On a generalization of the preconditioned Crank-Nicolson Metropolis algorithm

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Abstract

Metropolis algorithms for approximate sampling of probability measures on infinite dimensional Hilbert spaces are considered and a generalization of the preconditioned Crank-Nicolson (pCN) proposal is introduced. The new proposal is able to incorporate information of the measure of interest. A numerical simulation of a Bayesian inverse problem indicates that a Metropolis algorithm with such a proposal performs independent of the state space dimension and the variance of the observational noise. Moreover, a qualitative convergence result is provided by a comparison argument for spectral gaps. In particular, it is shown that the generalization inherits geometric ergodicity from the Metropolis algorithm with pCN proposal.

1 Introduction

Consider a target probability distribution $\mu$ defined on a possibly infinite dimensional separable Hilbert space $\mathcal{H}$. It is of interest to sample from this probability measure and assumed that there is a density of $\mu$ w.r.t. a Gaussian reference measure $\mu_0$ on $\mathcal{H}$ given by

$$ \frac{d\mu}{d\mu_0}(u) = \frac{1}{Z} \exp(-\Phi(u)), \quad u \in \mathcal{H}. \quad (1) $$
Here \( \Phi: \mathcal{H} \to \mathbb{R}_+ \) is a measurable function and \( Z = \int_{\mathcal{H}} \exp(-\Phi(u)) \mu_0(du) \) the normalizing constant. Such probability measures \( \mu \) arise as posterior distributions in Bayesian inference with \( \mu_0 \) as Gaussian prior. Common examples in infinite dimensional spaces are inferring spatially distributed properties of subsurface layers or stock prices.

Unfortunately, the fact that the normalizing constant \( Z \) is typically unknown and we can only ask for function values of \( \Phi \) makes it difficult to sample \( \mu \) directly. But Markov chains and in particular Metropolis-Hastings (MH) algorithms are applicable for approximate sampling. These algorithms consist of a proposal and an acceptance/rejection step. A state is proposed by the use of a proposal kernel but it is only accepted with a certain probability which depends on \( \frac{d\mu}{d\mu_0} \). The authors of [1] suggested a modification of a Gaussian random walk proposal which is \( \mu_0 \)-reversible. The latter property leads to a well-defined MH algorithm in infinite dimensional Hilbert spaces, see also [26]. This proposal was later [3] referred to as preconditioned Crank-Nicolson (pCN) proposal. Remarkably, the Markov chain of the resulting pCN Metropolis algorithm has dimension-independent sampling efficiency, see [3, 12]. This is a significant advantage compared to former, popular MH algorithms whose performance usually deteriorates with increasing state space dimension [3, 12, 21].

We extend the pCN proposal to incorporate information about the target measure \( \mu \). Such an adaption might exploit the anisotropy of the covariance of \( \mu \) or the local curvature of \( \Phi \). Intuitively, the resulting Markov chain has on average a larger step size and, thus, explores the state space faster. This idea is not entirely new. It is already mentioned in [25] where it is suggested to choose the covariance of the proposal adapted to the target measure. Later in [10] the authors explain how to propose new states using general local metric tensors. Moreover, in [18] the Hessian of the negative log density \( \Phi \) of \( \mu \) is employed as local curvature information to design a stochastic Newton MH method in finite dimensions and in [4, 15] a Gauss-Newton variant for capturing global curvature in an infinite dimensional setting is outlined.

Our approach for adapting the proposal to the target measure \( \mu \) has a similar motivation as the proposals considered in [4, 15]. It comes from a local linearization of the unknown-to-observable map in Bayesian inverse problems. This suggests a particular form for approximating the covariance of the target measure, namely \( (C + \Gamma)^{-1} \), where \( C \) denotes the covariance of the reference measure \( \mu_0 \) and \( \Gamma \) is a suitable self-adjoint and positive operator. We then consider the class of Gaussian proposals with covariance \( C_\Gamma = (C + \Gamma)^{-1} \). By enforcing \( \mu_0 \)-reversibility we derive our class of
generalized pCN (gpCN) proposal kernels $P_\Gamma$.

In a numerical simulation the resulting Metropolis algorithm performs dimension and variance independent. Here variance independence refers to the variance of the observational noise, which implicitly determines the covariance of the target distribution $\mu$. Particularly, if the variance of the noise decreases the measure $\mu$ becomes more concentrated. The numerical experiments also indicate that other popular MH or random walk algorithms perform worse, i.e., variance dependent.

Moreover, we present a convergence result for the gpCN Metropolis via spectral gaps. It is well known, see [20], that for Markov chains with reversible transition kernels $K$ a strictly positive spectral gap, in formulas $\text{gap}(K) > 0$, is equivalent to geometric ergodicity. The latter roughly means that the distribution of the $n$th step of a Markov chain converges exponentially fast to its stationary distribution. We refer to Section 2.1 for precise definitions and further details.

Our main theoretical result, see Theorem 20, is as follows: Let us assume that the transition kernel $M_0$ of the pCN algorithm is geometrically ergodic, i.e., $\text{gap}(M_0) > 0$. Then, for any $\varepsilon > 0$ there is an explicitly given probability measure $\mu_R$ which satisfies

$$\|\mu - \mu_L\|_{\text{tv}} \leq \varepsilon$$

with $\|\cdot\|_{\text{tv}}$ denoting the total variation distance. Furthermore, the transition kernel $M_{\Gamma,R}$ of the gpCN Metropolis algorithm with target distribution $\mu_R$ has a strictly positive spectral gap, that is, $\text{gap}(M_{\Gamma,R}) > 0$. In other words the resulting Markov chain converges exponentially fast to $\mu_R$.

The key for the proof is a new comparison theorem for spectral gaps of Markov chains generated by MH algorithms. In order to apply this comparison argument we show that the proposal kernels of the pCN and gpCN Metropolis are equivalent and that the density w.r.t. each other belongs to an $L_p$-space for a $p > 1$. We note that in [12] under additional assumptions on the density function $\frac{d\mu}{d\mu_0}$ it is proven that there exists a strictly positive spectral gap of the pCN Metropolis. Thus, in this setting the gpCN Metropolis algorithm targeting $\mu_R$ converges also exponentially.

The remainder of the paper is organized as follows. In Section 2 we state the precise framework, recall preliminary facts, and give a brief introduction into Markov chain Monte Carlo and MH algorithms including the pCN Metropolis algorithm. The gpCN Metropolis algorithm is motivated and defined in Section 3. Particularly, in Section 3.3 we illustrate its better performance compared to other popular MH algorithms. In Section
we state a general result for comparing spectral gaps of MH algorithms
and then apply it to the gpCN and pCN Metropolis. Section 5 provides an
outlook to gpCN algorithms in infinite dimensions which use Gaussian pro-
posals with state-dependent covariance. For the convenience of the reader
we recall some facts about Gaussian measures in Appendix A and present
more technical proofs in Appendix B.

2 Preliminaries

Let $\mathcal{H}$ be a separable Hilbert space with inner-product and norm denoted by
$\langle \cdot, \cdot \rangle$ and $\| \cdot \|$. By $\mathcal{B}(\mathcal{H})$ we denote the corresponding Borel $\sigma$-algebra and by
$\mathcal{L}(\mathcal{H})$ the set of all bounded, linear operators $A: \mathcal{H} \to \mathcal{H}$. Further, we have
a Gaussian measure $\mu_0 = N(0, C)$ on $(\mathcal{H}, \mathcal{B}(\mathcal{H}))$. Here and throughout the
whole paper $C: \mathcal{H} \to \mathcal{H}$ denotes a nonsingular covariance operator on $\mathcal{H}$, i.e.,
a linear, bounded, self-adjoint and positive trace class operator with $\ker C = \{0\}$. By $\mu$ we denote the probability measure of interest on $(\mathcal{H}, \mathcal{B}(\mathcal{H}))$ given
through the density defined in (1). Typically, the desired distribution is
complicated and the density only known up to a constant which makes
direct sampling with respect to $\mu$ difficult. That is the reason why Markov
chains are used for approximate sampling according to $\mu$.

2.1 Markov chains and spectral gaps

We give a short introduction to Markov chains and Markov chain Monte
Carlo (MCMC) methods on general state spaces.

Let $K: \mathcal{H} \times \mathcal{B}(\mathcal{H}) \to [0, 1]$ be a transition kernel, i.e., $K(x, \cdot)$ is for any
$x \in \mathcal{H}$ a probability measure on $(\mathcal{H}, \mathcal{B}(\mathcal{H}))$ and $K(\cdot, A)$ is for any $A \in \mathcal{B}(\mathcal{H})$
a measurable function. Then, a Markov chain with transition kernel $K$ is
a sequence of random variables $(X_n)_{n \in \mathbb{N}}$, mapping from some probability
space $(\Omega, \mathcal{F}, \mathbb{P})$ to $(\mathcal{H}, \mathcal{B}(\mathcal{H}))$, satisfying

$$\mathbb{P}(X_{n+1} \in A \mid X_1, \ldots, X_n) = \mathbb{P}(X_{n+1} \in A \mid X_n) = K(X_n, A)$$

almost surely for all $A \in \mathcal{B}(\mathcal{H})$. Most properties of a Markov chain can be
expressed as properties of its transition kernel. For example, we say the
transition kernel $K$ is $\mu$-reversible if

$$K(u, dv) \mu(du) = K(v, du) \mu(dv) \quad (2)$$

in the sense of measures on $\mathcal{H} \times \mathcal{H}$. This property is also known as detailed
balance condition and it implies that the distribution $\mu$ is a stationary or
invariant probability measure of a Markov chain with transition kernel $K$, i.e., if $X_1 \sim \mu$ then also $X_2 \sim \mu$.

Each $\mu$-reversible transition kernel $K$ on $(\mathcal{H}, \mathcal{B}(\mathcal{H}))$ induces a Markov operator, also denoted by $K$, given by

$$Kf(u) = \int_{\mathcal{H}} f(v) K(u, dv), \quad f \in L_2(\mu),$$

where

$$L_2(\mu) = \left\{ f: \mathcal{H} \to \mathbb{R} \mid \|f\|_{2, \mu} := \left( \int_{\mathcal{H}} |f(u)|^2 \mu(du) \right)^{1/2} < \infty \right\},$$

is the Hilbert space of measurable, square integrable functions with respect to $\mu$. By the $\mu$-reversibility we have that $K: L_2(\mu) \to L_2(\mu)$ is a linear, bounded and self-adjoint operator. We also introduce the closed subspace $L_0^2(\mu) = \{ f \in L_2(\mu) \mid \int_{\mathcal{H}} f(u) \mu(du) = 0 \}$ of $L_2(\mu)$ and the operator norm

$$\|K\|_\mu = \sup_{f \in L_0^2(\mu), f \neq 0} \frac{\|Kf\|_{2, \mu}}{\|f\|_{2, \mu}}$$

for $K: L_0^2(\mu) \to L_0^2(\mu)$. Let $\text{spec}(K \mid L_0^2(\mu))$ be the spectrum of $K$ on $L_0^2(\mu)$. Then, we also have

$$\|K\|_\mu = \sup\{|\lambda| : \lambda \in \text{spec}(K \mid L_0^2(\mu))\}.$$

We define $\text{gap}(K) = 1 - \|K\|_\mu$ as the spectral gap of $K$ (w.r.t. $\mu$). This is an important quantity which can be used to formulate conditions ensuring an exponentially fast convergence of the distribution of $X_n$ to $\mu$. To be more precise, we introduce the total variation distance of two probability measures $\nu_1, \nu_2$ on $(\mathcal{H}, \mathcal{B}(\mathcal{H}))$ by

$$\|\nu_1 - \nu_2\|_{tv} := \sup_{A \in \mathcal{B}(\mathcal{H})} |\nu_1(A) - \nu_2(A)|.$$

Let $\nu$ be the initial distribution of our Markov chain, i.e., $X_1 \sim \nu$. Then, with

$$K^n(u, A) = \int_{\mathcal{H}} K^{n-1}(v, A) K(u, dv), \quad A \in \mathcal{B}(\mathcal{H}),$$

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for \( n \in \mathbb{N} \), the distribution of \( X_{n+1} \) is given by

\[
\nu K^n(A) = \int_H K^n(u,A) \nu(du).
\]

Let \( \delta_u \) denote the probability measure concentrated at \( u \), so that \( \delta_u K^n(\cdot) = K^n(u,\cdot) \). In the setting above it is well known, see [20], that \( \|K\|_{\mu} < 1 \), or equivalently \( \text{gap}(K) > 0 \), holds, iff the transition kernel is geometrically ergodic, i.e., there is a measurable function \( c : \mathcal{H} \to (0,\infty) \) and a number \( \rho \in (0,1) \) such that

\[
\|K^n(u,\cdot) - \mu\|_{tv} \leq c(u)\rho^n, \quad n \in \mathbb{N}.
\]

If the distribution of \( X_n \) converges to \( \mu \), then the Markov chain \( (X_n)_{n \in \mathbb{N}} \) can be used for approximate sampling of \( \mu \). This leads to Markov chain Monte Carlo methods for the computation of expectations. The mean \( E_{\mu}(f) \) of \( f : \mathcal{H} \to \mathbb{R} \) w.r.t \( \mu \) can then be approximated by the time average

\[
S_{n,n_0}(f) = \frac{1}{n} \sum_{j=1}^{n} f(X_{j+n_0})
\]

where \( n \) is the sample size and \( n_0 \) a burn-in parameter to decrease the influence of the initial distribution. The spectral gap of \( K \) of the Markov chain \( (X_n)_{n \in \mathbb{N}} \) can then be applied to assess the error of the time average \( S_{n,n_0}(f) \).

