NOTE ON THE KNAPSACK MARKOV CHAIN

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Abstract. We show that for sufficiently large knapsacks the associated Markov chain on the state space of the admissible packings of the knapsack is rapidly mixing. Our condition basically states that at least half of all items should fit into the knapsack. This is much weaker than the condition assumed by Saloff-Coste in [12].

1. Introduction and Result

In this note we consider the following counting problem. For given $a \in \mathbb{N}^n$, $b \in \mathbb{N}$ count the number of combinations $x \in \{0,1\}^n$ such that $\sum_{i=1}^n a_i x_i \leq b$. As this can be thought of as n items with weights $a_1, \dots, a_n$ to be packed into a knapsack of capacity b this is also known as the *knapsack*-problem. The knapsack-problem is known to be $\#P$-complete. This makes it attractive to consider approximate counting algorithms. The basic idea of such approximate counting algorithms is to approximate the knapsack of capacity b by a sequence of knapsacks of decreasing size b_k (starting with $b_1 = b$ and up to $b_{b+1} = 0$) and to approximate the ratio of the sizes of two consecutive knapsacks by using a rapidly mixing homogeneous Markov chain.
Such a Markov chain $(Y_t)_{t\in\mathbb{N}}$ has been proposed by Sinclair in [13]. So, on the state space $X = \{x \in \{0,1\}^n \mid \sum_{i=1}^n a_i x_i \leq b\}$, we define its transition probability Q in the following way. Given that the Markov chain is in the state $x \in X$ at time t, the transition from x to a state y at time $t+1$ is given by

$$P(Y_{t+1} = y | Y_t = x) = Q(x,y) = \begin{cases} \frac{1}{2} + |\{\, i \,:\, x + e_i \notin X \,\}| / (2n) & : \quad y = x \\ 1/(2n) & : \quad y = x + e_i \in X \end{cases} \tag{1}$$

for all $t \in \mathbb{N}$. Here e_i denotes the i'th unit vector and the addition is to be understood "modulo 2". In other words the chain with a packing x does nothing with probability $1/2$ (this condition in the case $X = \{0,1\}^n$ assures aperiodicity, in the other cases it just gives handy non-trivial lower bound on the smallest eigenvalue). Otherwise it picks one of the items at random. If this item is not in the knapsack and still fits in, the algorithm puts it into the knapsack, while it is taken out when it is in the knapsack. As the starting point will not play any crucial rôle for our considerations we simply may assume that we start in the empty packing $0 \in \mathbb{N}^n$ at time one.

This Markov chain is time-reversible with respect to the uniform measure π on X, that is the detailed balance equations

$$\pi(x) Q(x,y) = \pi(y) Q(y,x)$$

hold true for every pair of states $x, y \in X$. To actually obtain an approximate counting algorithm from this Markov chain would require knowledge about whether it is also

Date: July 30, 1999.
1991 *Mathematics Subject Classification.* 60J10.
Key words and phrases. Markov chains, spectral estimates.

rapidly mixing for an arbitrary choice of the weights $a_1, \dots, a_n$ and the capacity b, that is whether there is a polynomial p in n and ε^{-1} such that

$$\|Q^t(x,\cdot) - \pi\|_{TV} \le \varepsilon \quad \text{for all } t \ge p(n,\varepsilon)$$

for any choice of x. This question which we also consider interesting in its own rights in general is wide open.
Here for two probability measures μ, ν on X the total variation distance is given by

$$\|\mu - \nu\|_{TV} = \frac{1}{2} \sum_{x \in X} |\mu(x) - \nu(x)|.$$

As is well known from the theory of Markov chains one way of proving such a result would be to bound the spectral gap of the chain by the inverse of a polynomial in n.

Let us explain this a little bit more in detail. Since Q is time-reversible with respect to the uniform measure π on X, irreducible and aperiodic we know that 1 is a simple eigenvalue of the linear operator $[\mathcal{Q}\cdot]$ on $L^2(\pi)$ induced by Q, that is the operator

$$[\mathcal{Q}f](x) = \sum_{y \in X} f(y) Q(x,y),$$

where $f \in L^2(\pi)$ (which in our case is, of course, the space of all functions).
By time-reversibility the operator $[\mathcal{Q}\cdot]$ is self-adjoint so that all the eigenvalues are real. We denote them by

$$1 = \beta_0 > \beta_1 \ge \ldots \ge \beta_{|X|-1} \ge -1$$

(note that they are, of course, also the eigenvalues Q).

Our aim is to give a lower estimate for the spectral gap, which in our case means we want to bound the eigenvalue

$$\lambda_1 = 1 - \beta_1 \tag{2}$$

of $Id - Q$ (in a slight abuse of language we will also speak about the spectral gap of the Markov chain (Y_t) and mean the spectral gap of Q). By a result of Diaconis and Stroock [5] a polynomial lower bound on λ_1 indeed implies the polynomial speed of convergence for Q as we have

$$\begin{aligned} \|Q^t(x,\cdot) - \pi\|_{TV} &\le \frac{1}{\pi(x)} (\beta_1^t \vee |\beta_{|X|-1}|^t) \\ &\le \frac{1}{\pi(x)} (\beta_1)^t \end{aligned}$$

as – due to the holding we added – we have $\beta_{|X|-1} \ge 0$.

