
tic;
for r = 1:gridSize
    for b = 1:gridSize
        thisRough = roughVector(r);
        thisBack =  backsVector(b);

        problem.params(1) = thisRough;
        problem.backgrounds(1) = thisBack;

        [outProblem,results] = RAT(problem,controls);
        thisChi = results.calculationResults.sum_chi;
```

```
        probArray(r,b) = exp(-thisChi/2);
        %percent = (counter/totalGrid)*100;
        %fprintf('Calculated %1.1f percent \n',percent);
        counter = counter + 1;
    end
end
toc;
```

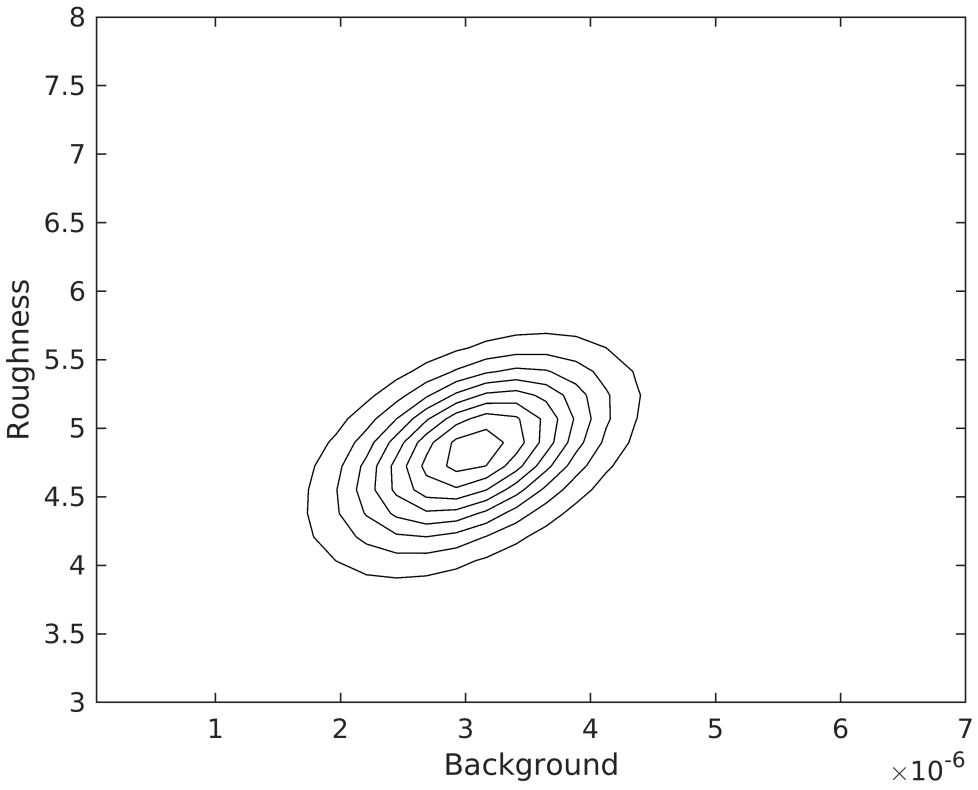
```
Elapsed time is 2.489519 seconds.
```

We can now plot this to see the resulting 2D posterior....

```
figure
contour(backsVector,roughVector,probArray,'k-');
```

```
Warning: MATLAB has disabled some advanced graphics rendering features by switching to software
 OpenGL. For more information, click here.
```