We assume \( \text{gap}(K) > 0 \) and mention two results. The first is rather classical and due to Kipnis and Varadhan [14]. If the initial distribution is \( \mu \) and \( f \in L^2(\mu) \), then the error \( \sqrt{n}(S_{n,n_0}(f) - E_{\mu}(f)) \) converges weakly to \( N(0,\sigma_{f,K}^2) \) with

\[
\sigma_{f,K}^2 = \langle (I + K)(I - K)^{-1}(f - E_{\mu}(f)),(f - E_{\mu}(f)) \rangle_{\mu} \leq \frac{2 \|f\|_{L^2(\mu)}^2}{\text{gap}(K)}
\]

where \( \langle \cdot , \cdot \rangle_{\mu} \) denotes the inner-product in \( L^2(\mu) \). The second result is more recent and provides a non-asymptotic bound of the mean square error. We have

\[
\sup_{\|f\|_{L^4} \leq 1} E |S_{n,n_0}(f) - E_{\mu}(f)|^2 \leq \frac{2}{n \cdot \text{gap}(K)} + \frac{C_{\nu} \|K\|_{\mu}^{n_0}}{n^2 \cdot \text{gap}(K)^2}
\]

with \( \|f\|_{L^4} = \left( \int_H |f(u)|^4 \mu(du) \right)^{1/4} \) and a number \( C_{\nu} \geq 0 \) depending on the initial distribution \( \nu \). We refer to [22] for more details.

This shows that \( \text{gap}(K) \) is a crucial quantity in the study of Markov chains and the numerical analysis of MCMC methods.
2.2 Metropolis algorithm with pCN proposal

In this work we focus on Markov chains derived from the Metropolis algorithm. Let $P$ be a transition kernel on $(\mathcal{H}, \mathcal{B}(\mathcal{H}))$ and $\alpha: \mathcal{H} \times \mathcal{H} \to [0, 1]$ be a measurable function. Then, a transition of such a Markov chain $(X_n)_{n \in \mathbb{N}}$ can be represented in algorithmic form:

1. Given the current state $X_n = u$, draw a sample $v$ of a random variable $V \sim P(u, \cdot)$ and a sample $a$ of a random variable $A \sim \text{Unif}[0, 1]$ independently.

2. If $a < \alpha(u, v)$, then set $X_{n+1} = v$, otherwise set $X_{n+1} = u$.

We call the kernel $P$ proposal kernel and $\alpha(u, v)$ acceptance probability. The transition kernel of such a Markov chain is then

$$M(u, dv) = \alpha(u, v)P(u, dv) + \delta_u(dv) \int_{\mathcal{H}} (1 - \alpha(u, w)) P(u, dw)$$

and we call it Metropolis kernel. It is well known, see [26], that $M$ is reversible w.r.t. $\mu$ if $\alpha(\cdot, \cdot)$ is chosen as

$$\alpha(u, v) = \min \left\{ 1, \frac{d\eta^\perp}{d\eta}(u, v) \right\}, \quad u, v \in \mathcal{H},$$

where $\frac{d\eta^\perp}{d\eta}$ denotes the Radon-Nikodym derivative – if existing – of the measures

$$\eta(du, dv) := P(u, dv) \mu(du) \quad \text{and} \quad \eta^\perp(du, dv) := P(v, du) \mu(dv).$$

For finite dimensional state spaces the condition of absolute continuity of $\eta^\perp$ w.r.t. $\eta$ is often easily satisfied. However, for infinite dimensional state spaces this becomes a real issue, since there measures tend to be singular. As pointed out in [1, 3] a possible way to ensure the existence of $\frac{d\eta^\perp}{d\eta}$ is to choose a proposal kernel $P$ which is $\mu_0$-reversible, i.e.,

$$P(u, dv) \mu_0(du) = P(v, du) \mu_0(dv).$$

Then, due to the fact that $\frac{d\mu}{d\mu_0}$ and $\frac{d\mu_0}{d\mu}$ exist, see (1), it follows that

$$\frac{d\eta^\perp}{d\eta}(u, v) = \frac{d\mu}{d\mu_0}(v) \frac{d\mu_0}{d\mu}(u) = \exp(\Phi(u) - \Phi(v))$$

and, hence, $\alpha(u, v) = \min \{1, \exp(\Phi(u) - \Phi(v))\}$. 
Now we explain the Metropolis algorithm with *preconditioned Crank-Nicolson* (pCN) proposal, see also [3] for details. The pCN proposal kernel is given by

\[ P_0(u, \cdot) = N(\sqrt{1 - s^2 u}, s^2 C) \]  

(7)

where \( s \in [0, 1] \) denotes a variance or stepsize parameter. It is straightforward to verify that \( P_0 \) is \( \mu_0 \)-reversible. Namely, by applying (28) from the Appendix A we derive

\[ P_0(u, dv) \mu_0(du) = N\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} C & \sqrt{1 - s^2} C \\ \sqrt{1 - s^2} C & C \end{bmatrix}\right) = P_0(v, du) \mu_0(dv). \]

In the following we call the resulting Metropolis algorithm with proposal \( P_0 \) simply pCN Metropolis algorithm or only pCN Metropolis and denote its Metropolis kernel by \( M_0 \).

Next, we want to generalize the pCN Metropolis algorithm to allow proposal kernels which employ a different covariance structure than the covariance of \( \mu_0 \).

### 3 Metropolis with gpCN proposals

In recent years many authors proposed and pursued the idea to construct proposals which try to exploit certain geometrical features of the target measure, see for example [10, 18, 15, 4].

We consider generalized pCN (gpCN) proposals which aim to adapt to the covariance structure of the target measure \( \mu \). We motivate our gpCN proposal, show that it is well-defined in function spaces and illustrate its higher performance in a simple but common setting.

#### 3.1 Motivation from Bayesian inference

We briefly recall the Bayesian framework and refer to [8] for an overview and to [24] for a comprehensive introduction to the topic.

Assume \( X \) is a random variable on \((\mathcal{H}, \mathcal{B}(\mathcal{H}))\) with distribution \( \mu_0 = N(0, C) \). Here \( \mu_0 \) is called the prior distribution and describes our initial uncertainty about \( X \). Let \( Y \) be a random variable on \( \mathbb{R}^m \) given by

\[ Y = G(X) + \varepsilon \]

(8)

with a continuous map \( G : \mathcal{H} \to \mathbb{R}^m \) and \( \varepsilon \sim N(0, \Sigma) \), independent of \( X \), with \( \Sigma \in \mathbb{R}^{m \times m} \). The variable \( Y \) models an observable quantity related
to $X$ via the map $G$ which is perturbed by additive noise $\varepsilon$. Then, given some observation $y \in \mathbb{R}^m$ of $Y$ we want to infer $X$, i.e., we are interested in the conditional distribution of $X$ given the event $Y = y$. We denote this conditional distribution by $\mu$ and call it posterior distribution. In particular, in this setting $\mu$ admits a representation of the form (1) with

$$\Phi(u) = \frac{1}{2} |y - G(u)|^2_{\Sigma^{-1}}$$

where $|x|^2_{\Sigma^{-1}} = x^T \Sigma^{-1} x$ for $x \in \mathbb{R}^m$.

A special situation appears if $G(u) = Lu + b$ with a linear mapping $L: \mathcal{H} \to \mathbb{R}^m$ and $b \in \mathbb{R}^m$. Then, it is known from [17] that $\mu = N(m, \tilde{C})$ with

$$m = CL^*(LCL^* + \Sigma)^{-1}(y - b), \quad \tilde{C} = (C^{-1} + L^*\Sigma^{-1}L)^{-1}. \quad (10)$$

If a Metropolis algorithm with Gaussian proposal is applied to sample approximately from a Gaussian target measure as above we know from [21] that it is advantageous to use $s^2\tilde{C}$ with $s \in \mathbb{R}$ as proposal covariance. The affine case indicates how we can construct good Gaussian proposal kernels if the map $G$ is nonlinear but smooth.

For a fixed $u_0 \in \mathcal{H}$ local linearization leads to

$$G(u) = G(u_0) + \nabla G(u_0) (u - u_0) + r(u)$$

with a residual term $r(u) \in \mathbb{R}^m$. For a sufficiently smooth $G$ the residual $r$ is small (in a neighborhood of $u_0$), so that

$$\tilde{G}(u) = G(u_0) + \nabla G(u_0) (u - u_0)$$

is close to $G(u)$ (in a neighborhood of $u_0$). The substitution of $G$ by $\tilde{G}$ in the model (8) leads to a Gaussian target measure $\tilde{\mu} = N(\tilde{m}, \tilde{C})$ with covariance

$$\tilde{C} = (C^{-1} + L^*\Sigma^{-1}L)^{-1}, \quad L = \nabla G(u_0).$$

By the fact that $G$ and $\tilde{G}$ are close to each other, we also have that the actual target measure $\mu$ and $\tilde{\mu}$ are close to each other. Then, it is reasonable to use $\tilde{C}$ in the covariance operator of the proposal in a Metropolis algorithm. Of course, there might be other choices than a simple linearization of $G$ at one point. For example, averaging linearizations at several points $u_1, \ldots, u_n \in \mathcal{H}$ leads to

$$\tilde{C} = \left( C^{-1} + \frac{1}{N} \sum_{n=1}^N L_n^* \Sigma^{-1} L_n \right)^{-1}, \quad L_n = \nabla G(u_n).$$
One could also think of a state-dependent covariance $C(u)$. This motivates to study proposals which use covariances of the form $C_\Gamma = (C^{-1} + \Gamma)^{-1}$ for suitably chosen operators $\Gamma$.

3.2 Well-defined gpCN proposals

In this section we introduce the gpCN proposal kernel and prove that the Metropolis algorithm with this proposal is well-defined, in the sense that it leads to a $\mu$-reversible transition kernel.

For this we introduce the set $\mathcal{L}_+(\mathcal{H})$ of all linear, bounded, self-adjoint and positive operators $\Gamma : \mathcal{H} \to \mathcal{H}$. We define the operators

$$C_\Gamma := (C^{-1} + \Gamma)^{-1}, \quad \Gamma \in \mathcal{L}_+(\mathcal{H}),$$

motivated in Section 3.1, for which we also use the representation

$$C_\Gamma = C^{1/2} (I + H_\Gamma)^{-1} C^{1/2}, \quad H_\Gamma := C^{1/2} \Gamma C^{1/2}.$$

In the following we prove that $C_\Gamma$ can be considered as covariance operator.

