Analysis of the Gibbs Sampler for Hierarchical Inverse Problems

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Outline

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Hierarchical Inverse Problems with Gaussian Noise and Prior

\[ y = G(u) + \eta \]

- \( G : X \rightarrow Y \) continuous, \( X \) separable Hilbert, \( Y = X \) or \( \mathbb{R}^M \).

- \( \eta \sim N(0, \lambda^{-1}I) \).

- Prior \( u \sim N(0, \delta^{-1}C_\theta) \), \( \delta^{-1} > 0 \) amplitude, \( \sigma(C_\theta) \preceq \{j^{-2\theta-1}\}_{j \in \mathbb{N}}, \theta > 0 \) regularity.

- Fix \( \theta \). Hyper-prior \( \delta \sim \mathbb{P}(\delta) \). (can also fix \( \delta = 1 \), hyper-prior on \( \theta \))

- Stuart '10 conditions on \( G \)

\[ \mathbb{P}(u|y, \delta) \ll \mathbb{P}(u|\delta). \]
Sampling the Posterior

AIM: efficiently sample \( P(u, \delta | y) \propto P(u | y, \delta)P(\delta | y) \)

Natural to use Metropolis within Gibbs algorithm; range of possible parametrizations.

Centered MwG Algorithm

- update \( u^{(k+1)} | y, \delta^{(k)} \)
- update \( \delta^{(k+1)} | y, u^{(k+1)} \)

Individually each Metropolis step well understood, study interplay.

Bardsley ’12
Sampling the Posterior - Intuition

Think $\infty$-dim, discretize unknown in $\mathbb{R}^N$: study mixing as $N \rightarrow \infty$.

Centered MwG Algorithm: In continuum limit

- $\delta$ almost sure property of $u|\delta$.
- Abs ctty $\Rightarrow$ $\delta$ almost sure property of $u|y, \delta$.
- 2nd step, CA estimates $\delta$ pretending to know $u$; in fact know $u^{(k+1)}|y, \delta^{(k)}$.
- $\delta^{(k+1)}|y, u^{(k+1)}$ point mass on $\delta^{(k)}$.

$$\delta^{(k+1)}_N \sim \delta^{(k)}_N,$$ for large $N$.

- Intuition independent of dim($Y$) and $\mathbb{P}(\delta)$. 
Sampling the Posterior - Intuition

- Bad mixing of CA due to strong dependence of $u|\delta$ and $\delta$ as $N \to \infty$.
- Break dependence: $u = \delta^{-\frac{1}{2}} v$, $v \sim N(0, C_{\theta})$, $\delta \sim \mathbb{P}(\delta)$.

**Non-Centered MwG Algorithm**
- update $u^{(k+1)}|y, \delta^{(k)}$, compute $\nu^{(k+1)} = (\delta^{(k)})^{\frac{1}{2}} u^{(k+1)}$;
- update $\delta^{(k+1)}|y, \nu^{(k+1)}$.

Roberts and Stramer '01, Papaspiliopoulos, Roberts and Sköld '07

- NCA robust wrt $N$. 
Sampling the Posterior - Hierarchical Regularity

Intuition applies also for sampling $\mathbb{P}(u, \theta|y)$ when $\theta \sim \mathbb{P}(\theta)$ and $\delta = 1$ fixed.

- $\theta$ almost sure property of $u|\theta$.
- Conditions on $\mathcal{G}$ secure $\mathbb{P}(u|y, \theta) \ll \mathbb{P}(u|\theta)$.
- CA deteriorates as $N \to \infty$.
- Reparametrize, $u = C_\theta^{\frac{1}{2}} v$, $v \sim \mathcal{N}(0, I)$, $\theta \sim \mathbb{P}(\theta)$.
- NCA robust wrt $N$.

Analysis of GS difficult, no convergence results in limit $N \to \infty$ in nontrivial settings.
Linear Setting - Conditional Conjugacy

\[ G = K : X \rightarrow Y \ \text{linear bounded}, \ \delta \sim \text{Ga}(\alpha, \beta). \]

- Discretize unknown in \( \mathbb{R}^N \) and data in \( \mathbb{R}^M \), approximate operators \( K, C_\theta, I \).
- Bayes' theorem gives density of posterior on \( \mathbb{R}^N \times \mathbb{R} \)

\[
p(u, \delta | y) \propto \delta^{\alpha + \frac{N}{2} - 1} \exp\left( -\beta \delta - \frac{\lambda}{2} \| Ku - y \|^2 - \frac{\delta}{2} \| C_\theta^{-\frac{1}{2}} u \|^2 \right)
\]

- Conditional conjugacy

\[
u | y, \delta \sim N(m, C)
\]

\[
delta | y, u \sim \text{Ga}\left( \alpha + \frac{N}{2}, \beta + \frac{1}{2} \| C_\theta^{-\frac{1}{2}} u \|^2 \right)
\]

- Use understanding developed in A, Larsson, Stuart '13 to analyze.
Assume prior regular enough, $\mathbb{P}(u|y, \delta) = N(m, C) \ll \mathbb{P}(u|\delta) = N(0, \delta^{-1}C_\theta)$ in limit.