```
hold on
xlabel('Background');
ylabel('Roughness')
```



We can now calculate the individual posterior distributions by margnalising along the other dimension. For roughness we sum over columns..

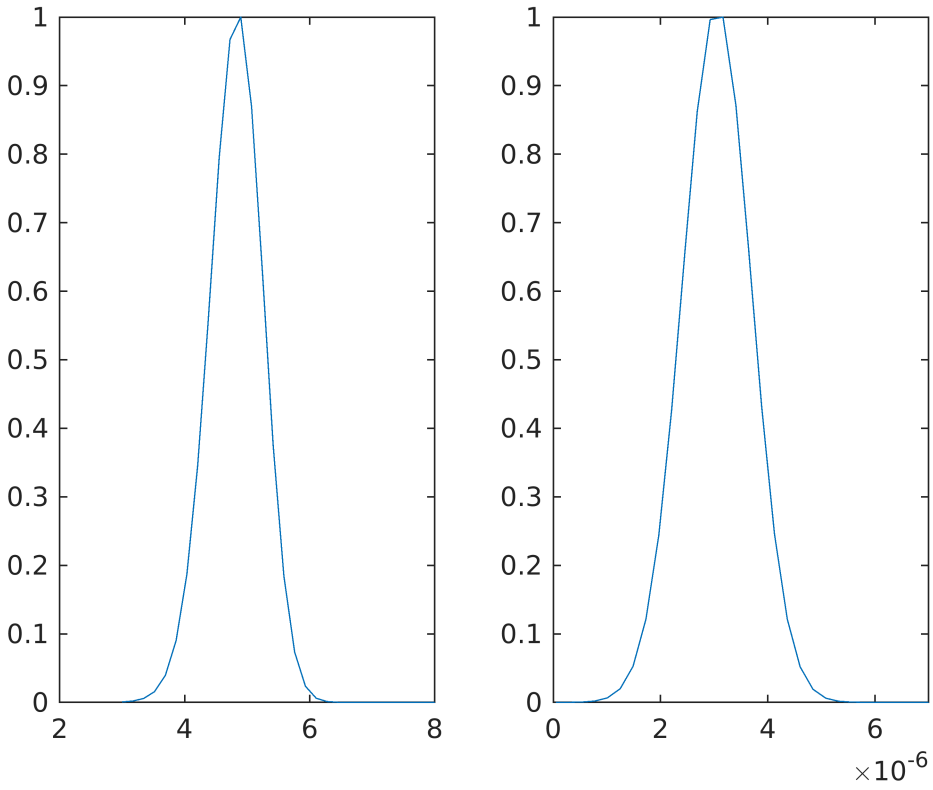
```
roughDist = sum(probArray,1);   % Sum over columns
backsDist = sum(probArray,2);   % Sum over rows
```

Normalise each distribution by simply dividing by the maximum value.

```
roughDist = roughDist ./ max(roughDist);
backsDist = backsDist ./ max(backsDist);

roughPosterior = [roughVector(:) backsDist(:)];
backsPosterior = [backsVector(:) roughDist(:)];

subplot(1,2,1);
plot(roughPosterior(:,1), roughPosterior(:,2));
subplot(1,2,2);
plot(backsPosterior(:,1), backsPosterior(:,2));
```



2. Delayed Rejection Adaptive Metropolis.

Now run the analysis using DRAM, and compare the resulting posteriors to the calculated ones.

```
problem.scalefactorFitYesNo = 0;

controls.procedure = 'bayes'
```

```
controls =
  controlsDef with properties:

           parallel: 'single'
          procedure: 'bayes'
    calcSldDuringFit: 'no'
             method: 'dram'
              nsimu: 1000
           adaptint: 1000
             burnin: 100
```

```
            repeats: 1
```

```
tic;
[outProb,results] = RAT(problem,controls)
```

```
Running loop 1 of 1
Sampling these parameters:
name   start [min,max] N(mu,s^2)
Substrate Roughness: 8 [3,8] N(0,Inf)
Background 1: 7e-06 [5e-08,7e-06] N(0,Inf)
outProb =
  problemDef with properties:

         experimentType: 'standard'
     experimentGeometry: 'air/substrate'
                nParams: 1
                 params: 8
              paramNames: {'Substrate Roughness'}
             paramConstr: {[3 8]}
           paramFitYesNo: 1
            nBackgrounds: 1
             backgrounds: 7.0000e-06
        backgroundNames: {'Background 1'}
       backgroundConstr: {[5.0000e-08 7.0000e-06]}
     backgroundFitYesNo: 1
          nScalefactors: 1
           scalefactors: 0.1014
       scalefactorNames: {'Scalefactor 1'}
      scalefactorConstr: {[0.0100 0.3000]}
    scalefactorFitYesNo: 0
              nQzshifts: 1
               qzshifts: 0
            qzshiftNames: {'Qz Shifts 1'}
           qzshiftConstr: {[-0.0300 0.0300]}
         qzshiftFitYesNo: 0
           nbairFitYesNo: 0
                 nNbsubs: 1
                  nbsubs: 6.3500e-06
              nbsubNames: {'D2O'}
             nbsubConstr: {[6.3000e-06 6.4000e-06]}
           nbsubFitYesNo: 0
       numberOfContrasts: 1
            nResolutions: 1
             resolutions: 0.0300
        resolutionNames: {'Resolution 1'}
       resolutionConstr: {[0.0100 0.0500]}
     resolutionFitYesNo: 0
                allData: {[53×3 double]}
             dataPresent: 1
                resample: 0
              dataLimits: {[0.0489 0.6117]}
               simLimits: {[0.0489 0.6117]}
           contrastBacks: {[1 1]}
          contrastShifts: 1
          contrastScales: 1
            contrastNbas: 1
            contrastNbss: 1
             contrastRes: 1
     contrastRepeatSLDs: {[0 1]}
              modelType: 'layers'
          numberOfLayers: 0
           layersDetails: {0×1 cell}
          contrastLayers: {[]}
results = struct with fields:
```