**Proposition 1.** Let $C$ be a nonsingular covariance operator on $\mathcal{H}$, $\Gamma \in \mathcal{L}_+(\mathcal{H})$ and $C_\Gamma$ with $H_\Gamma$ given as in (12). Then $H_\Gamma \in \mathcal{L}_+(\mathcal{H})$ is trace class and $C_\Gamma$ is also a nonsingular covariance operator on $\mathcal{H}$.

**Proof.** That $H_\Gamma \in \mathcal{L}_+(\mathcal{H})$ follows by construction. Furthermore, since $H_\Gamma$ is a composition of two Hilbert-Schmidt and one bounded operator, $C^{1/2}$ and $\Gamma$, respectively, it is trace class [5, Proposition 1.1.2]. Since $H_\Gamma$ is positive and self-adjoint, we have $\langle (I + H_\Gamma)u, u \rangle \geq \langle u, u \rangle$ and, thus, $(I + H_\Gamma)^{-1} \in \mathcal{L}_+(\mathcal{H})$ with $\| (I + H_\Gamma)^{-1} \| \leq 1$. Therefore, the self-adjointness and positivity of $C_\Gamma$ follows. Moreover, since $C_\Gamma$ is a composition of two nonsingular Hilbert-Schmidt and one nonsingular bounded operator, $C^{1/2}$ and $(I + H)^{-1}$, respectively, it is trace class and nonsingular, too.

By Proposition 1 we can use the covariance operator $C_\Gamma$ rather than $C$, as in the pCN Metropolis, for the proposal kernel. We consider

$$P(u, \cdot) = N(Au, s^2 C_\Gamma), \quad s \in [0, 1), \quad \Gamma \in \mathcal{L}_+(\mathcal{H}),$$

where $A : \mathcal{H} \to \mathcal{H}$ denotes a suitably chosen linear, bounded operator on $\mathcal{H}$. Here $A$ should be chosen such that $P$ is $\mu_0$-reversible, which means that a Metropolis kernel with proposal $P$ is $\mu$-reversible, see Section 2.2. By applying (28) we obtain in this setting

$$P(u, dv) \mu_0(du) = N \left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} C & CA^* \\ AC & ACA^* + s^2 C_\Gamma \end{bmatrix} \right)$$
and
\[ P(v, du) \mu_0(dv) = N \left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} ACA^* + s^2 C_{\Gamma} & AC \\ CA^* & C \end{bmatrix} \right). \]

Thus, for satisfying (5) we need to choose \( A \) so that
\[ AC = CA^*, \quad ACA^* + s^2 C_{\Gamma} = C. \tag{14} \]

By straightforward calculation we obtain as solution to (14) that
\[ A = A_{\Gamma} = C^{1/2} \sqrt{I - s^2 (I + H_{\Gamma})^{-1} C^{-1/2}}. \tag{15} \]

The next lemma ensures that this choice of \( A \) is well-defined, i.e., the positive square root operator exists and \( A \) is a bounded operator on \( \mathcal{H} \). The boundedness is non-trivial since \( C^{-1/2} \) is the inverse of a Hilbert-Schmidt operator. Namely, one easily can construct a bounded \( B \in \mathcal{L}(\mathcal{H}) \) such that \( C^{1/2} BC^{-1/2} \) is unbounded on \( \mathcal{H} \). Since the proof is rather technical, we state it in Appendix B.1.

**Lemma 2.** Let the assumptions of Proposition 1 be satisfied and let \( s \in [0, 1) \). Then \( A_{\Gamma} \) given by (15) is a bounded linear operator on \( \mathcal{H} \) which satisfies condition (14).

**Definition 3** (gpCN proposal). For \( s \in [0, 1) \) and \( \Gamma \in \mathcal{L}_+(\mathcal{H}) \) the **generalized pCN proposal kernel** is given by
\[ P_{\Gamma}(u, \cdot) := N(A_{\Gamma} u, s^2 C_{\Gamma}). \tag{16} \]

For the zero operator \( \Gamma = 0 \) we have the pCN proposal. By Lemma 2 and the arguments stated in Section 2.2 we obtain the following important result.

**Corollary 4.** Let \( \mu_0 = N(0, C) \) and \( \mu \) be given by (1). Let the assumptions of Lemma 2 be satisfied. Then, a gpCN proposal kernel \( P_{\Gamma} \) given by (16) and an acceptance probability \( \alpha(u, v) = \min \{1, \exp(\Phi(u) - \Phi(v))\} \) induce a \( \mu \)-reversible Metropolis kernel denoted by \( M_{\Gamma} \).

For simplicity we also call the Metropolis algorithm with transition kernel \( M_{\Gamma} \) just gpCN Metropolis. There are connections of the gpCN Metropolis to other recently developed Metropolis algorithms for general Hilbert spaces which also use more sophisticated choices for the proposal than the pCN proposal. The following two remarks address these connections.
Remark 5. The gpCN proposals form a subclass of the *operator weighted proposals* introduced in [4, 15]. The particular form of the gpCN proposal allows us to derive properties such as boundedness of the “proposal mean operator” $A_T$ and the convergence of the resulting Markov chain, see Section 4. These issues were left open in [4, 15].

Remark 6. In [19] the authors compute a Gaussian measure $\mu_* = N(m_*, C_*)$ which comes closest to $\mu$ w.r.t. the Kullback-Leibler distance. The admissible class of Gaussian measures considered there is closely related to our parametrized proposal covariances $C_\Gamma$, although the former set is slightly broader. Then, they use the knowledge of $\mu_*$ in the proposal kernel $P_*(u, \cdot) = N(m_* + \sqrt{1 - s^2(u - m_*)}, s^2 C_*)$ for the Metropolis algorithm. Note that $P_*$ is not $\mu_0$-reversible but $\mu_*$-reversible, since it is like a pCN proposal for the prior $\mu_*$. In order to obtain $\mu$-reversible Markov chains the authors need to adapt the acceptance probability in the Metropolis algorithm by including terms of $\frac{d\mu_*}{d\mu_0}$, cf. Section 5.

### 3.3 Numerical illustrations

We illustrate the gpCN Metropolis algorithm for approximating samples of a posterior distribution in Bayesian inference. In particular, we compare different Metropolis algorithms and investigate which of those algorithms perform independent of the state space dimension and of the variance of the involved perturbation.

We consider the same setting and inference problem as in [19, Section 6.1]. Assume noisy observations $y_j = p(0.2j) + \varepsilon_j$ with $j = 1, \ldots, 4$, of the solution $p$ of

$$\frac{d}{dx} \left(e^{u(x)} \frac{d}{dx} p(x)\right) = 0, \quad p(0) = 0, \quad p(1) = 2,$$

(17)

on $D = [0, 1]$ are given and we want to infer on $u$. Here the $\varepsilon_j$ are independent realizations of the normal distribution $N(0, \sigma_\varepsilon^2)$. We place a Gaussian prior $N(0, \Delta^{-1})$ with $\Delta = \frac{d^2}{dx^2}$ on the completion $\mathcal{H}_c$ of $H^1_0(D) \cap H^2(D)$ in $L^2(D)$. Recall that $(\Omega, \mathcal{F}, \mathbb{P})$ is a probability space and let $U : \Omega \to \mathcal{H}_c \subset L^2(D)$ be a random function with distribution $N(0, \Delta^{-1})$. This allows us to represent the random function $U$ as

$$U(\omega)(x) = \frac{\sqrt{2}}{\pi} \sum_{k=1}^{\infty} \xi_k(\omega) \sin(k\pi x), \quad \xi_k \sim N(0, k^{-2}), \quad (18)$$

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\( \mathbb{P} \)-a.s. where all random variables \( \xi_k \) are independent. Thus, inference on \( u \) is equivalent to inference on \( \xi = (\xi_k)_{k \in \mathbb{N}} \). This leads to the prior \( \mu_0 \) for \( \xi \) on \( \mathcal{H} := \ell^2(\mathbb{R}) \) given by \( \mu_0 = N(0, C) \) with \( C = \text{diag}\{k^{-2} : k \in \mathbb{N}\} \). Further, we denote by \( \mu \) the resulting conditional distribution of \( \xi \) given the observed data \( y_1, \ldots, y_4 \). The measure \( \mu \) is given by a density of the form (1) with \( \Phi \) as in (9) where \( \Sigma = \sigma^2 \varepsilon I \) and \( G(\xi) \) is the mapping \( \xi \mapsto u(\cdot, \xi) \mapsto p(\cdot | 0.2 j, \xi) \) for \( j = 1, \ldots, 4 \).

We test the performance of \( \mu \)-reversible Metropolis algorithms for computing expectations w.r.t. \( \mu \) of a function \( f : \ell^2(\mathbb{R}) \to \mathbb{R} \). We consider 4 Metropolis algorithms denoted by RW, pCN, GN-RW and gpCN with different proposal kernels:

- **RW**: Gaussian random walk proposal \( P_1(\xi, \cdot) = N(\xi, s^2 C) \),
- **pCN**: pCN proposal \( P_2(\xi, \cdot) = N(\sqrt{1 - s^2} \xi, s^2 C) \),
- **GN-RW**: Gauss-Newton random walk proposal \( P_3(\xi, \cdot) = N(\xi, s^2 C_T) \),
- **gpCN**: gpCN proposal \( P_4(\xi, \cdot) = N(A_T \xi, s^2 C_T) \).

Here we choose \( \Gamma = \sigma^{-2} \varepsilon LL^\top \) with \( L = \nabla G(\xi_{\text{MAP}}) \) and

\[
\xi_{\text{MAP}} = \arg\min_{\xi \in \text{Im} C^{1/2}} \left( \sigma^{-2} |y - G(\xi)|^2 + \|C^{-1/2} \xi\|^2 \right).
\]

For all Metropolis algorithms we tune \( s \) such that the average acceptance rate is about 0.25\(^1\). As a metric for comparison we consider and estimate the **effective sample size**

\[
\text{ESS} = \text{ESS}(n, f, (\xi_k)_{k \in \mathbb{N}}) = n \left[ 1 + 2 \sum_{k \geq 0} \gamma_f(k) \right]^{-1}.
\]

Here \( n \) is the number of samples taken from a Markov chain \( (\xi_k)_{k \in \mathbb{N}} \) with, say, a Markov transition kernel \( M \) and \( \gamma_f \) denotes the autocorrelation function \( \gamma_f(k) = \text{Corr}(f(\xi_{n_0}), f(\xi_{n_0+k})) \) for a quantity of interest \( f \).

The value of ESS corresponds to the number of independent samples w.r.t. \( \mu \) which would approximately yield the same mean squared error as the MCMC estimator \( S_{n,n_0}(f) \) for computing \( \mathbb{E}_\mu(f) \). This can be justified \(^1\)The empirical performance of each algorithm was best for this particular tuning.
under the assumption that \( \xi_{n_0} \sim \mu \), since then by virtue of \([22, \text{Proposition 3.26}]\) we have

\[
\lim_{n \to \infty} n \cdot \mathbb{E} |S_{n,n_0}(f) - \mathbb{E}_\mu(f)|^2 = \sigma_{f,M}^2,
\]

\[
1 + 2 \sum_{k \geq 0} \gamma_f(k) = \frac{\sigma_{f,M}^2}{\mathbb{E}_\mu(f^2) - \mathbb{E}_\mu(f)^2}
\]

where \( \sigma_{f,M}^2 \) denotes the asymptotic variance of the estimator \( S_{n,n_0}(f) \) as in Section 2.1.

For numerical simulations we use an equidistant discretization of \([0, 1]\) with \( \Delta x = 2^{-9} \). The solution of (17) is given by \( p(x) = 2S_x(e^{-u})/S_1(e^{-u}) \) with \( S_x(f) = \int_0^x f(y)dy \) and is evaluated employing the trapezoidal rule. Furthermore, we truncate the expansion (18) after \( N \) terms where we vary \( N \) in order to test the Metropolis algorithms for dimension independent performance. The unperturbed observations are generated by \( u(x) = 2\sin(2\pi x) \).

