

A Multivariate Gaussian Sampler in High Dimensions

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Reference: C. Gilavert, S. Moussaoui, J. Idier, Efficient Gaussian Sampling for Solving Large-Scale Inverse Problems using MCMC, IEEE Trans. Signal Processing, vol. 63, No. 1, pp. 70-80, 2015 ([Arxiv preprint:1409.0606](#)).

Introduction

Draw K samples $\{\mathbf{x}_k\}_{k=1}^K$, from a N -dimensional Gaussian distribution

$$\mathbf{x}_k \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{R})$$

with a mean vector $\boldsymbol{\mu} \in \mathbb{R}^N$ and a symmetric definite positive covariance matrix $\mathbf{R} \in \mathbb{R}^{N \times N}$.

⊗ **Classical approach** [Wold 1948 ; Scheuer and Stoller, 1962]

1. perform the Cholesky factorization, $\mathbf{R} = \mathbf{L}_r \mathbf{L}_r^t, \rightsquigarrow \mathcal{O}(N^3)$
2. draw a sample from a standard Gaussian distribution, $\boldsymbol{\omega} \sim \mathcal{N}(\mathbf{0}_N, \mathbf{I}_N)$,
3. retain $\mathbf{x} = \mathbf{L}_r \boldsymbol{\omega} + \boldsymbol{\mu}$.

◁ *Main purpose: reduce the computation complexity of MCMC algorithms involving repeated application of high-dimensional Gaussian sampling*

Outline

1. Gaussian sampling for a Bayesian inference
 - Context of inverse problems
 - Main approaches
2. Gaussian sampling within the Reversible Jump MCMC framework
 - The Reversible Jump MCMC framework
 - Proposed sampler
3. Sampler cost optimization and its adaptive tuning
 - Targeting an acceptance rate
 - Optimization of the computation cost
4. Concluding remarks

1. Gaussian sampling for a Bayesian inference

1.1 Context of inverse problems

The *observations* $\mathbf{y} \in \mathbb{R}^M$ are expressed according to

$$\mathbf{y} = \mathbf{H} \mathbf{x} + \mathbf{n} \quad (1)$$

with $\mathbf{x} \in \mathbb{R}^N$ the *sought variable* and $\mathbf{H} \in \mathbb{R}^{M \times N}$ the *observation matrix* (convolution, projection, mixing)

- Gaussian likelihood: $\mathbf{y} | (\mathbf{x}, \boldsymbol{\mu}_n, \mathbf{R}_n) \sim \mathcal{N}(\mathbf{H}\mathbf{x} + \boldsymbol{\mu}_n, \mathbf{R}_n)$,
- Gaussian prior: $\mathbf{x} | (\boldsymbol{\mu}_x, \mathbf{R}_x) \sim \mathcal{N}(\boldsymbol{\mu}_x, \mathbf{R}_x)$
 - Simple Gaussian model,
 - Gaussian Markov random fields,
 - Hierarchical Gaussian model (scale/location Gaussian mixtures).

- Inference from the posterior distribution,

$$P(\mathbf{x}, \Theta | \mathbf{y}) \propto P(\mathbf{y} | \mathbf{x}, \Theta) P(\mathbf{x} | \Theta) P(\Theta) \quad (2)$$

with Θ hyperparameter set, $\Theta = \{\boldsymbol{\mu}_x, \mathbf{R}_x, \boldsymbol{\mu}_n, \mathbf{R}_n\}$

- Gibbs sampler: for $k = 1, \dots, K$,

$$\begin{cases} \text{sample } \Theta_k \sim P(\Theta | \mathbf{y}, \mathbf{x}_{k-1}) \\ \text{sample } \mathbf{x}_k \sim P(\mathbf{x} | \mathbf{y}, \Theta_k) \end{cases}$$

According to the Bayesian model,

$$\mathbf{x} | (\mathbf{y}, \Theta) \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{R} = \mathbf{Q}^{-1})$$

with

$$\mathbf{Q} = \mathbf{H}^t \mathbf{R}_n^{-1} \mathbf{H} + \mathbf{R}_x^{-1}, \quad \rightsquigarrow \mathbf{Q} = \mathbf{F}^t \mathbf{F} \quad (3)$$

$$\mathbf{Q}\boldsymbol{\mu} = \mathbf{H}^t \mathbf{R}_n^{-1} (\mathbf{y} - \boldsymbol{\mu}_n) + \mathbf{R}_x^{-1} \boldsymbol{\mu}_x. \quad \rightsquigarrow \mathbf{Q}\boldsymbol{\mu} = \mathbf{b} \quad (4)$$

◁ *The calculation of the distribution involves the precision matrix \mathbf{Q} , instead of \mathbf{R}*

◁ *A matrix inversion is necessary to apply the classical sampling approach*

◁ *The posterior mean is given as the solution of a linear system depending on \mathbf{Q}*

⊗ **Solution 1.** *Avoid high-dimensionnal matrix inversion.* [Rue, 2001]

1. perform the Cholesky factorization of $\mathbf{Q} = \mathbf{L}_q \mathbf{L}_q^t$, instead of \mathbf{R} ,
2. draw a sample from a standard Gaussian distribution, $\boldsymbol{\omega} \sim \mathcal{N}(\mathbf{0}_N, \mathbf{I}_N)$,
3. solve $\mathbf{L}_q \mathbf{z} = \mathbf{b}$ and get \mathbf{z} ,
4. retain \mathbf{x} , solution of $\mathbf{L}_q^t \mathbf{x} = \mathbf{z} + \boldsymbol{\omega}$.