```
          res: [1×1 struct]
        chain: [5000×2 double]
      s2chain: []
      sschain: [5000×1 double]
    bestPars: [4.8270 3.0541e-06]
```

```
toc
```

```
Elapsed time is 7.466652 seconds.
```

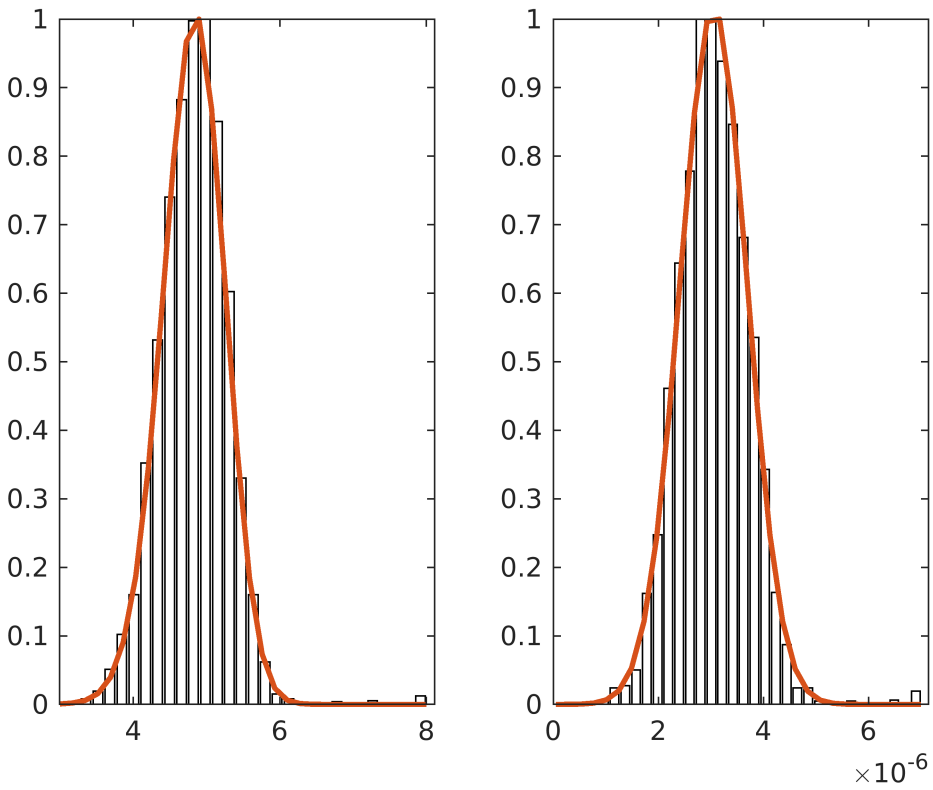
We can get the posteriors from results.chain...

```
roughPostDram = results.chain(:,1);
backPostDram = results.chain(:,2);

[roughCounts,roughBins] = hist(roughPostDram,30);
roughCounts = roughCounts ./ max(roughCounts);

[backCounts,backBins] = hist(backPostDram,30);
backCounts = backCounts ./ max(backCounts);

subplot(1,2,1); bar(roughBins,roughCounts,'w');
hold on; plot(roughPosterior(:,1), roughPosterior(:,2), 'LineWidth', 2.0)
subplot(1,2,2); bar(backBins,backCounts,'w');
hold on; plot(backsPosterior(:,1), backsPosterior(:,2), 'LineWidth',2.0);
```



3. Nested Sampling

Nested sampling is primarily for model selection, but can be used to obtain the posteriors also. We do the same comparison as for DRAM.

In order to switch to NS, we just need to change the relevant flag in controlsDef...