We also consider different noise levels \( \sigma_\varepsilon \) to examine the effect of smaller variances \( \sigma_\varepsilon^2 \), leading to more concentrated posterior distributions \( \mu \), to the performance of the Metropolis algorithms. In all cases we take \( n_0 = 10^5 \) as burn-in length and \( n = 10^6 \) as sample size. We set \( f(\xi) := \int_0^1 e^{u(x, \xi)} dx \) as quantity of interest\(^2\). To estimate the ESS we use the initial monotone sequence estimators\(^3\), for details we refer to \([9, \text{Section 3.3}]\).

The results of the simulations are illustrated in Figure 1 and Figure 2. The former displays the estimated autocorrelation functions \( \gamma_f \) resulting from the four Metropolis algorithms for \( N = 50 \) and \( \sigma_\varepsilon = 0.1 \) in (a), for \( N = 50 \) and \( \sigma_\varepsilon = 0.01 \) in (b), for \( N = 400 \) and \( \sigma_\varepsilon = 0.1 \) in (c) and for \( N = 400 \) and \( \sigma_\varepsilon = 0.01 \) in (d). In Figure 2 we display the estimated ESS for varying \( \sigma_\varepsilon = 0.1, 0.05, 0.025, 0.01 \) with fixed \( N = 100 \) in (a) and varying \( N = 50, 100, 200, 400 \) with fixed \( \sigma_\varepsilon = 0.1 \) in (b).

We see in both figures that the pCN and gpCN perform dimension independent and only the GN-RW and gpCN perform variance independent. Thus, the gpCN Metropolis is the only algorithm with both desirable properties. Moreover, it performs best among the four algorithms also in absolute terms of the ESS.

\(^2\)We also studied other functions such as \( f(\xi) = \xi_1, f(\xi) = \max_x e^{u(x, \xi)} \) and \( f(\xi) = p(0.5, \xi) \) but the results of the comparison were essentially the same.

\(^3\)We also estimated the ESS by batch means (100 batches of size \( 10^4 \)) to control our simulations. This lead to similar results.
Figure 1: Autocorrelation of $f$ given samples generated by the four Metropolis algorithms denoted by RW, pCN, GN-RW and gpCN for: (a) state dimension $N = 50$ and noise standard deviation $\sigma_\varepsilon = 0.1$; (b) $N = 50$ and $\sigma_\varepsilon = 0.01$; (c) $N = 400$ and $\sigma_\varepsilon = 0.1$; (d) $N = 400$ and $\sigma_\varepsilon = 0.01$.

4 Qualitative comparison of gpCN Metropolis

In this section we develop qualitative comparison arguments for Metropolis algorithms in a general setting and apply those results to the gpCN Metropolis algorithms. In particular, we relate the existence of a spectral gap for the gpCN to the existence of a spectral gap of the pCN Metropolis. Here it is worth to mention that in [12] sufficient conditions for the latter were proven.

We start with stating a general comparison result for the spectral gaps of Metropolis algorithms with equivalent proposals. Then, we verify the corresponding assumptions for the gpCN Metropolis: positivity and equivalence to the pCN proposal. In order to derive our main theorem, we consider in
Figure 2: Dependence of empirical ESS for each Metropolis algorithm RW, pCN, GN-RW and gpCN w.r.t.: (a) noise variance with fixed state dimension $N = 100$; (b) state dimension with fixed noise variance $\sigma^2 = 0.01$.

Section 4.4 restrictions of the target measure $\mu$ to arbitrary $R$-balls in $\mathcal{H}$ and prove convergence of the gpCN Metropolis to those restricted measures.

4.1 Comparison of spectral gaps

Let $K$ be a $\mu$-reversible transition kernel on $(\mathcal{H}, \mathcal{B}(\mathcal{H}))$, i.e., the associated Markov operator $K: L^2(\mu) \rightarrow L^2(\mu)$ is self-adjoint. Let the largest element of the spectrum $\text{spec}(K|L^0_2(\mu))$ be given by

$$\Lambda(K) := \sup \{\lambda: \lambda \in \text{spec}(K|L^0_2(\mu))\}$$

and define the conductance of $K$ (w.r.t. $\mu$) by

$$\varphi(K) := \inf_{\mu(A) \in (0,1/2]} \frac{\int_A K(u, A^c)\mu(du)}{\mu(A)}.$$

Under the assumptions above the Cheeger inequality for Markov operators, see [16], given by

$$\frac{\varphi(K)^2}{2} \leq 1 - \Lambda(K) \leq 2\varphi(K)$$

provides a useful relation between $\Lambda(K)$ and the conductance $\varphi(K)$.

Let us assume that $M_1$ and $M_2$ are $\mu$-reversible transition kernels of Metropolis algorithms with the same acceptance probability $\alpha$ and proposals $P_1$ and $P_2$, respectively, Then, we obtain the following result.
Lemma 7. Let $\mu$ be a probability measure on $(\mathcal{H}, \mathcal{B}(\mathcal{H}))$ and for $i = 1, 2$ let

$$M_i(u, dv) = \alpha(u, v) P_i(u, dv) + \delta_u(dv) \int_{\mathcal{H}} (1 - \alpha(u, w)) P_i(u, dw)$$

be Metropolis kernels. If the proposal kernels $P_1$ and $P_2$ admit a density

$$\rho(u, v) = \frac{dP_1(u)}{dP_2(u)}(v), \quad u, v \in \mathcal{H},$$

such that for a $p > 1$ we have

$$\kappa_p := \sup_{\mu(A) \in (0, 1/2]} \frac{\int_A \int_{A^c} \rho(u, v)^p P_2(u, dv) \mu(du)}{\mu(A)} < \infty, \quad (20)$$

then

$$\varphi(M_1) \leq \kappa_p^{1/p} \varphi(M_2)^{(p-1)/p}.$$ 

Proof. Let $A \in \mathcal{B}(\mathcal{H})$ with $\mu(A) \in (0, 1/2]$. Further, let $q = p/(p - 1)$ such that $1/q + 1/p = 1$. Then

$$\int_A M_1(u, A^c) d\mu(u) = \int_{\mathcal{H}} \int_{\mathcal{H}} 1_{A^c}(v) 1_A(u) \alpha(u, v) P_1(u, dv) d\mu(u)$$

$$= \int_{\mathcal{H}} \int_{\mathcal{H}} 1_{A^c}(v) 1_A(u) \alpha(u, v) \rho(u, v) P_2(u, dv) d\mu(u).$$

Note that $P_2(u, dv)\mu(du)$ is a probability measure on $(\mathcal{H} \times \mathcal{H}, \mathcal{B}(\mathcal{H} \times \mathcal{H}))$ and we can apply Hölder’s inequality according to this measure with parameters $p$ and $q$. Thus, by using $\alpha(u, v) = \alpha(u, v)^{1/q} \alpha(u, v)^{1/p}$ we obtain

$$\int_A M_1(u, A^c) d\mu(u)$$

$$\leq \left( \int_A M_2(u, A^c) d\mu(u) \right)^{1/q} \left( \int_{A} \int_{A^c} \rho(u, v)^p \alpha(u, v) P_2(u, dv) d\mu(u) \right)^{1/p}$$

$$\leq \left( \int_A M_2(u, A^c) d\mu(u) \right)^{1/q} \left( \int_{A} \int_{A^c} \rho(u, v)^p P_2(u, dv) d\mu(u) \right)^{1/p}$$

Dividing by $\mu(A)$, applying $\mu(A)^{-1} = \mu(A)^{-1/q} \mu(A)^{-1/p}$ and taking the infimum yields

$$\varphi(M_1) \leq \varphi(M_2)^{1/q} \kappa_p^{1/p}. \quad \Box$$
An immediate consequence of Lemma 7 and (19) is the following theorem.

**Theorem 8** (Spectral gaps comparison). Let the assumptions of Lemma 7 be satisfied and let the associated Markov operators to $M_1$ and $M_2$ be positive and self-adjoint on $L_2(\mu)$. Then

$$\left( \frac{\text{gap}(M_1)}{2} \right)^p \leq \kappa_p \left( 2 \text{gap}(M_2) \right)^{(p-1)/2}.$$  

We apply Theorem 8 to prove our convergence result of the gpCN Metropolis. We therefore verify in the following section the condition that the corresponding Markov operator is positive.

### 4.2 Positivity of Metropolis with Gaussian proposals

Recall that $\langle f, g \rangle_\mu = \int_H fg \, d\mu$ denotes the inner-product of $L_2(\mu)$ and that a Markov operator $K : L_2(\mu) \to L_2(\mu)$ is positive if $\langle Kf, f \rangle_\mu \geq 0$ for all $f \in L_2(\mu)$.

**Lemma 9** (Positivity of proposals). Let $\mu_0 = N(0, C)$ be a Gaussian measure on a separable Hilbert space $\mathcal{H}$ and let $P(u, \cdot) = N(Au, Q)$ be a $\mu_0$-reversible proposal kernel with bounded, linear operator $A : \mathcal{H} \to \mathcal{H}$. If there exists a bounded, linear operator $B : \mathcal{H} \to \mathcal{H}$ such that

$$B^2 = A, \quad BC = CB^*,$$

and $D := C - BCB^*$ is positive and trace class, then, the Markov operator associated to the proposal $P$ is positive on $L_2(\mu_0)$.

**Proof.** Because of the assumptions on $B$ and $D$ we obtain that the proposal kernel $P_1(u, \cdot) = N(Bu, D)$ is well-defined. Further, since $BCB^* + D = C$ we derive

$$P_1(u, dv)\mu_0(du) = N\left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} C & CB^* \\ BC & C \end{bmatrix} \right),$$

which leads by $BC = CB^*$ to the $\mu_0$-reversibility of $P_1$ and, thus, to the self-adjointness of its associated Markov operator in $L_2(\mu_0)$. It remains to prove that $P_1^2 = P$ holds for the associated Markov operators which then immediately yields the assertion. The equality of the Markov operators is equivalent to the equality of the measures $P_1^2(u, \cdot)$ and $P(u, \cdot)$ for all $u \in \mathcal{H}$. In order to show $P_1^2(u, \cdot)$ and $P(u, \cdot)$, we take $(\xi_n)_{n \in \mathbb{N}}$ to be an i.i.d. sequence with $\xi_1 \sim N(0, D)$ and construct an auxiliary Markov chain by

$$X_{n+1} = BX_n + \xi_n, \quad n \geq 1,$$
where $X_1 = u$ for an arbitrary $u \in \mathcal{H}$. The transition kernel of the chain $(X_n)_{n\in\mathbb{N}}$ is the kernel $P_1$. In particular, for $G \in \mathcal{B}(\mathcal{H})$ holds $\mathbb{P}[X_3 \in G] = P_1^2(u,G)$. By

$$X_3 = BX_2 + \xi_2 = B^2 u + B\xi_1 + \xi_2$$

and $B\xi_1 + \xi_2 \sim N(0, BDB^* + D)$ we obtain $X_3 \sim N(B^2 u, BDB^* + D)$. Due to the assumptions we have $B^2 = A$ and

$$BDB^* + D = B(C - BCB^*)B^* + C - BCB^* = C - ACA^*.$$

The last step $C - ACA^* = Q$ follows by the assumed $\mu_0$-reversibility of $P$, because we know from Section 3.2 that $P$ being $\mu_0$-reversible is equivalent to $A$ and $Q$ satisfying $AC = CA^*$ and $ACA^* + Q = C$. We thus arrive at $X_3 \sim N(Au, Q)$ which proves $P_1^2(u,\cdot) = P(u,\cdot)$. 

The previous two lemma lead to the following result about the gpCN Metropolis.

**Theorem 11** (Positivity of gpCN Metropolis). Let $\mu_0 = N(0, C)$ and $\mu$ as in (1) and let $M_\Gamma$ denote the gpCN Metropolis kernel as in Corollary 4. Then the associated Markov operator $M_\Gamma$ is self-adjoint and positive on $L_2(\mu)$.

**Proof.** It is enough to verify the assumptions of Lemma 9 for the gpCN proposal. Recall that $P_\Gamma(u,\cdot) = N(A_\Gamma u, C_\Gamma)$ which is $\mu_0$-reversible by construction with bounded $A_\Gamma = C^{1/2} \sqrt{I - s^2(I + H)^{-1}}$ $C^{-1/2}$. By choosing

$$B := C^{1/2} \sqrt{I - s^2(I + H)^{-1}} C^{-1/2},$$

the next lemma extends the previous result to Markov operators associated to Metropolis algorithms. The proof follows by the same line of arguments as developed in [23, Section 3.4] and is therefore omitted.