⊗ **Solution 2. Perturbation-Optimization** [Orioux et al., 2012 ; Lalanne 2001]

1. draw a sample from a standard Gaussian distribution, $\omega \sim \mathcal{N}(\mathbf{0}_{M+N}, \mathbf{I}_{M+N})$,
2. get a sample from a Gaussian distribution, $\eta \sim \mathcal{N}(Q\mu, Q)$, according to $\eta = F^t\omega + Q\mu$,
3. retain x , solution of $Qx = \eta$.

◁ *The complexity of both solutions (1 and 2) is $\mathcal{O}(N^3)$ unless matrix Q exhibits an exploitable structure,*

◁ *Matrix Q depends on Θ and, thus, varies during Gibbs sampler iterations.*

⊗ **Practical alternative.** [Bardsley, 2010 ; Papandreou et al., 2010 ; Tan et al., 2010]

Numerical complexity reduction by applying an early stopped iterative solver (conjugate gradient) in Step 3.

◁ *Question 1. Correctness of the sampler?*

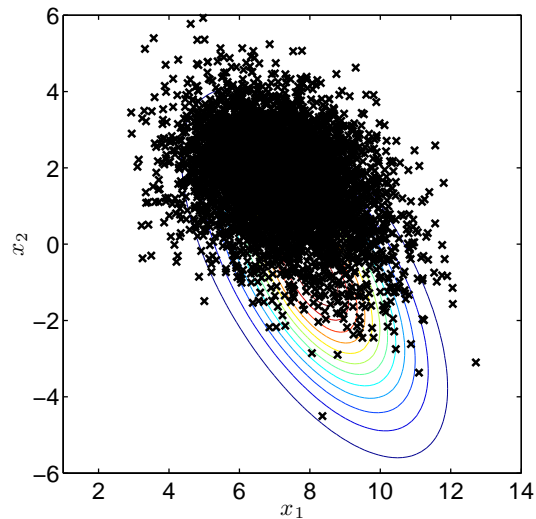
◁ *Question 2. Choice of the truncation level?*

◁ *Approximate resolution induces an incorrect sampling !*

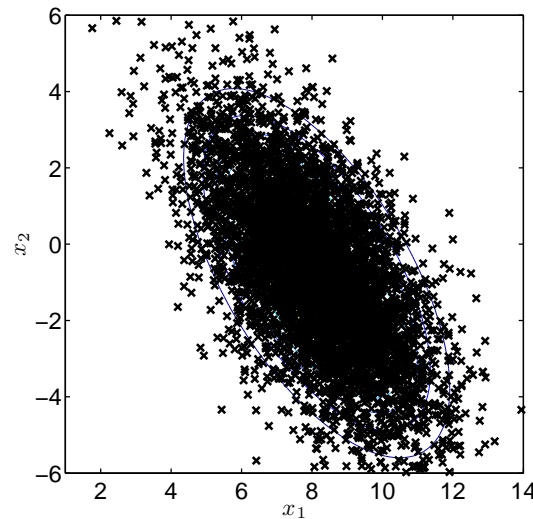
Let Q and μ be defined by

$$Q = R^{-1} \text{ with } R_{ij} = \sigma^2 \rho^{|i-j|} \text{ and } \mu_i \sim \mathcal{U}[0, 10], \quad (\forall i, j = 1, \dots, N) \quad (5)$$

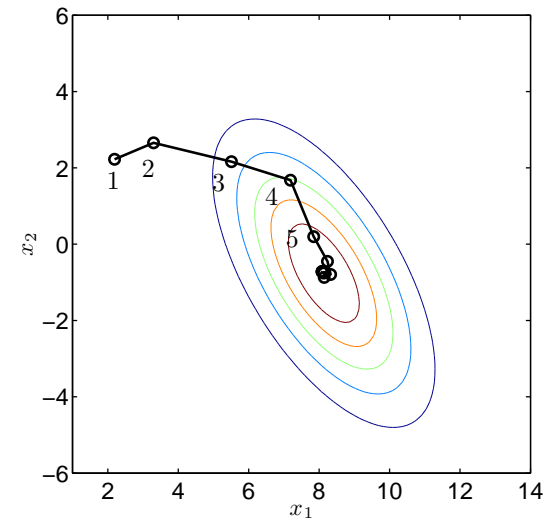
with $N = 20$, $\sigma^2 = 1$ and $\rho = 0.8$. Draw $K = 10,000$ samples.



$J = 4$ CG iterations



$J = 10$ CG iterations



Sample mean

Our proposal: Introduce an accept-reject step to correct this behavior.