In [12] Saloff-Coste proved by comparison with the simple walk on the n-dimensional cube $W_n = \{0,1\}^n$ that for knapsacks satisfying that any subset $J \subset \{1, \dots, n\}$ of objects of size $|J| \le n - \sqrt{n}$ is a valid packing, i.e. $\sum_{j \in J} a_j \le b$, the spectral gap satisfies

$$\lambda_1 \ge 2e^{-4} \frac{1}{n}.$$

So, for knapsacks where the set of valid packings looks "almost like the whole cube W_n" Q is indeed rapidly mixing.

Our main assumption will be the following.

Assumption 1.1. *There is $1 \geq \alpha > 1/2$ such that whenever $J \subset \{1, \ldots, n\}$ with $|J| \leq \alpha n$ the inequality*

$$\sum_{j \in J} a_j \leq b$$

holds. In other words any packing consisting of at most αn many objects is a valid packing.

Remark 1.2. *Indeed, assuming that Assumption 1.1 holds simply means that we restrict our attention to such knapsacks $X \subseteq \{0,1\}^n$ that contain all x with*

$$|x| := \sum_{i=1}^{n} x_i \leq \alpha n$$

for some $1/2 < \alpha \leq n$. On the other hand in the above form Assumption 1.1 is more related to the original knapsack problem.

With this assumption our result reads as follows.

Theorem 1.3. *For any knapsack X satisfying Assumption 1.1 the spectral gap of the transition matrix Q on X given by (1) satisfies*

$$\lambda_1 \geq \kappa \left[n \log(n)\right]^{-1} \tag{3}$$

for a positive constant κ. In particular, the Markov chain (Y_t) is rapidly mixing in this situation.

Remark 1.4.
1. *Observe that we only need to show (and will show) Theorem 1.3 for all n large enough, say larger than some number N. It then holds for all n by just choosing a different κ.*
2. *Comparing our result with Saloff-Coste's bound mentioned above, we see that it contains an additional factor $\log n$. Neither could we get rid of this factor, nor can we give any examples to illustrate that it is really necessary. As a matter of fact the central method of this paper, the so-called distance method to be introduced below, yields a bound of order $\frac{1}{n}$ for the spectral gap. Therefore, we strongly conjecture that indeed $\frac{1}{n}$ is the right order which is also supported by Saloff-Coste's result cited above. The additional $\log n$ term only shows up in a lemma where we prepare for employing the distance method.*
3. *The rapidly mixing property is essential for the construction of approximate counters, so-called fpras-algorithms, cf.* [7] *and* [13]. *Using such algorithms it is possible to approximate the total number of elements of X in polynomial time. Unfortunately, the result of Theorem 1.3 is not sufficient to construct an fpras-algorithm. To this end we would also need to show the rapidly mixing property for the Markov chain Q on smaller knapsacks.*
   On the other hand Assumption 1.1 drastically improves Saloff-Coste's condition cited above.

Theorem 1.3 will be proved in the following Section. The proof relies on two techniques which are rather new in the theory of Markov chains.

Acknowledgement: We are extraordinarily grateful to two anonymous referees. Their comments on an earlier draft of the paper largely improved its readability.

2. Proof

In this section we will prove Theorem 1.3. The proof uses a combination of two methods. On the one hand we will use a *martingale method*, as it has first been used in [11] on the other hand a *distance method*, which has been introduced to the theory of Markov chains in [10] and [8] to investigate the spectral gap of algorithms from group theory. Both methods have their origin in the theory of diffusions on manifolds (cf. [2], [3]). Moreover, we will finally use a comparison technique that allows us to translate the result for knapsacks of even size to knapsacks of an odd size.

To be more precise we will first use the martingale method to see that on the "middle level" of the knapsack, that is the level where exactly half of the items are in the knapsack, every eigenfunction to β_1 essentially varies like it varies on the whole space X. This knowledge will be used in the distance method introduced next. It will help us to concentrate on states which are not on the boundary of the knapsack (for others the coupling needed for the distance method would be hard to find).

So, we will first give the proof for knapsacks with an even number of items. The rest will then follow easily.

Let us start by introducing some basic notations. First let us decompose our state space X in the following way.

$$L = \{\, x \in X \,:\, |x| < n/2 \,\}$$

denotes the lower half of the cube (here and in the following, for $x \in W_n$ we write $|x|$ for the number of 1's in x – so $|x| = \sum_{i=1}^{n} x_i$),

$$M = \{\, x \in X \,:\, |x| = n/2 \,\}$$

its middle level and

$$B = \{\, x \in X \,:\, \exists i \,:\, x + e_i \notin X \,\}$$

is the upper boundary of X. Clearly, for $x \in B$ we have $|x| + 1 > \alpha n$.