**Lemma 10** (Positivity of Metropolis kernels). Let $\mu$ be a measure on $\mathcal{H}$ given by (1) and let $P$ be a $\mu_0$-reversible proposal kernel whose associated Markov operator is positive on $L_2(\mu_0)$. Then, the Markov operator associated to a $\mu$-reversible Metropolis kernel

$$M(u, dv) = \alpha(u, v)P(u, dv) + \delta_u(dv) \int_\mathcal{H} (1 - \alpha(u, w))P(u, dw)$$

with $\alpha(u, v) = \min\{1, \frac{d\mu}{d\mu_0}(v) \frac{d\mu_0}{d\mu}(u)\}$ is positive on $L_2(\mu)$. 

The previous two lemma lead to the following result about the gpCN Metropolis.

**Theorem 11** (Positivity of gpCN Metropolis). Let $\mu_0 = N(0, C)$ and $\mu$ as in (1) and let $M_\Gamma$ denote the gpCN Metropolis kernel as in Corollary 4. Then the associated Markov operator $M_\Gamma$ is self-adjoint and positive on $L_2(\mu)$.

**Proof.** It is enough to verify the assumptions of Lemma 9 for the gpCN proposal. Recall that $P_\Gamma(u,\cdot) = N(A_\Gamma u, C_\Gamma)$ which is $\mu_0$-reversible by construction with bounded $A_\Gamma = C^{1/2} \sqrt{I - s^2(I + H)^{-1}}$ $C^{-1/2}$. By choosing

$$B := C^{1/2} \sqrt{I - s^2(I + H)^{-1}} C^{-1/2},$$
we obtain $B^2 = A_\Gamma$ and $BC = CB^*$. Moreover,

\[ D = C - BCB^* = C^{1/2}(I - \sqrt{I - s^2(I + H)^{-1}})C^{1/2}. \]

The eigenvalues of $I - \sqrt{I - s^2(I + H)^{-1}}$ take the form $1 - \sqrt{1 - s^2} \geq 0$ with $\lambda \geq 0$ being an eigenvalue of $H_\Gamma$. Thus, $I - \sqrt{I - s^2(I + H)^{-1}}$ is positive and bounded which yields $D$ being positive and trace class since $D$ is then a product of two Hilbert-Schmidt and one bounded operator. Thus, the conditions of Lemma 9 are satisfied and the assertion follows. \hfill \square

### 4.3 Density between pCN and gpCN proposal

In this section we show that for any state $u \in \mathcal{H}$ the gpCN proposal is equivalent to the pCN proposal in the sense of measures. Moreover, we will also derive an integrability result for the corresponding density. For proving the equivalence we need the following technical result.

**Lemma 12.** Let the assumptions of Corollary 4 be satisfied and define the bounded, linear operator $\Delta_\Gamma : \mathcal{H} \rightarrow \mathcal{H}$ by

\[ \Delta_\Gamma := A_0 - A_\Gamma = \sqrt{1 - s^2}I - C^{1/2}\sqrt{I - s^2(I + H_\Gamma)^{-1}}C^{-1/2}. \]  

(21)

Then $\text{Im} \Delta_\Gamma \subseteq \text{Im} C^{1/2}$, i.e., $C^{-1/2}\Delta_\Gamma$ is a bounded operator on $\mathcal{H}$.

The proof of this lemma can be found in Appendix B.2. It is similar to the proof of Lemma 2 and again rather technical. However, Lemma 12 ensures that we can apply the Cameron-Martin theorem, Theorem 21 in Appendix A, in the proof of the following result. The other main tool for deriving the next theorem is a variant of the Feldman-Hajek theorem as stated in Theorem 22 in Appendix A.

**Theorem 13** (Density of pCN w.r.t. gpCN). With the notation and assumptions of Corollary 4 holds the following.

1. The measures $\mu_0 = N(0, C)$ and $\mu_\Gamma = N(0, C_\Gamma)$ are equivalent with

\[ \pi_\Gamma(v) := \frac{d\mu_0}{d\mu_\Gamma}(v) = \frac{\exp \left( \frac{1}{2} \langle H_\Gamma C^{-1/2}v, C^{-1/2}v \rangle \right)}{\sqrt{\det(I + H_\Gamma)}}. \]  

(22)

2. For $u \in \mathcal{H}$ the measures $P_0(u, \cdot)$ and $P_\Gamma(u, \cdot)$ are equivalent with

\[ \frac{dP_0(u)}{dP_\Gamma(u)}(v) = \pi_{\text{CM}} \left( \Delta_\Gamma u, \frac{1}{s}(v - A_\Gamma u) \right) \pi_\Gamma \left( \frac{1}{s}(v - A_\Gamma u) \right). \]  

(23)

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where $\Delta_{\Gamma}$ as in (21) and

$$
\pi_{CM}(h, v) := \exp \left( -\frac{1}{2} \|C^{-1/2}h\|^2 + \langle C^{-1}h, v \rangle \right). \tag{24}
$$

(The subscript in $\pi_{CM}$ indicates the Cameron-Martin formula.)

**Proof.** We prove (22) by verifying the assumptions of Theorem 22 from Appendix A. We observe

$$
I - C^{-1/2}C_{\Gamma}C^{-1/2} = I - (I + H_{\Gamma})^{-1}
$$

and set $T_{\Gamma} := I - (I + H_{\Gamma})^{-1}$. The eigenvalues $(t_n)_{n \in \mathbb{N}}$ of the self-adjoint operator $T_{\Gamma}$ are given by

$$
t_n = 1 - \frac{1}{1 + \lambda_n} = \frac{\lambda_n}{1 + \lambda_n} < 1
$$

where $(\lambda_n)_{n \in \mathbb{N}}$ are the eigenvalues of the positive trace class operator $H_{\Gamma}$. Thus, $T_{\Gamma}$ is also trace class and satisfies $\langle T_{\Gamma}u, u \rangle < \|u\|^2$ for any $u \in \mathcal{H}$. Then, the assertion follows by Theorem 22 and

$$
T_{\Gamma}(I - T_{\Gamma})^{-1} = (I - (I + H_{\Gamma})^{-1}) (I + H_{\Gamma}) = H_{\Gamma}.
$$

To show the equivalence of $P_0(u, \cdot)$ and $P_{\Gamma}(u, \cdot)$ for any $u \in \mathcal{H}$ we introduce the auxiliary kernel $K_{\Gamma}(u, \cdot) = N(A_{\Gamma}u, s^2C)$. Lemma 23 from the appendix combined with (22) leads to

$$
\frac{dK_{\Gamma}(u)}{dP_{\Gamma}(u)}(v) = \pi_{\Gamma} \left( \frac{1}{s} [v - A_{\Gamma}u] \right), \quad u, v \in \mathcal{H}.
$$

Thus, it remains to prove the equivalence of $K_{\Gamma}(u, \cdot)$ and $P_0(u, \cdot)$ for any $u \in \mathcal{H}$. By the Cameron-Martin formula, see Theorem 21 in Appendix A, this holds iff

$$
\text{Im}(A_{\Gamma} - \sqrt{1 - s^2I}) \subseteq \text{Im}(C^{1/2})
$$

which was shown in Lemma 12. Theorem 21 combined with Lemma 23 then yields

$$
\frac{dP_0(u)}{dK_{\Gamma}(u)}(v) = \pi_{CM} \left( [\sqrt{1 - s^2I} - A_{\Gamma}]u, \frac{1}{s} (v - A_{\Gamma}u) \right)
$$

and the assertion follows by

$$
\frac{dP_0(u)}{dP_{\Gamma}(u)}(v) = \frac{dP_0(u)}{dK_{\Gamma}(u)}(v) \frac{dK_{\Gamma}(u)}{dP_{\Gamma}(u)}(v).
$$

$\square$
Note that Theorem 13 implies that for any $\Gamma_1, \Gamma_2 \in \mathcal{L}_+(\mathcal{H})$ there exists a density between the two gpCN proposals $P_{\Gamma_1}(u)$ and $P_{\Gamma_2}(u)$. However, for the application of Theorem 8 we still have to verify condition (20). This is partly addressed in the following result.

**Theorem 14 (Integrability of gpCN density).** Let the assumptions of Lemma 12 be satisfied and set

$$\rho_{\Gamma}(u, v) := \frac{dP_0(u)}{dP_{\Gamma}(u)}(v), \quad u, v \in \mathcal{H}.$$ 

Then, for any $0 < p < 1 + \frac{1}{\|H_{\Gamma}\|}$ there exist constants $c = c(p, H_{\Gamma}) < \infty$ and $b = b(p, \|C^{-1/2} \Delta_{\Gamma}\|) < \infty$ such that

$$\int_{\mathcal{H}} \rho^p_{\Gamma}(u, v) P_{\Gamma}(u, dv) \leq c \exp \left( \frac{b^2}{2} \|u\|^2 \right).$$

**Proof.** By Theorem 13 we know

$$\rho_{\Gamma}(u, v) = \pi_{CM}(\Delta_{\Gamma} u, \frac{1}{s}(v - A_{\Gamma} u)) \pi_{\Gamma}(\frac{1}{s}(v - A_{\Gamma} u))$$

where $\pi_{\Gamma}$ and $\pi_{CM}$ as in (22) and (24), respectively. By first applying a change of variable, see Lemma 23, and then the Cauchy-Schwarz inequality we obtain

$$\int_{\mathcal{H}} \rho^p_{\Gamma}(u, v) P_{\Gamma}(u, dv) = \int_{\mathcal{H}} \pi^p_{CM}(\Delta_{\Gamma} u, v) \pi^p_{\Gamma}(v) \mu_{\Gamma}(dv)$$

$$= \int_{\mathcal{H}} \pi^p_{CM}(\Delta_{\Gamma} u, v) \pi^{p-1}_{\Gamma}(v) \mu_{0}(dv)$$

$$\leq \left( \int_{\mathcal{H}} \pi^{2p}_{CM}(\Delta_{\Gamma} u, v) \mu_{0}(dv) \right)^{1/2} \left( \int_{\mathcal{H}} \pi^{2p-2}_{\Gamma}(v) \mu_{0}(dv) \right)^{1/2}.$$ 

Furthermore, we have by applying (29) from Appendix A

$$\int_{\mathcal{H}} \pi^{2p}_{CM}(\Delta_{\Gamma} u, v) \mu_{0}(dv) = \int_{\mathcal{H}} e^{-\frac{2p}{2} \|C^{-1/2} \Delta_{\Gamma} u\|^2} e^{2p \langle C^{-1} \Delta_{\Gamma} u, v \rangle} \mu_{0}(dv)$$

$$= \exp \left( (2p^2 - p) \|C^{-1/2} \Delta_{\Gamma} u\|^2 \right).$$

We apply $\|C^{-1/2} \Delta_{\Gamma} u\| \leq \|C^{-1/2} \Delta_{\Gamma}\| \|u\|$ and set

$$b := \sqrt{2p^2 - p} \|C^{-1/2} \Delta_{\Gamma}\|$$

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Due to the assumptions on $p$ we have
\[
\langle (2p - 2)H_Gv, v \rangle < \frac{\langle H_Gv, v \rangle}{\|H_G\|} \leq \|v\|^2, \quad v \in \mathcal{H}.
\]
Thus, we can apply (30) from Appendix A and get
\[
\int_{\mathcal{H}} \pi_{2p-2}(v)\mu_0(dv) = \int_{\mathcal{H}} \frac{\exp \left( \frac{1}{2} \langle (2p - 2)H_G C^{-1/2}v, C^{-1/2}v \rangle \right)}{\det(I + H_G)^{(2p-2)/2}} \mu_0(dv)
= (\det(I - (2p - 2)H_G) \det(I + H_G)^{2p-2})^{-1/2}
=: c^2
\]
which proves the assertion.