2. Sampling within the Reversible Jump MCMC framework

2.1 Reversible Jump MCMC [Green, 1995 ; Waagepetersen and Sorensen, 2001]

- Construct a Markov chain whose distribution asymptotically converges to the target distribution $P_{\mathbf{X}}(\cdot)$.
- Introduce an auxiliary variable $\mathbf{z} \in \mathbb{R}^L \sim f_{\mathbf{Z}}(\mathbf{z}|\mathbf{x}_{\text{old}})$ and define a differentiable transformation $\phi(\cdot)$

$$\begin{aligned}\phi : (\mathbb{R}^N \times \mathbb{R}^L) &\mapsto (\mathbb{R}^N \times \mathbb{R}^L) \\ (\mathbf{x}_{\text{old}}, \mathbf{z}) &\mapsto (\mathbf{x}, \mathbf{s})\end{aligned}$$

that must be reversible $\phi(\mathbf{x}, \mathbf{s}) = (\mathbf{x}_{\text{old}}, \mathbf{z})$.

- The transition from \mathbf{x}_{old} to \mathbf{x}_{new} is governed by an acceptance probability

$$\alpha(\mathbf{x}_{\text{old}}, \mathbf{x}) = \min \left(1, \frac{P_{\mathbf{X}}(\mathbf{x})P_{\mathbf{Z}}(\mathbf{s}|\mathbf{x})}{P_{\mathbf{X}}(\mathbf{x}_{\text{old}})P_{\mathbf{Z}}(\mathbf{z}|\mathbf{x}_{\text{old}})} |J_{\phi}(\mathbf{x}_{\text{old}}, \mathbf{z})| \right).$$

where $J_{\phi}(\cdot)$ is the Jacobian determinant of $\phi(\cdot)$.

2.2 Gaussian sampling within RJMCMC

To sample from a Gaussian distribution $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{Q}^{-1})$,

- An auxiliary variable $\boldsymbol{z} \in \mathbb{R}^N$ is sampled from

$$P_{\boldsymbol{Z}}(\boldsymbol{z}|\boldsymbol{x}_{\text{old}}) = \mathcal{N}(\boldsymbol{A}\boldsymbol{x}_{\text{old}} + \boldsymbol{c}, \boldsymbol{B}). \quad (6)$$

The choice of $\boldsymbol{A} \in \mathbb{R}^{N \times N}$, $\boldsymbol{B} \in \mathbb{R}^{N \times N}$ and $\boldsymbol{c} \in \mathbb{R}^{N \times N}$ will be discussed later.

- The deterministic move is performed using the transformation $\phi(\cdot)$, such that

$$\begin{pmatrix} \boldsymbol{x} \\ \boldsymbol{s} \end{pmatrix} = \begin{pmatrix} \phi_1(\boldsymbol{x}_{\text{old}}, \boldsymbol{z}) \\ \phi_2(\boldsymbol{x}_{\text{old}}, \boldsymbol{z}) \end{pmatrix} = \begin{pmatrix} -\boldsymbol{x}_{\text{old}} + \boldsymbol{f}(\boldsymbol{z}) \\ \boldsymbol{z} \end{pmatrix}, \quad (7)$$

with functions $(\boldsymbol{f} : \mathbb{R}^N \mapsto \mathbb{R}^N)$, $(\phi_1 : (\mathbb{R}^N \times \mathbb{R}^N) \mapsto \mathbb{R}^N)$ and $(\phi_2 : (\mathbb{R}^N \times \mathbb{R}^N) \mapsto \mathbb{R}^N)$.

$\triangleleft \boldsymbol{f}(\boldsymbol{z})$ must be independent from $\boldsymbol{x}_{\text{old}}$ to ensure the reversibility condition

⊛ **Proposition** [Gilavert 2014]

Let an auxiliary variable \mathbf{z} be obtained according to (6) and a proposed sample \mathbf{x} according to the transformation defined by (7). Then the acceptance probability is

$$\alpha(\mathbf{x}_{old}, \mathbf{x}) = \min \left(1, e^{-\mathbf{r}(\mathbf{z})^t(\mathbf{x}_{old} - \mathbf{x})} \right),$$

with $\mathbf{r}(\mathbf{z}) = \mathbf{Q}\boldsymbol{\mu} + \mathbf{A}^t \mathbf{B}^{-1} (\mathbf{z} - \mathbf{c}) - \frac{1}{2} (\mathbf{Q} + \mathbf{A}^t \mathbf{B}^{-1} \mathbf{A}) \mathbf{f}(\mathbf{z})$.

In particular, the acceptance probability equals one when $\mathbf{f}(\mathbf{z})$ is the exact solution of the linear system

$$\frac{1}{2} (\mathbf{Q} + \mathbf{A}^t \mathbf{B}^{-1} \mathbf{A}) \mathbf{f}(\mathbf{z}) = \mathbf{Q}\boldsymbol{\mu} + \mathbf{A}^t \mathbf{B}^{-1} (\mathbf{z} - \mathbf{c}). \quad (8)$$

⊛ **Proof.** See paper [Gilavert 2015].