```
controls.procedure = 'NS';
controls.Nlive = 200
```

```
controls =
  controlsDef with properties:

           parallel: 'single'
          procedure: 'NS'
    calcSldDuringFit: 'no'
              Nlive: 200
              Nmcmc: 0
          propScale: 0.1000
        nsTolerance: 1
```

.. and run RAT..

```
tic;
[outNS,results] = RAT(problem,controls)
```

```
outNS =
  problemDef with properties:

        experimentType: 'standard'
    experimentGeometry: 'air/substrate'
               nParams: 1
                params: 8
            paramNames: {'Substrate Roughness'}
           paramConstr: {[3 8]}
         paramFitYesNo: 1
          nBackgrounds: 1
           backgrounds: 7.0000e-06
       backgroundNames: {'Background 1'}
      backgroundConstr: {[5.0000e-08 7.0000e-06]}
    backgroundFitYesNo: 1
         nScalefactors: 1
          scalefactors: 0.1014
      scalefactorNames: {'Scalefactor 1'}
     scalefactorConstr: {[0.0100 0.3000]}
   scalefactorFitYesNo: 0
             nQzshifts: 1
              qzshifts: 0
          qzshiftNames: {'Qz Shifts 1'}
         qzshiftConstr: {[-0.0300 0.0300]}
       qzshiftFitYesNo: 0
         nbairFitYesNo: 0
               nNbsubs: 1
                nbsubs: 6.3500e-06
            nbsubNames: {'D2O'}
           nbsubConstr: {[6.3000e-06 6.4000e-06]}
         nbsubFitYesNo: 0
     numberOfContrasts: 1
          nResolutions: 1
           resolutions: 0.0300
       resolutionNames: {'Resolution 1'}
```

```
       resolutionConstr: {[0.0100 0.0500]}
     resolutionFitYesNo: 0
                allData: {[53×3 double]}
            dataPresent: 1
               resample: 0
             dataLimits: {[0.0489 0.6117]}
              simLimits: {[0.0489 0.6117]}
          contrastBacks: {[1 1]}
         contrastShifts: 1
         contrastScales: 1
           contrastNbas: 1
           contrastNbss: 1
            contrastRes: 1
     contrastRepeatSLDs: {[0 1]}
              modelType: 'layers'
         numberOfLayers: 0
          layersDetails: {0×1 cell}
         contrastLayers: {[]}
results = struct with fields:
             logX: -5.0870
    nest_samples: [914×3 double]
    post_samples: [242×4 double]
        fitNames: {2×1 cell}
```

```
toc
```

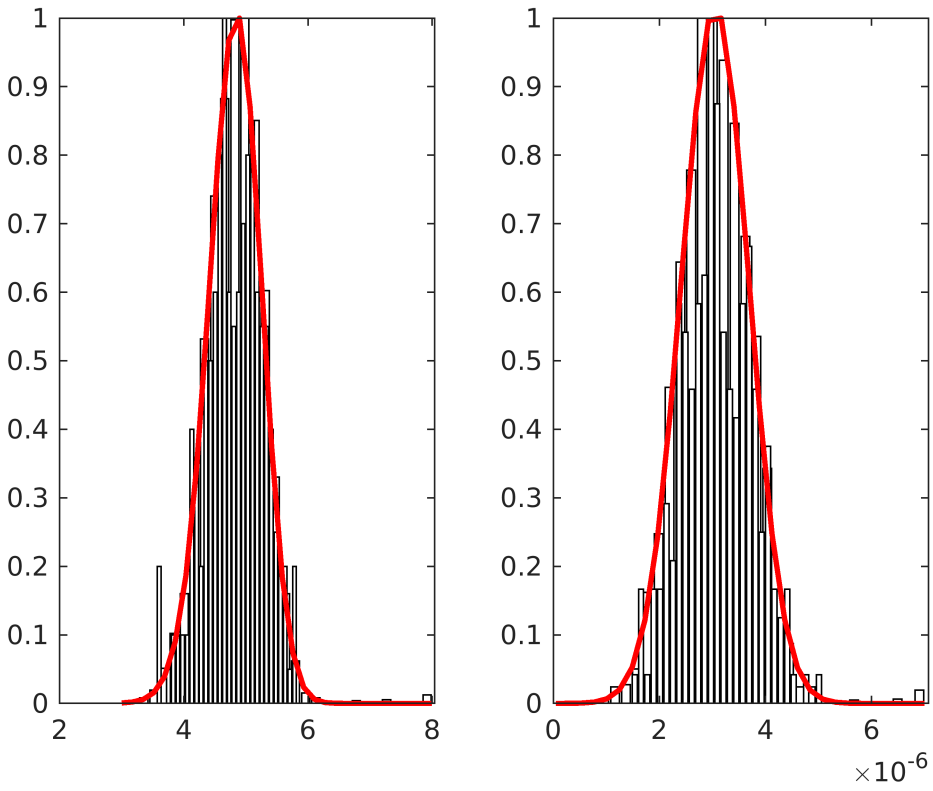
```
Elapsed time is 16.236259 seconds.
```