Thus, the above theorem allows us to estimate the integral in (20). We obtain for $0 < p < 1 + 1/(2\|H_G\|)$ that
\[
\int_A \int_{A^c} \rho^p(u; v)p_G(u, dv) \mu(du) \leq \int_A \exp \left( \frac{b^2}{2} \|u\|^2 \right) \mu(du).
\]
Unfortunately, if we divide the right-hand side by $\mu(A)$ and take the supremum over all $\{A : 0 < \mu(A) \leq 0.5\}$ this is unbounded. In the next section we introduce restrictions of the target measure for which we come around this problem.

### 4.4 Restrictions of the target measure

In order to show boundedness of $\kappa_p$ from (20) for the gpCN proposal we consider restrictions of the target measure to bounded sets. For appropriately chosen sets, the restricted measures become arbitrarily close to the target measure. Let $R \in (0, \infty]$ and set
\[
\mathcal{H}_R := \{u \in \mathcal{H} : \|u\| < R\}.
\]

**Definition 15 (Restricted measure).** Let $\mu$ be a probability measure on $(\mathcal{H}, \mathcal{B}(\mathcal{H}))$ and $R \in (0, \infty]$. We define its restriction to $\mathcal{H}_R$ as the probability measure $\mu_R$ on $\mathcal{H}$ given by
\[
\mu_R(du) := \frac{1}{\mu(\mathcal{H}_R)} 1_{\mathcal{H}_R}(u) \mu(du). \quad (25)
\]
For sufficiently large $R$ the measure $\mu_R$ is close to $\mu$, because

$$\|\mu_R - \mu\|_{tv} = \int_{\mathcal{H}} \left| \frac{d\mu_R}{d\mu}(u) - 1 \right| d\mu(u) = \mu(H_R^c) + 1 - \mu(H_R) = 2\mu(H_R^c)$$

and since $\mu$ is a probability measure on $(\mathcal{H}, \mathcal{B}(\mathcal{H}))$ there exists for any $\varepsilon > 0$ a number $R > 0$ such that $2\mu(H_R^c) < \varepsilon$.

We ask now whether good convergence properties of a $\mu$-reversible transition kernel $K$ are inherited on a suitably modified $\mu_R$-reversible transition kernel $K_R$.

**Definition 16** (Restricted transition kernel). Let $K$ be a transition kernel on $\mathcal{H}$ and $R \in (0, \infty]$. We define its restriction to $H_R$ as the following transition kernel $K_R: H \times \mathcal{B}(\mathcal{H}) \to [0, 1]$ given by

$$K_R(u, dv) := 1_{H_R}(v) K(u, dv) + K(u, H_R^c) \delta_u(dv). \quad (26)$$

Note that if $K$ is $\mu$-reversible, then $K_R$ is $\mu_R$-reversible and if $K$ is of Metropolis form (3), then so is $K_R$.

**Proposition 17.** Let $\mu$ be a probability measure on $(\mathcal{H}, \mathcal{B}(\mathcal{H}))$ and $K$ be a $\mu$-reversible transition kernel. Then for any $R > 0$ the transition kernel $K_R$ given in (26) is $\mu_R$-reversible with $\mu_R$ as in (25). Moreover, for a Metropolis kernel $M$ of the form (3) the corresponding restricted kernel $M_R$ is again a Metropolis kernel

$$M_R(u, dv) = \alpha_R(u, v) P(u, dv) + \delta_u(dv) \left( 1 - \int_{\mathcal{H}} \alpha_R(u, w) P(u, dw) \right)$$

with $\alpha_R(u, v) := 1_{H_R}(v) \alpha(u, v)$.

*Proof.* Recall that $K$ is $\mu$-reversible iff

$$\int_{A} K(u, B) d\mu(u) = \int_{B} K(u, A) d\mu(u), \quad \forall A, B \in \mathcal{B}(\mathcal{H}).$$

Let $A, B \in \mathcal{B}(\mathcal{H})$. We have

$$\int_{A} K_R(u, B) d\mu_R(u) = \int_{A} K(u, B \cap H_R) d\mu_R(u) + \int_{A \cap B} K(u, H_R^c) d\mu_R(u)$$

$$= \frac{Z_R}{Z_R} \int_{A \cap H_R} K(u, B \cap H_R) d\mu(u) + \int_{A \cap B} K(u, H_R^c) d\mu_R(u).$$
Because of the $\mu$-reversibility of $K$ we can interchange $A$ and $B$ which leads to the first assertion. The second statement follows by

$$M_R(u, dv) = 1_{\mathcal{H}_R}(v)M(u, dv) + \delta_u(dv)M(u, \mathcal{H}_R^c)$$

$$= 1_{\mathcal{H}_R}(v)\alpha(u, v)P(u, dv)$$

$$+ \delta_u(dv) \left( 1 - \int_{\mathcal{H}} \alpha(u, w)P(u, dw) + \int_{\mathcal{H}_R^c} \alpha(u, w)P(u, dw) \right)$$

$$= 1_{\mathcal{H}_R}(v)\alpha(u, v)P(u, dv) + \delta_u(dv) \left( 1 - \int_{\mathcal{H}_R} \alpha(u, w)P(u, dw) \right).$$

Now we ask whether a spectral gap of $K$ on $L_2(\mu)$ implies a spectral gap of the Markov operator associated to $K_R$ on $L_2(\mu_R)$. Note, that

$$K_RF(u) = \int_{\mathcal{H}} f(v) K_R(u, dv) = \int_{\mathcal{H}_R} f(v) K(u, dv) + f(u) K(u, \mathcal{H}_R^c).$$

We have the following relation between $\|K_R\|_{\mu_R}$ and $\|K\|_\mu$.

**Lemma 18.** With the notation and assumptions from above holds

$$\|K_R\|_{\mu_R} \leq \|K\|_\mu + \sup_{u \in \mathcal{H}_R} K(u, \mathcal{H}_R^c). \quad (27)$$

Furthermore, if the Markov operator $K$ is positive on $L_2(\mu)$, then $K_R$ is also positive on $L_2(\mu_R)$.

**Proof.** For $f \in L_2(\mu_R)$ let

$$(Ef)(u) := 1_{\mathcal{H}_R}(u)f(u) \in L_2(\mu).$$

Note that $\|f\|_{2,\mu_R} = \frac{1}{\sqrt{\mu(\mathcal{H}_R)}} \|Ef\|_{2,\mu}$ and for $\int_{\mathcal{H}_R} f \, d\mu_R = 0$ follows $\int_{\mathcal{H}} Ef \, d\mu = 0$. Further, for any $f \in L_2(\mu_R)$ we have

$$\|K_Rf\|_{2,\mu_R}^2 = \int_{\mathcal{H}_R} \left( \int_{\mathcal{H}_R} f(v) K(u, dv) + f(u) K(u, \mathcal{H}_R^c) \right)^2 \, d\mu_R(u)$$

$$= \int_{\mathcal{H}_R} \left( \int_{\mathcal{H}} Ef(v) K(u, dv) + Ef(u) K(u, \mathcal{H}_R^c) \right)^2 \, d\mu_R(u)$$

$$= \|K(Ef) + g Ef\|_{2,\mu_R}^2.$$
with \( g(u) := 1_{\mathcal{H}_R}(u) K(u, \mathcal{H}_R^c) \). Then

\[
\| K_R f \|_{2, \mu_R} \leq \| K(E f) \|_{2, \mu} + \| g Ef \|_{2, \mu}
\]

By taking the supremum over all \( f \in L^2_0(\mu_R) \) and because of \( E(L^2_0(\mu_R)) \subseteq L^2_0(\mu) \) the first assertion follows. Moreover, we have for \( f \in L^2_0(\mu_R) \) that

\[
\langle K_R f, f \rangle_{\mu_R} = \int_{\mathcal{H}} K_R f(u) f(u) \mu_R(du)
\]

The second term is always positive since \( f^2(u) K(u, \mathcal{H}_R^c) \geq 0 \) for all \( u \in \mathcal{H} \) and the first term coincides with \( \langle K(E f), Ef \rangle_{\mu} / \mu(\mathcal{H}_R) \). Thus, the second statement is proven. \( \square \)

Lemma 18 tells us that there exists an absolute spectral gap of \( K_R \) if there exists an absolute spectral gap of \( K \) and \( \sup_{u \in \mathcal{H}_R} K(u, \mathcal{H}_R^c) \) is sufficiently small. Indeed, we can apply this result to the pCN Metropolis algorithm.

**Theorem 19** (Spectral gap of restricted pCN Metropolis). Let \( \mu \) be as in (1) and let \( M_0 \) denote the \( \mu \)-reversible pCN Metropolis kernel. If there exists a spectral gap of \( M_0 \) in \( L^2_2(\mu) \), then for any \( \varepsilon > 0 \) there exists a number \( R \in (0, \infty) \) such that \( M_{0,R} \) possesses a spectral gap in \( L^2_2(\mu_R) \), i.e.,

\[
\text{gap}(M_{0,R}) = 1 - \| M_{0,R} \|_{\mu_R} \geq \text{gap}(M_0) - \varepsilon,
\]

where \( \mu_R \) as in (25) and \( M_{0,R} \) according to Definition 16.

**Proof.** Given the results of Proposition 17 and Lemma 18 it suffices to prove that for any \( \varepsilon > 0 \) there exists an \( R > 0 \) such that \( \sup_{u \in \mathcal{H}_R} M_{0}(u, \mathcal{H}_R^c) \leq \varepsilon. \)
We recall that the proposal kernel of $M_0$ is $P_0(u, \cdot) = N(\sqrt{1-s^2}u, s^2C)$ and obtain with $\mu^s := N(0, s^2C)$ that

$$
\sup_{u \in \mathcal{H}_R} M_0(u, \mathcal{H}_R^c) \leq \sup_{u \in \mathcal{H}_R} P_0(u, \mathcal{H}_R^c) = \sup_{u \in \mathcal{H}_R} \int_{\|\sqrt{1-s^2}u+v\| \geq R} \mu^s(v) \, dv \\
\leq \sup_{u \in \mathcal{H}_R} \int_{\|\sqrt{1-s^2}u+v\| \geq R} \mu^s(v) \, dv \\
= \sup_{u \in \mathcal{H}_R} \int_{\|v\| \geq R - \sqrt{1-s^2}u} \mu^s(v) \, dv \\
\leq \int_{\|v\| \geq (1-\sqrt{1-s^2})R} \mu^s(v) = \mu_0(\mathcal{H}_R^c)
$$

where $R_s = \frac{1-\sqrt{1-s^2}}{s}$ and $\mu_0 = N(0, C)$. Again, since $\mu_0$ is a probability measure on $\mathcal{H}$ we know that there exists a number $R$, such that $\mu_0(\mathcal{H}_R^c) \leq \varepsilon$.

### 4.5 Spectral gap of restricted gpCN Metropolis

Now, we are able to formulate and to prove our main convergence result.

**Theorem 20** (Convergence of gpCN Metropolis). Let $\mu$ be as in (1) and assume that the pCN Metropolis kernel possesses a spectral gap in $L_2(\mu)$, i.e., $\text{gap}(M_0) > 0$. Then, for any $\Gamma \in \mathcal{L}_+(\mathcal{H})$ and any $\varepsilon \in (0, \text{gap}(M_0))$ there exists a number $R_0 = R_0(\varepsilon) \in (0, \infty)$ such that for any $R \geq R_0$ holds

$$
\|\mu - \mu_R\|_{tv} < \varepsilon \quad \text{and} \quad \text{gap}(M_{\Gamma,R}) > 0
$$

where $\text{gap}(M_{\Gamma,R}) = 1 - \|M_{\Gamma,R}\|_{\mu_R}$ denotes the spectral gap of $M_{\Gamma,R}$ in $L_2(\mu_R)$.