⊛ Consequence

Setting $A = B = Q$ and $c = Q\mu$

- defines $z \sim \mathcal{N}(Qx_{\text{old}} + Q\mu, Q)$, which can also be expressed as $z = Qx_{\text{old}} + \eta$,
- simplifies equation (8) to a linear system $Qf(z) = z$,
- cancels the correlation between successive samples when the acceptance probability equals one,
- by substituting $x = f(z) - x_{\text{old}}$ in (8), the latter becomes $Qx = \eta$.

2.3 Reversible Jump Perturbation-Optimization algorithm

1. Sample $\eta \sim \mathcal{N}(Q\mu, Q)$.
2. Solve the linear system $Qx = \eta$ in an approximate way. Let \hat{x} denote the obtained solution and $r(z) = \eta - Q\hat{x}$.
3. With probability $\min\left(1, e^{-r(z)^t(x_{\text{old}} - \hat{x})}\right)$, set $x_{\text{new}} = \hat{x}$, otherwise set $x_{\text{new}} = x_{\text{old}}$.

◁ To ensure reversibility of the deterministic move, the initial point x_0 of the solver must be such that $u_0 = x_0 + x_{\text{old}}$ does not depend on x_{old} .

◁ Consequence: setting $x_0 = \mathbf{0}$ or $x_0 = x_{\text{old}}$ is not allowed, while $x_0 = -x_{\text{old}}$ is the default choice corresponding to $u_0 = \mathbf{0}$.

⊛ Comparison with the T-PO algorithm

Similarly to the T-PO, the proposed RJPO algorithm relies on the approximate resolution of the same linear system $Qx = \eta$, but with two additional features:

- An accept-reject strategy to ensure the sampler convergence,
- An initial point x_0 of the linear solver such that $x_0 + x_{\text{old}}$ does not depend on x_{old} .

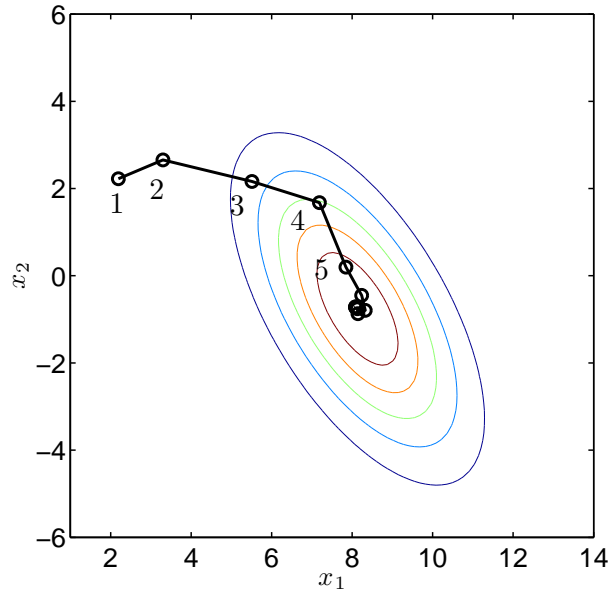
⊛ Implementation issues

- The linear conjugate gradient algorithm is used for the system resolution since it permits a matrix-free implementation with reduced memory requirements,
- A stopping rule based on a threshold on the relative residual norm is applied:

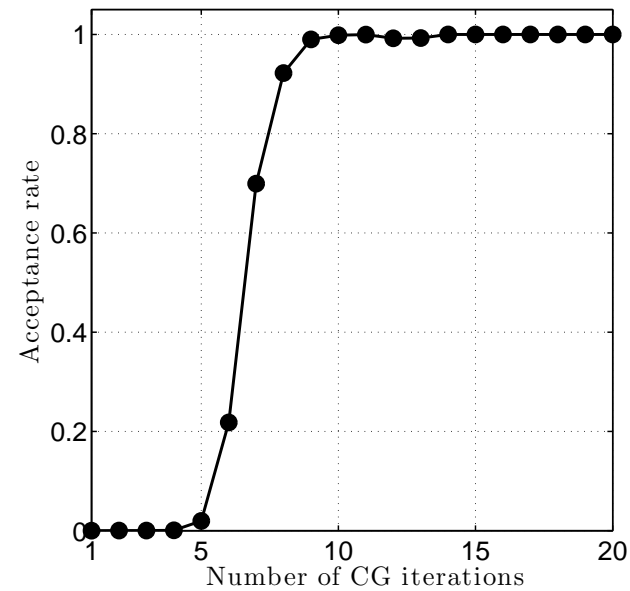
$$\epsilon = \frac{\|\eta - Qx\|_2}{\|\eta\|_2}.$$

1) Application to the toy example

⊛ Acceptance probability



Sample mean



acceptance rate

◁ The acceptance rate curve indicates a required minimal number of CG iterations,