```
posteriors = results.post_samples;
roughPostNS = posteriors(:,1);
backPostNS = posteriors(:,2);

[roughCountsNS,roughBinsNS] = hist(roughPostNS,30);
roughCountsNS = roughCountsNS ./ max(roughCountsNS);

[backCountsNS,backBinsNS] = hist(backPostNS,30);
backCountsNS = backCountsNS ./ max(backCountsNS);

subplot(1,2,1); bar(roughBinsNS,roughCountsNS,'w');
hold on; plot(roughPosterior(:,1), roughPosterior(:,2),'r-', 'LineWidth', 2.0)
subplot(1,2,2); bar(backBinsNS,backCountsNS,'w');
hold on; plot(backsPosterior(:,1), backsPosterior(:,2),'r-', 'LineWidth',2.0);
```

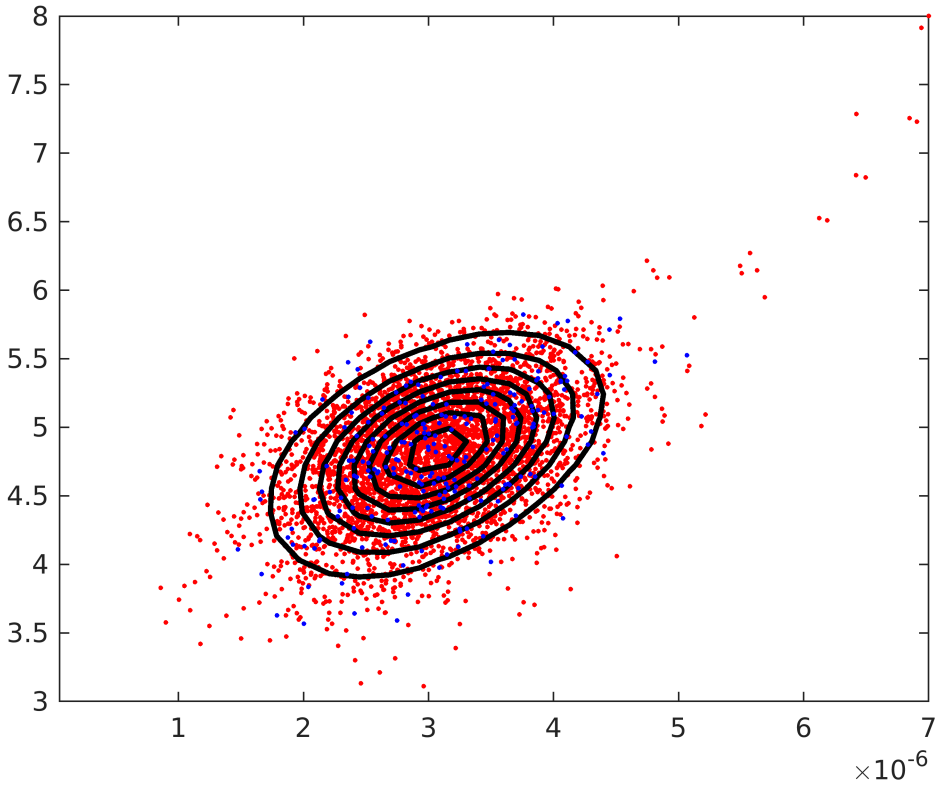


3. Overall Comparison

```
figure

hold on; box on

plot(backPostDram,roughPostDram,'r.')
contour(backsVector,roughVector,probArray,'k-','LineWidth',2);
plot(backPostNS,roughPostNS,'b.')
```


8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
1
2
3
4
5
6
7
×10-6