**Proof.** By Theorem 19 we have that for any $\varepsilon \in (0, \text{gap}(M_0))$ there exists a number $R_0 \in (0, \infty)$ such that for any $R \geq R_0$ holds

$$
\|\mu - \mu_R\|_{tv} \leq \varepsilon \quad \text{and} \quad \text{gap}(M_{0,R}) > 0.
$$

Moreover, Proposition 17, Theorem 19 and Theorem 11 yield that for any $\Gamma \in \mathcal{L}_+(\mathcal{H})$ the Markov operator associated to $M_{\Gamma,R}$ is self-adjoint and positive on $L_2(\mu_R)$. In particular, $M_{\Gamma,R}$ is again a Metropolis kernel with proposal $P_{\Gamma}$ and acceptance probability $\alpha_R$. Thus, in order to apply Theorem 8 to $M_{0,R}$ and $M_{\Gamma,R}$ it remains to verify that there exists a $p > 1$ so that

$$
\kappa_{p,R} := \sup_{\mu_R(A) \in (0,1/2]} \frac{\int_A \int_{A^c} \rho_{\Gamma}(u, v)^p P_{\Gamma}(u, dv) \, d\mu_R(u)}{\mu_R(A)} < \infty
$$
where \( \rho_{\Gamma}(u, v) = \frac{dP_0(u)}{d(P_0(u))}(v) \). By Theorem 14 we have for any \( p < 1 + \frac{1}{2\|H_{\Gamma}\|} \) that

\[
\kappa_{p,R} \leq \sup_{\mu_R(A) \in (0, 1/2]} \int_A \exp \left( \frac{b^2}{2} \|u\|^2 \right) \frac{d\mu_R(u)}{\mu_R(A)} \leq \exp \left( \frac{b^2}{2} R^2 \right) < \infty.
\]

Hence, Theorem 8 leads to

\[
gap(M_{\Gamma,R})^{(p-1)/2} \geq \frac{1}{2^{3(p-1)/2}} \frac{\gap(M_{0,R})^p}{\kappa_{p,R}} > 0
\]

which proves the assertion. \( \Box \)

Theorem 20 tells us that the corresponding restricted gpCN Metropolis converges exponentially fast to any, arbitrarily close, restriction \( \mu_R \) of \( \mu \) whenever the pCN Metropolis converges exponentially fast to \( \mu \) itself. In particular, under the conditions of [12, Theorem 2.14] we have that for sufficiently large \( R \) the gpCN Metropolis algorithm, given by \( M_{\Gamma,R} \), is geometrically ergodic, i.e., the distribution of the \( n \)th step of the corresponding Markov chain converges exponentially fast to \( \mu_R \). We argued with restrictions of \( \mu \), since we need that \( \kappa_p \) of Theorem 8 is bounded.

However, let us mention here that in simulations when \( R \) is sufficiently large one cannot distinguish between \( \mu \) and \( \mu_R \) as well as between Markov chains with transition kernels \( M_{\Gamma} \) and \( M_{\Gamma,R} \).

Moreover, we conjecture that the gpCN Metropolis targeting \( \mu \) has a strictly positive spectral gap whenever the pCN Metropolis has one. Recalling the results of the numerical simulations in Section 3.3 we even conjecture that the spectral gap of the gpCN Metropolis with suitably chosen \( \Gamma \in \mathcal{L}_+(\mathcal{H}) \) is much larger than the one of the pCN Metropolis.

5 Outlook on proposals with state-dependent covariances

In this section we further comment on the idea of state-dependent proposal covariances. Consider the proposal kernel

\[
P_{\text{loc}}(u, \cdot) = \mathcal{N}(A_{\Gamma(u)}u, s^2C_{\Gamma(u)})
\]

where we assume that for \( u \in \mathcal{H} \) we have \( \Gamma(u) \in \mathcal{L}_+(\mathcal{H}) \) and that the corresponding mapping \( u \mapsto \Gamma(u) \) is measurable. Further, by \( A_{\Gamma(u)} \) and \( C_{\Gamma(u)} \) we denote the components of the gpCN proposal for \( \Gamma = \Gamma(u) \). When
considering the measure $\eta_{loc}(du, dv) = P_{loc}(u, dv)\mu_0(du)$ we notice that $\eta$ is no longer a Gaussian measure due to the dependence of $\Gamma$ on $u$. However, to construct a $\mu$-reversible Metropolis kernel with the proposal $P_{loc}$ above, we can apply the same trick as in [1, Theorem 4.1], namely, with $\rho_{\Gamma}(u, v) = \frac{dP_0(u)}{dP_{\Gamma}(u)}(v)$ we have

$$P_{loc}(u, dv)\mu_0(du) = \frac{1}{\rho_{\Gamma(u)}(u, v)} P_0(u, dv)\mu_0(du)$$

$$= \frac{1}{\rho_{\Gamma(u)}(u, v)} P_0(v, du)\mu_0(du)$$

$$= \frac{\rho_{\Gamma(v)}(v, u)}{\rho_{\Gamma(u)}(u, v)} P_{loc}(v, du)\mu_0(du),$$

where we used the $\mu_0$-reversibility of the pCN Proposal $P_0$. Hence, according to the general Metropolis kernel construction outlined in Section 2.2, we have that a Metropolis kernel $M_{loc}$ with proposal $P_{loc}$ and acceptance probability

$$\alpha_{loc}(u, v) = \min\left\{1, \exp(\Phi(u) - \Phi(v)) \frac{\rho_{\Gamma(u)}(u, v)}{\rho_{\Gamma(v)}(v, u)} \right\}$$

is $\mu$-reversible. Note, that the same construction can analogously be applied to proposals of the form

$$P'_{loc}(u, \cdot) = N(\sqrt{1 - s^2u}, s^2C_{\Gamma(u)}),$$

where the modified acceptance probability includes terms of $\pi_{\Gamma(\cdot)}$ from (22) rather than of $\rho_{\Gamma(\cdot)}$. The arguments above show that this type of algorithms are well-posed in infinite dimensions.

The advantage of this approach is that the resulting Metropolis algorithm might be even better adapted to the target measure by allowing locally different proposal covariances. For a motivation of state-dependent proposal covariances we refer to [10, 18]. Of course, the question arises if the additionally computational costs of evaluating $\Gamma(u)$, $\rho_{\Gamma(u)}$ etc. in each step pays off in a significantly higher statistical efficiency. We leave this open for future research.
Appendix
A Gaussian measures

The following brief introduction to Gaussian measures is based on the presentations given in [5, Section 1] and [11, Section 3]. Another comprehensive reference for this topic is [2].

Let $H$ be a Hilbert space with norm $\| \cdot \|$ and inner-product $\langle \cdot, \cdot \rangle$ and let $L^1_+(H)$ denote the set of all linear, bounded, self-adjoint, positive and trace class operators $A : H \to H$.

Let $\mu$ be a measure on $(H, B(H))$ and for simplicity let us assume that $\int_H \|v\|^2 \mu(dv) < \infty$. The mean $m \in H$ of $\mu$ is defined as the Bochner integral $m = \int_H v \mu(dv)$ and the covariance of $\mu$ is the unique operator $C \in L^1_+(H)$ given by

$$\langle Cu, u' \rangle = \int_H \langle u, v - m \rangle \langle u', v - m \rangle \mu(dv), \quad \forall u, u' \in H.$$ 

A measure $\mu$ on $H$ is called a Gaussian measure with mean $m \in H$ and covariance operator $C \in L^1_+(H)$, denoted by $N(m, C)$, iff

$$\int_H e^{i\langle u, v \rangle} \mu(dv) = e^{i\langle m, u \rangle - \frac{1}{2} \langle Cu, u \rangle}, \quad \forall u \in H.$$ 

This definition is equivalent to $\langle u \rangle_*\mu = N(\langle u, m \rangle, \langle Cu, u \rangle)$ for all $u \in H$ where $\langle u \rangle : H \to \mathbb{R}$ with $\langle u \rangle(v) := \langle u, v \rangle$ and where $\langle u \rangle_*\mu$ denotes the pushforward measure of $\mu$ under the mapping $\langle u \rangle$. Gaussian measures are uniquely determined by their mean and covariance, i.e., for any $m \in H$ and any $C \in L^1_+(H)$ there exists a unique Gaussian measure $\mu = N(m, C)$ on $H$. Moreover, the set of random variables on $H$ distributed according to a Gaussian measure is closed w.r.t. affine transformations. In detail, let $X \sim N(m, C)$ be a Gaussian random variable on $H$ and let $b \in H$ and $T : H \to H$ be a bounded, linear operator, then due to [5, Proposition 1.2.3] we have

$$b + TX \sim N(b + Tm, TCT^*). \quad (28)$$

The Cameron-Martin space $H_\mu$ of a Gaussian measure $\mu = N(m, C)$ on $H$ is defined as the image space $\text{Im} C^{1/2}$ which forms equipped with $\langle u, v \rangle_{C^{-1}} := \langle C^{-1/2}u, C^{-1/2}v \rangle$ again a Hilbert space. The space $H_\mu$ has some surprising properties: it is the intersection of all measurable linear subspaces $X \subseteq H$ with $\mu(X) = 1$; if $\ker C = \{0\}$ then $H_\mu$ is dense in $H$ and if $H$ is infinite dimensional then $\mu(H_\mu) = 0$. Moreover, the space $H_\mu$ plays
an important role for the equivalence of Gaussian measures as rigorously expressed in the Cameron-Martin theorem below. Before stating the result we need some more notation.

In the following let \( \mu = N(0, C) \). For \( u \in \mathcal{H} \) we set 

\[
W_u(v) := \langle C^{-1/2}u, v \rangle, \quad \forall v \in \mathcal{H},
\]

and understand \( W_u \) as an element of \( L^2(\mu) \). Since the mapping \( \mathcal{H} \ni u \mapsto W_u \in L^2(\mu) \) is an isometry \([5, \text{Section } 1.2.4]\), we can define for any \( u \in \mathcal{H} \)

\[
\langle C^{-1/2}u, \cdot \rangle := \lim_{n \to \infty} W_{u_n},
\]

where \( u_n \in \mathcal{H} \) and \( u_n \to u \) in \( \mathcal{H} \) as \( n \to \infty \). And by \([5, \text{Proposition } 1.2.7]\) it holds that

\[
\int_{\mathcal{H}} e^{\langle C^{-1/2}u, v \rangle} \, d\mu(v) = e^{\frac{1}{2} \| u \|^2}, \quad \forall u \in \mathcal{H}.
\]

(29)

Hence, if \( h \in \mathcal{H} \), we understand \( \langle C^{-1/2}h, \cdot \rangle \) as \( \langle C^{-1/2}(C^{-1/2}h), \cdot \rangle \in L^2(\mu) \).

**Theorem 21** (Cameron-Martin formula, \([5, \text{Theorem } 1.3.6]\)). Let \( \mu = N(0, C) \) and \( \mu_h = N(h, C) \) be Gaussian measures on a separable Hilbert space \( \mathcal{H} \). Then, \( \mu \) and \( \mu_h \) are equivalent iff \( h \in \mathcal{H} \) in which case

\[
\frac{d\mu_h}{d\mu}(v) = \exp \left( -\frac{1}{2} \| C^{-1/2}h \|^2 + \langle C^{-1/2}h, v \rangle \right).
\]

Thus, two Gaussian measures \( N(m, C) \) and \( N(m+h, C) \) are only equivalent if \( h \in \text{Im } C^{1/2} \). Consider now \( \mu = N(0, C) \) and \( \nu = N(0, Q) \) with \( C \neq Q \). Before stating a theorem about the equivalence of \( \mu \) and \( \nu \), we need some more notations. Let \( T : \mathcal{H} \to \mathcal{H} \) be in the following a self-adjoint trace class operator and let \( (t_n)_{n \in \mathbb{N}} \) denote the sequence of its eigenvalues. We set

\[
\det(I + T) := \prod_{n=1}^{\infty} (1 + t_n)
\]

and define

\[
\langle TC^{-1/2}u, C^{-1/2}u \rangle := \lim_{N \to \infty} \langle TC^{-1/2} \Pi_N u, C^{-1/2} \Pi_N u \rangle, \quad \mu\text{-a.e.}
\]

where \( \Pi_N \) denotes the projection operator to \( \text{span}\{e_1, \ldots, e_N\} \) with \( e_n \) denoting the \( n \)th eigenvector of \( C \). The existence of the \( \mu\text{-a.e.-limit} \) above is
proven in [5, Proposition 1.2.10] and, furthermore, if \( \langle Tu, u \rangle < \|u\|^2 \) holds for any \( u \in \mathcal{H} \), then by [5, Proposition 1.2.11] we have
\[
\int_{\mathcal{H}} e^{\frac{1}{2}\left(TC^{-1/2}u,C^{-1/2}u\right)} \, d\mu(u) = \frac{1}{\sqrt{\det(1 - T)}}. \tag{30}
\]

**Theorem 22 ([5, Proposition 1.3.11])**. Let \( \mu = N(0, C) \) and \( \nu = N(0, Q) \) be Gaussian measures on a separable Hilbert space \( \mathcal{H} \). If \( T := I - C^{-1/2}QC^{-1/2} \) is self-adjoint, trace class and satisfies \( \langle Tu, u \rangle < \|u\|^2 \) for any \( u \in \mathcal{H} \), then \( \mu \) and \( \nu \) are equivalent with
\[
\frac{d\nu}{d\mu}(u) = \frac{1}{\sqrt{\det(I - T)}} \exp\left(-\frac{1}{2}(T(I - T)^{-1}C^{-1/2}u, C^{-1/2}u)\right), \quad u \in \mathcal{H}.
\]

We note that the assumptions of Theorem 22 can be relaxed to \( I - C^{-1/2}QC^{-1/2} \) being Hilbert-Schmidt which is known as Feldman-Hajek theorem. Also in this case expression for the Radon-Nikodym derivative can be obtained, see [2, Corollary 6.4.11].