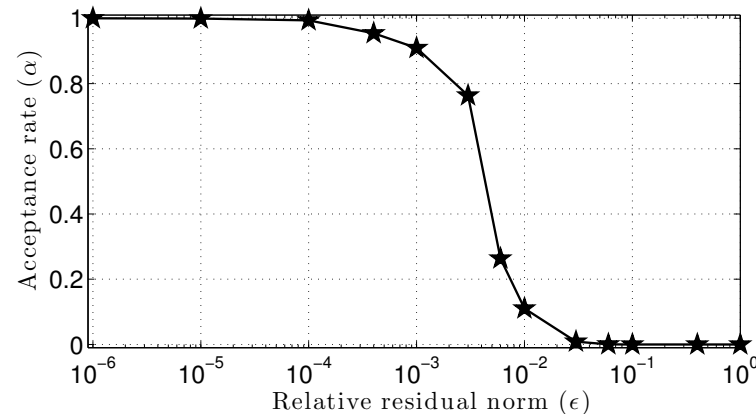
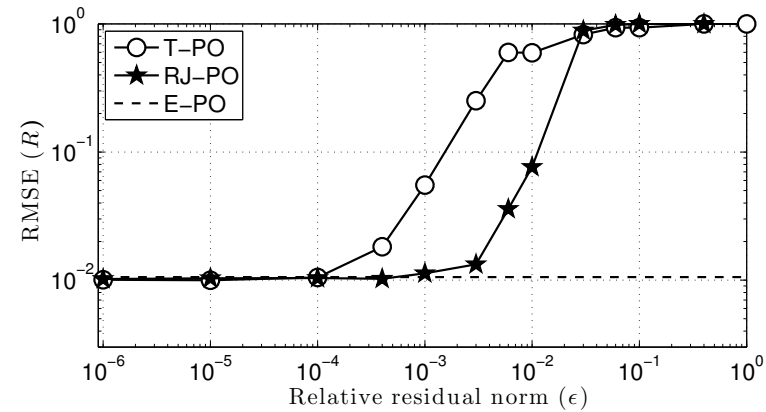
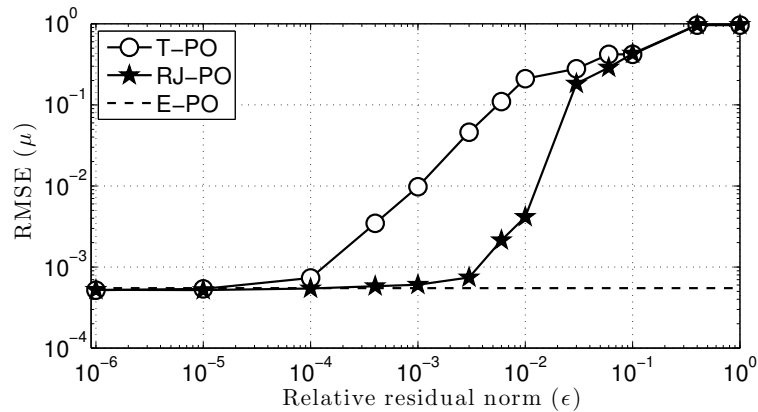
◁ How to choose the appropriate truncation level to maximize efficiency?

2) Influence of the relative residual norm

⊗ Estimation error

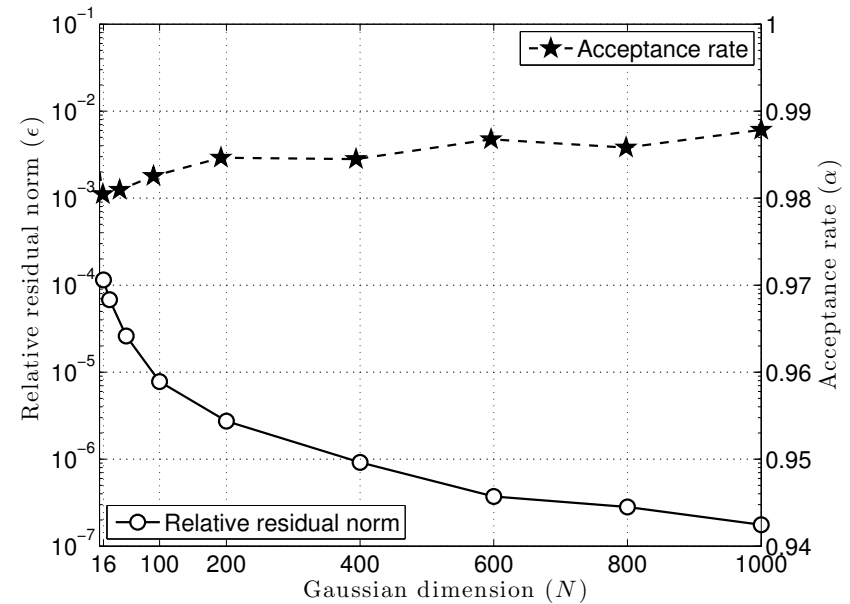
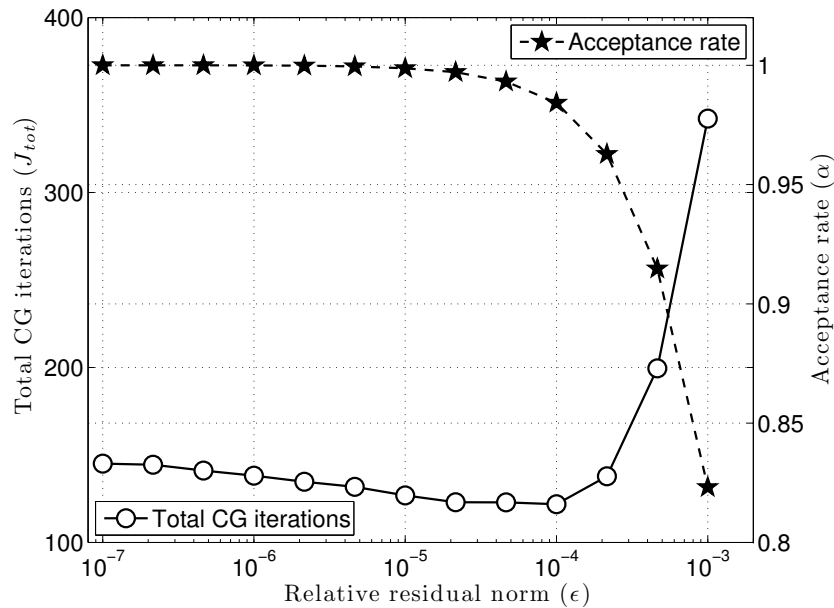
$$\text{RMSE}(\boldsymbol{\mu}) = \frac{\|\boldsymbol{\mu} - \hat{\boldsymbol{\mu}}\|_2}{\|\boldsymbol{\mu}\|_2} \quad \text{and} \quad \text{RMSE}(\mathbf{R}) = \frac{\|\mathbf{R} - \hat{\mathbf{R}}\|_F}{\|\mathbf{R}\|_F},$$