Use consistent discretizations of operators.

Lemma

$$\frac{1}{2}\|C_\theta^{-\frac{1}{2}}u^{(k+1)}\|^2 = (\delta^{(k)})^{-1}\frac{N}{2} + (\delta^{(k)})^{-1}\sqrt{\frac{N}{2}}W_{1,N} + F_N(\delta^{(k)})$$

i) 1st and 2nd terms LLN and CLT terms if $u^{(k+1)}$ drawn from prior $\mathbb{P}(u|\delta^{(k)})$;

ii) $F_N(\delta^{(k)})$ well controlled correction term since $u^{(k+1)}$ drawn from $\mathbb{P}(u|y, \delta^{(k)})$.

Property: $\text{Ga}(\alpha + \frac{N}{2}, \beta + \mu^{-1}\frac{N}{2}) \sim \text{Dirac}(\mu)$, for large $N$.

Combine $\mathbb{P}(\delta^{(k+1)}|y, u^{(k+1)}) \sim \text{Ga}(\alpha + \frac{N}{2}, \beta + (\delta^{(k)})^{-1}\frac{N}{2}) \sim \text{Dirac}(\delta^{(k)})$, for large $N$. 
Result - $\delta$ Evolves Slowly

Theorem (A, Bardsley, Papaspiliopoulos, Stuart '13)

For $N \to \infty$, for any $\delta > 0$ we have $y$ almost surely

$$\frac{N}{2} \mathbb{E} \left[ \delta_N^{(k+1)} - \delta_N^{(k)} | \delta_N^{(k)} = \delta \right] = (\alpha + 1)\delta - f(\delta; y)\delta^2 + o(1)$$

$$\frac{N}{2} \text{Var} \left[ \delta_N^{(k+1)} - \delta_N^{(k)} | \delta_N^{(k)} = \delta \right] = 2\delta^2 + O(N^{-\frac{1}{2}}).$$

All expectations taken wrt the randomness in the algorithm.

Looks like numerical discretization of

$$d\delta = \left( (\alpha + 1)\delta - f(\delta; y)\delta^2 \right) dt + \sqrt{2}\delta \, dW$$

with time-step $2N^{-1}$; hence $O(N)$ steps to sample posterior.
Marginal Algorithm

In linear case can analytically find $y|\delta$ by integrating out $u$ from likelihood.

**Marginal algorithm**

- update $u^{(k+1)}|y, \delta^{(k)}$;
- draw $\delta^{(k+1)}|y$.

MA optimal (in principle i.i.d $\delta$ samples) robust in $N$, use as gold standard.
Hierarchical Amplitude, $X = L^2[0, 1], Y = \mathbb{R}^{15}$

Figure: $K = P_{15} \circ (I + c(-\Delta))^{-1}, C_\theta = (-\Delta)^{-1}, \delta \sim \text{Ga}(1, 10^{-4}), \lambda = 100, N = 1023$
Centered Algorithm, $N = 15, 1023$
Non-Centered Algorithm, $N = 15, 1023$
Conclusions

- CA easy to implement, deteriorates for large dimension.
- NCA easy to implement, robust wrt dimension, but deteriorates for small noise.

δ (resp. θ) and ν a posteriori dependent via data; for exact data strong dependence.

**Figure:** Non-Centered Algorithm Amplitude, Small Noise $\lambda = 100^2$
Further Work

More research needed in small noise limit.

- MA optimal but in nonlinear setting marginalization is intractable, approximate using importance sampling leading to Pseudo-Marginal approach, Andrieu and Roberts '09, Filippone and Girolami '13.

- Interweaving method of Yu and Meng '11, PNCA of Papaspiliopoulos Roberts and Sköld '03 do not improve significantly.

- Random truncation of prior and use of Reversible Jump algorithm promising.

Further analysis of GS in high dimensions, extending theory to nonlinear setting, other parameters in prior, other priors...
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Hierarchical Regularity, $X = Y = L^2[0, 1]$

Figure: $K = I, C_\theta = (-\Delta)^{-\theta - \frac{1}{2}}, p(\theta) = e^{-\theta}, \lambda = 200, N = 512, \theta_{true} = 1.75$
Centered Algorithm, $N = 32, 8192$
Non-Centered Algorithm, $N = 32, 8192$
Non-Centered Algorithm Regularity, Small Noise $\lambda = 200^2$