Finally, we recall two simple but useful results.

**Lemma 23.** Let \( \mathcal{H} \) be a separable Hilbert space, \( 0 < s < \infty \) and \( h \in \mathcal{H} \).

- Assume \( \mu = N(m, C) \), \( \nu = N(m + h, s^2C) \) on \( \mathcal{H} \) and \( f : \mathcal{H} \to \mathbb{R} \). Then
  \[
  \int_{\mathcal{H}} f(v) \mu(dv) = \int_{\mathcal{H}} f\left(\frac{1}{s}(v - h)\right) \nu(dv).
  \]

- Assume \( \mu_1 = N(m_1, C_1) \) and \( \mu_2 = N(m_2, C_2) \) are equivalent with \( \frac{d\mu_2}{d\mu_1}(u) = \pi(u) \). Then the measures \( \nu_1 = N(m_1 + h, s^2C_1) \) and \( \nu_2 = N(m_2 + h, s^2C_2) \) are also equivalent with
  \[
  \frac{d\nu_2}{d\nu_1}(u) = \pi\left(\frac{u - h}{s}\right).
  \]

**B Proofs**

The following proofs are rather operator theoretic and rely heavily on the holomorphic functional calculus. We refer to [7, Section VII.3] for a comprehensive introduction.
B.1 Proof of Lemma 2

The square root operator in (15) exists, because \( I - s^2 (I + H_\Gamma)^{-1} \) is self-adjoint and positive where the latter holds due to \( I + H_\Gamma \) being compact and \( \|(I + H_\Gamma)^{-1}\| \leq 1 \). That \( A_\Gamma \) satisfies (14) can also be easily verified and it remains to show the boundedness of \( A_\Gamma \). For \( s = 0 \) the assertion is obvious, so that we assume \( s \in (0, 1) \). Let us define \( f : \mathbb{C} \setminus \{-1\} \to \mathbb{C} \) by

\[
f(z) = \sqrt{1 - s^2 (1 + z)^{-1}}.
\]

The function \( f \) is analytic in the complex half plane \( \{ z \in \mathbb{C} : \Re(z) > s^2 - 1 \} \), since \( \Re(1 + z) > s^2 \) implies \( \Re((1 + z)^{-1}) = \frac{\Re(1 + z)}{|1 + z|^2} \leq \frac{1}{\Re(1 + z)} < \frac{1}{s^2} \).

Denoting \( \gamma := \|H_\Gamma\| \) the spectrum of \( H_\Gamma = C^{1/2} \Gamma C^{1/2} \) is contained in \([0, \gamma] \). Then, since \( s < 1 \) we have that \( f \) is analytic in a neighborhood, say, \( N[0, \gamma] \). Hence, by functional calculus we obtain

\[
\sqrt{I - s^2 (I + H_\Gamma)^{-1}} = f(H_\Gamma) = \frac{1}{2\pi i} \int_{\partial N[0, \gamma]} f(\zeta) (\zeta I - H_\Gamma)^{-1} \, d\zeta,
\]

Due to analyticity we can approximate \( f \) by a sequence of polynomials \( p_n \) with degree \( n \) which converge uniformly on \( N[0, \gamma] \) to \( f \) for \( n \to \infty \). Then, by [7, Lemma VII.3.13] holds

\[
\|p_n(H_\Gamma) - f(H_\Gamma)\|_{\mathcal{H} \to \mathcal{H}} \to 0,
\]

for \( n \to \infty \). Since the polynomials \( p_n \) can be represented as \( p_n(z) = \sum_{k=0}^{n} a_k^{(n)} z^k \), we obtain further

\[
C^{1/2} p_n(H_\Gamma) = C^{1/2} \sum_{k=0}^{n} a_k^{(n)} (C^{1/2} \Gamma C^{1/2})^k = p_n(C \Gamma) C^{1/2}.
\]

By [13, Proposition 1] we have

\[
\text{spec}(C \Gamma | \mathcal{H}) = \text{spec}(C^{1/2} \Gamma C^{1/2} | \mathcal{H}) \subseteq [0, \gamma]
\]

where \( \text{spec}(\cdot | \mathcal{H}) \) denotes the spectrum on \( \mathcal{H} \), and, thus, we can conclude \( \|p_n(C \Gamma) - f(C \Gamma)\|_{\mathcal{H} \to \mathcal{H}} \to 0 \) as \( n \to \infty \) again by [7, Lemma VII.3.13]. Hence,

\[
C^{1/2} f(H_\Gamma) = \lim_{n \to \infty} C^{1/2} p_n(H_\Gamma) = \lim_{n \to \infty} p_n(C \Gamma) C^{1/2} = f(C \Gamma) C^{1/2}
\]

and

\[
A_\Gamma = C^{1/2} f(H_\Gamma) C^{-1/2} = f(C \Gamma) C^{1/2} C^{-1/2} = f(C \Gamma)
\]

where \( f(C \Gamma) \) is by construction a bounded operator. \( \square \)
B.2 Proof of Lemma 12

By [6, Theorem 1] the relation \( \text{Im}(\Delta \Gamma) \subseteq \text{Im}(C^{1/2}) \) holds iff there exists a bounded operator \( B : \mathcal{H} \rightarrow \mathcal{H} \) such that

\[
\Delta \Gamma = C^{1/2}B. \tag{31}
\]

Thus, \( \text{Im}(\Delta \Gamma) \subseteq \text{Im}(C^{1/2}) \) is equivalent to \( C^{-1/2} \Delta \Gamma \) being bounded on \( \mathcal{H} \).

In order to construct and analyze the operator \( B \), we define \( f : \mathbb{C} \backslash \{-1\} \rightarrow \mathbb{C} \) by

\[
f(z) := \sqrt{1 - s^2(1 + z)^{-1}} - \sqrt{1 - s^2},
\]

which is analytic in \( \{ z \in \mathbb{C} : \Re(z) > s^2 - 1 \} \), cf. the proof of Lemma 2, and particularly in

\[
V = \{ z \in \mathbb{C} : \text{dist}(z, [0, \gamma]) \leq \varepsilon \}, \quad 0 < \varepsilon < 1 - s^2,
\]

where \( \gamma := \| H_{\Gamma} \| \). We have the following representation

\[
-\Delta \Gamma = A_{\Gamma} - \sqrt{1 - s^2} I
= C^{1/2} \left( \sqrt{I - s^2 (I + H_{\Gamma})^{-1}} - \sqrt{1 - s^2} I \right) C^{-1/2}
= C^{1/2} f(H_{\Gamma}) C^{-1/2}
\]

with

\[
f(H_{\Gamma}) = \frac{1}{2\pi i} \int_{\partial V} f(\zeta) (\zeta I - H_{\Gamma})^{-1} d\zeta
\]

see [7, Chapter VII.3]. Hence, if we can prove that \( B = -f(H_{\Gamma}) C^{-1/2} \) is a bounded operator on \( \mathcal{H} \), we have shown the assertion.

For this let \( p_n(z) = \sum_{k=0}^{n} a_k^{(n)} z^k \) be polynomials of degree \( n \), with \( n \in \mathbb{N} \), which converge uniformly on \( V \) to \( f \). Such polynomials exist due to the analyticity of \( f \) and by the fact that \( f(0) = 0 \) we can assume w.l.o.g. that \( a_0^{(n)} = 0 \) for all \( n \in \mathbb{N} \). This leads to

\[
p_n(H_{\Gamma}) = C^{1/2} \Gamma^{1/2} \left( \sum_{k=1}^{n} a_k^{(n)} (\Gamma^{1/2} C \Gamma^{1/2})^{k-1} \right) \Gamma^{1/2} C^{1/2}
= C^{1/2} \Gamma^{1/2} q_{n-1}(\Gamma^{1/2} C \Gamma^{1/2}) \Gamma^{1/2} C^{1/2}
\]

with \( q_{n-1}(z) := \sum_{k=1}^{n} a_k^{(n)} z^{k-1} = p_n(z)/z \). Now, [13, Proposition 1] implies that the operators \( C^{1/2} \Gamma C^{1/2} \) and \( \Gamma^{1/2} C \Gamma^{1/2} \) share the same spectrum, since \( C \) and \( \Gamma \) are positive. Thus, \( \text{spec}(\Gamma^{1/2} C \Gamma^{1/2} | \mathcal{H}) \subset [0, \gamma] \) and we have

\[
q_n(\Gamma^{1/2} C \Gamma^{1/2}) = \frac{1}{2\pi i} \int_{\partial V} q_n(\zeta) (\zeta I - \Gamma^{1/2} C \Gamma^{1/2})^{-1} d\zeta, \quad n \in \mathbb{N}.
\]
Moreover, the polynomials $q_n$ are a Cauchy sequence in $C(\partial V)$, since

$$
\sup_{\zeta \in \partial V} |q_n(\zeta) - q_m(\zeta)| \leq \sup_{\zeta \in \partial V} \frac{|\zeta|}{\min_{\eta \in \partial V} |\eta|} |q_n(\zeta) - q_m(\zeta)| \\
= \frac{1}{\min_{\eta \in \partial V} |\eta|} \sup_{\zeta \in \partial V} |\zeta q_n(\zeta) - \zeta q_m(\zeta)| \\
= \frac{1}{\min_{\eta \in \partial V} |\eta|} \sup_{\zeta \in \partial V} |p_{n+1}(\zeta) - p_{m+1}(\zeta)|
$$

where $\min_{\eta \in \partial V} |\eta| = \varepsilon > 0$ due to our choice of $V$. Thus, the polynomials $q_n$ converge uniformly on $\partial V$ to a function $g$. This implies that the operators $q_n(\Gamma^{1/2}C\Gamma^{1/2})$ converge in the operator norm to a bounded operator

$$
g(\Gamma^{1/2}C\Gamma^{1/2}) := \frac{1}{2\pi i} \int_{\partial V} g(\zeta) (\zeta I - \Gamma^{1/2}C\Gamma^{1/2})^{-1} d\zeta.
$$

We arrive at

$$
f(H_T) = \lim_{n \to \infty} p_n(C^{1/2}\Gamma^{1/2}C^{1/2}) \\
= \lim_{n \to \infty} C^{1/2}\Gamma^{1/2} q_{n-1}(\Gamma^{1/2}C\Gamma^{1/2}) \Gamma^{1/2}C^{1/2} \\
= C^{1/2}\Gamma^{1/2} g(\Gamma^{1/2}C\Gamma^{1/2}) \Gamma^{1/2}C^{1/2},
$$

which yields

$$
B = -f(H_T)C^{-1/2} = -C^{1/2}\Gamma^{1/2} g(\Gamma^{1/2}C\Gamma^{1/2})\Gamma^{1/2}
$$

being bounded on $\mathcal{H}$.

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