where $\hat{\boldsymbol{\mu}}$ and $\hat{\mathbf{R}}$ the empirical estimates using 10^5 generated Markov chain samples.



* Convergence diagnosis and computation cost

- Assess the total (cumulated) number of conjugate gradient iterations before convergence (diagnosis based on Gelman-Rubin convergence criterion on 100 parallel chains)



◁ A lower acceptance rate induces a higher number of iterations due to slow convergence.

◁ A minimal cost can be reached and it corresponds to an acceptance rate of almost one.

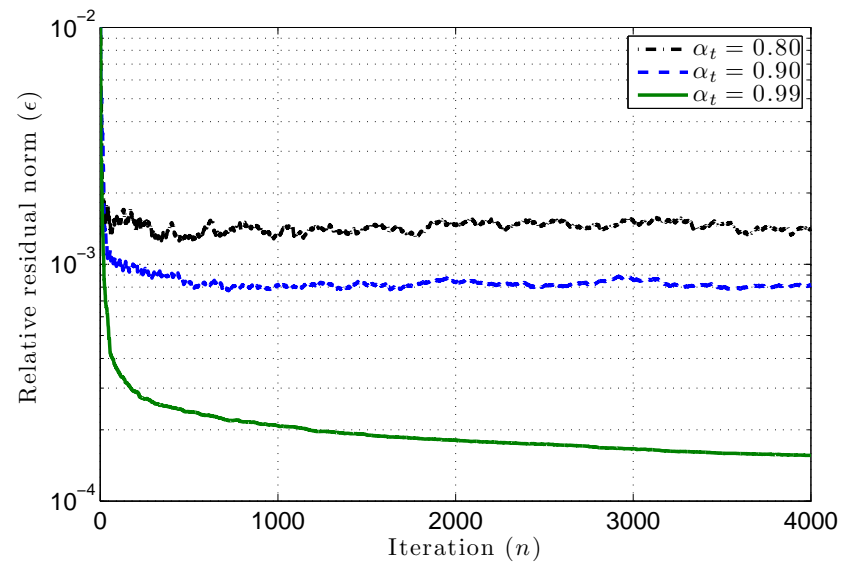
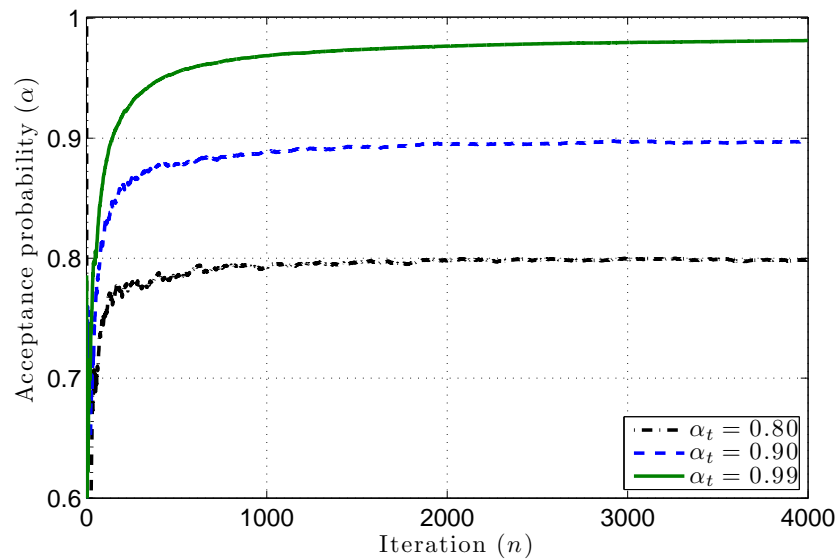
3. Adaptive tuning of the Gaussian sampler

3.1 Targeting a predefined acceptance rate

Adjust recursively the relative residual norm ϵ to achieve a desired acceptance rate α_t using a stochastic approximation procedure [Andrieu and Robert 2001]

$$\log(\epsilon_{k+1}) = \log(\epsilon_k) + \gamma_k [\alpha(\mathbf{x}_k, \mathbf{x}) - \alpha_t] \tag{9}$$

with $\gamma_k = K_0 k^{-\beta}$. (Take $K_0 = 1$ and $\beta = 0.5$.)



3.2 Minimization of the computation cost per effective sample

1) Statistical efficiency

- Effective sample size (ESS) [Goodman and Sokal, 1989]: number n_{eff} of independent samples, that would yield the same estimation variance in approximating the Bayesian estimator as n_{max} samples of the simulated chain:

$$n_{\text{eff}} = \frac{n_{\text{max}}}{1 + 2 \sum_{k=1}^{\infty} \rho_k} \quad (10)$$

where ρ_k the autocorrelation coefficient at lag k . For a first-order autoregressive chain, $\rho_k = \rho^k$,

$$n_{\text{eff}} = n_{\text{max}} \frac{1 - \rho}{1 + \rho} \implies \text{ESS Ratio} = \frac{n_{\text{eff}}}{n_{\text{max}}}. \quad (11)$$

- It defines how many iterations n_{max} are needed for each resolution accuracy in order to get chains having the same effective sample size.

2) Computation cost per effective sample

We propose to define the *computing cost per effective sample* (CCES) as

$$\text{CCES} = \frac{J_{\text{tot}}}{n_{\text{eff}}} = J \cdot \frac{1 + \rho}{1 - \rho}. \quad (12)$$

where $J = J_{\text{tot}}/n_{\text{max}}$ is the average number of CG iterations per sample.

- The chain correlation ρ is an implicit function of the acceptance rate α . It has two terms:
 - With a probability $(1 - \alpha)$, the accept-reject procedure produces identical (*i.e.*, maximally correlated) samples in case of rejection.
 - In case of acceptance, the new sample is slightly correlated with the previous one, because of the early stopping of the CG algorithm.
- The correlation induced in the case of acceptance is negligible compared to the correlation

induced by rejection.

Thus, $\rho = (1 - \alpha)$ and

$$\text{CCES} = J \frac{1 + \rho}{1 - \rho} = \frac{2 - \alpha}{\alpha}$$

- The best tuning of the relative residual norm leading to the lowest CCES satisfies

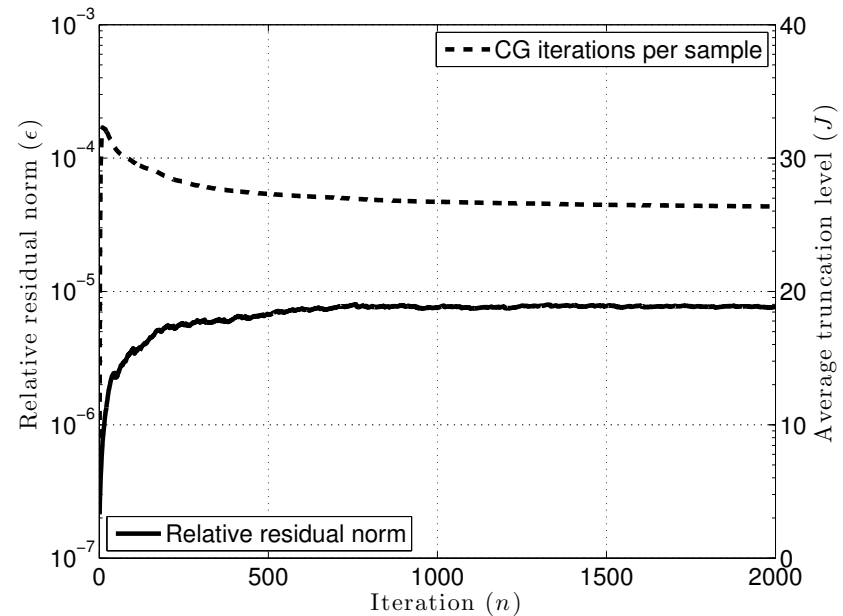
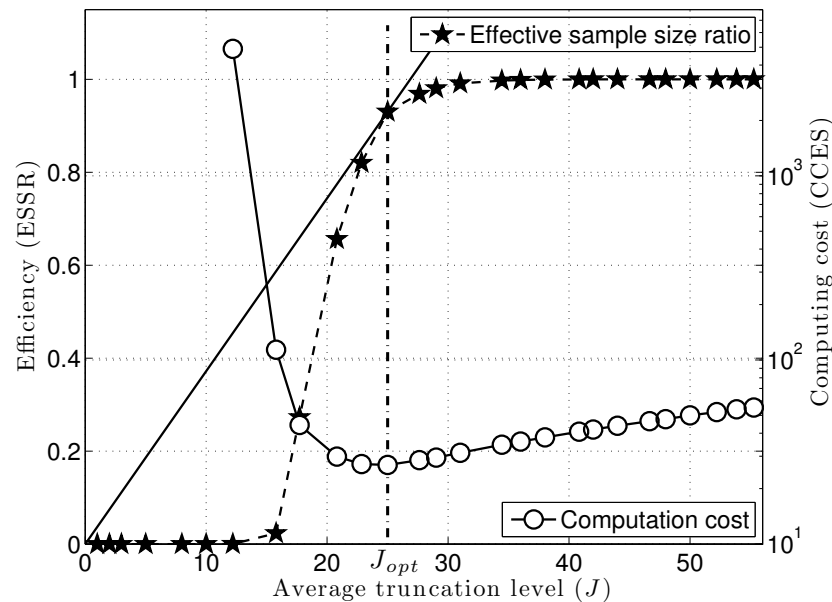
$$J \frac{d\alpha}{dJ} - \alpha + \frac{\alpha^2}{2} = 0.$$

◁ The solution can not be calculated analytically.

⊛ Adaptive tuning

The stochastic approximation procedure is now applied to adaptively adjust the optimal value of ϵ ,

$$\log \epsilon_{k+1} = \log \epsilon_k + \gamma_k \left(J_k \frac{d\alpha_k}{dJ} - \alpha_k + \frac{\alpha_k^2}{2} \right), \quad (13)$$

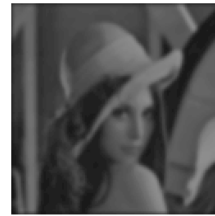


◁ *There is no need to define the target acceptance probability.*

3.3 Example of image superresolution



Original image



One observation



Reconstructed image

Having 5 images of size 128×128 pixels ($M = 81920$) we reconstruct the original one of size 256×256 ($N = 65536$ pixels).

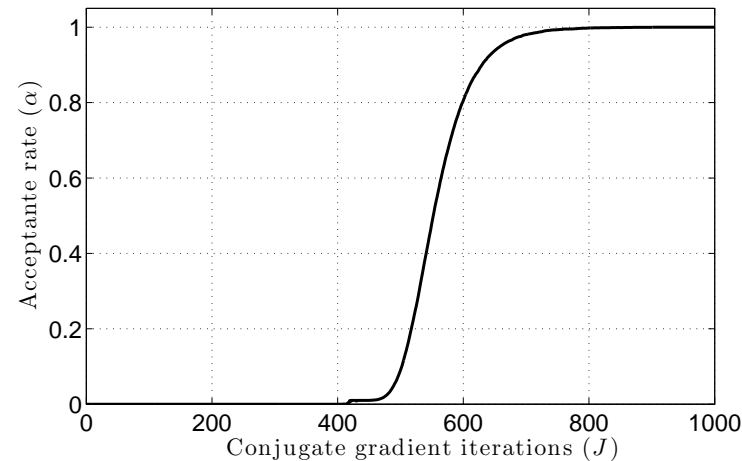
- The noise is assumed zero mean, Gaussian with an unknown precision matrix $Q_n = \gamma_n \mathbf{I}$,
- A zero-mean Gaussian distribution x , with a precision matrix $Q_x = \gamma_x \mathbf{D}^t \mathbf{D}$ assigned to x , with \mathbf{D} a circulant convolution matrix associated to a Laplacian filter.

- Non-informative Jeffrey's priors are assigned to the two hyper-parameters γ_n and γ_x .
- A Gibbs sampler is run for 1000 iterations and a burn-in period of 100 iterations.

⊛ **Sampled posterior statistics.** Mean (standard deviation)

	γ_n	$\gamma_x \times 10^{-4}$	x_i
Cholesky	102.1 (0.56)	6.1 (0.07)	104.6 (9.06)
T-PO $\epsilon = 10^{-4}$	0.3 (0.06)	45 (0.87)	102.2 (3.30)
T-PO $\epsilon = 10^{-6}$	6.8 (0.04)	32 (0.22)	104.8 (2.34)
T-PO $\epsilon = 10^{-8}$	71.7 (0.68)	21 (0.29)	102.7 (2.51)
RJPO $\alpha_t = 0.99$	101.2 (0.55)	6.1 (0.07)	101.9 (8.89)

⊛ Acceptance rate



⊛ Computation time and memory usage

- The computation time per sample, on a Intel Core i7-3770 with 8 GB of RAM and a 64bit system :
 - Cholesky sampler: 20.3s and the required memory is about 6 GB
 - RJPO algorithm: 15.1s and the memory usage is less than 200 MB
- This last result is due to the use of a conjugate gradient on which each matrix-vector product is performed without explicitly writing the matrix Q .

4. Conclusions

- Convergent multivariate Gaussian sampling suitable for high-dimensional problems
- Empirical analysis of the statistical efficiency,
- Set an adaptive tuning allowing to optimize the computation cost.

⊗ Open questions

- Establish a link between the proposed strategy and random walk Metropolis Hastings (RWMH), Metropolis Adjusted Langevin Algorithm (MALA)?
- Use of the computation cost per effective sample for an adaptive scaling of RWMH and MALA?