For any two points $x, y \in X$ (or in W_n) let $d_H(x, y)$ denote their Hamming distance – that is the number of coordinates where they are different or, more formally,

$$d_H(x, y) := \sum_{i=1}^{n} |x_i - y_i|$$

for $x, y \in X$. As usual, for a set $A \subset X$ let $d_H(v, A) = \min\{\, d_H(v, a) \,:\, a \in A \,\}$ be the minimal Hamming distance from v to the set A. Moreover, the following distance (by which we only understand a positive function of two variables - as opposed to a metrics where the triangle inequality has to be fulfilled; in particular the Hamming distance d_H is indeed a metrics) will be central in the proof:

$$\begin{aligned} d(v, w) &:= d_H(v, w)^{1/2} + c\frac{(d_H(v, L) \vee d_H(w, L) \vee 1)^2}{n} \\ &=: d_H(v, w)^{1/2} + d'(v, w) \end{aligned} \tag{4}$$

where c denotes a positive constant. Note that both summands in (4) decrease whenever the Hamming distance included in their definition decreases. Also note that for $v, w \in L$ the distance $d(v, w)$ basically agrees with the square root of the Hamming distance of v and w (up to an additive constant $\frac{c}{n}$).

A central argument in the proof will rely on coupling the random walk induced by Q starting in some point x to another random walk induced by Q starting in some other point y.

The proof will combine this coupling with considerations of an eigenfunction f to the second-largest eigenvalue β_1 of Q.
First let us show that we can assume, that the minimum and maximum of f on the middle level M up to a multiplicative constant behave like the minimum and maximum of f on the whole space X.

Lemma 2.1. *Fix $\gamma \in (0,1)$. Suppose that for all $x_1, y_1 \in M$ one of the the inequalities*

$$f(x_1) \leq \max_{v\in X} f(v)\gamma \tag{5}$$

or

$$f(y_1) \geq \min_{v\in X} f(v)\gamma, \tag{6}$$

hold. Then we have for sufficiently large n,

$$\lambda_1 \geq (1-\gamma)\left[\kappa n \log(n)\right]^{-1},$$

where κ is a constant.

Remark 2.2. *Note that as f is an eigenvalue to β_1 we have that*

$$\min_{v\in X} f(v) < 0 < \max_{v\in X} f(v).$$

Proof of Lemma 2.1. Indeed, suppose that for all $w \in M$ we had

$$f(w) \leq \max_{v\in X} f(v)\gamma. \tag{7}$$

Observe that clearly

$$Z_t = f(X_t) + \lambda_1 \sum_{i=0}^{t-1} f(X_i)$$

is a martingale under Q. So, starting the Markov chain Q in the state x satisfying $f(x) = \max_{v\in X} f(v)$ and stopping this martingale at time $t = p \wedge T_M$ where $p \in \mathbb{N}$ and T_M is the first hitting time of the set M we obtain by the martingale property of Z_t

$$\begin{aligned} f(x) &= E_x\left(f\left(X_{p\wedge T_M}\right)\right) + \lambda_1 E_x\left(\sum_{i=0}^{p\wedge T_M - 1} f(X_i)\right) \\ &\leq E_x\left(f\left(X_{p\wedge T_M}\right)\right) + \lambda_1 E_x\left(p \wedge T_M\right) f(x). \end{aligned}$$

As T_M has finite expectation taking the limit p to infinity yields by dominated convergence

$$f(x) - E_x\left(f\left(X_{T_M}\right)\right) \leq \lambda_1 E_x\left(T_M\right) f(x).$$

Clearly by (7) we have

$$E_x\left(f\left(X_{T_M}\right)\right) \leq f(x)\gamma$$

and thus, as $f(x) > 0$ (see the above remark)

$$\lambda_1 E_x\left(T_M\right) \geq 1 - \gamma.$$

Finally, we can couple the Markov chain Y_t to a simple random walk Y_t' on W_n in such a way that Y_t removes the i'th item from the knapsack whenever the random walk Y_t'

on W_n changes the i'th coordinate from 1 to 0 and that Y_t adds the i'th item to the knapsack whenever Y'_t writes a 1 in the i'th coordinate and this results in an admissible packing of the knapsack. Otherwise Y stands still. So, if we start in $x \in L$ the random walks Y_t and Y'_t will reach the middle level L simultaneously. If $x \in X \setminus (L \cup B)$ it may happen that Y'_t exits X and Y_t cannot follow. Observe, however, that as removing things from the knapsack is always allowed, whenever Y_t is in a state $x \in X$ with $x_i = 1$ for some i then by this coupling Y'_t is in a state $x' \in W_n$ with $x'_i = 1$. Hence we see that if we start above the middle level by the above coupling Y will always be closer to M than the random walk on W_n (in the sense that $Y_t = x$ and $Y'_t = x'$ then $|x| \leq |x'|$), in particular T_M is bounded from above by the entrance time T'_M of Y'_t into M. As for the latter we have that

$$E(T'_M) = \mathcal{O}(n \log n)$$

(this seems to be somehow mathematical folklore, at least we were assured several times that this result would be true, but couldn't find a proof; hence we have added a proof in the Appendix) we obtain the bound

$$E_x\left(T_M\right) \leq \kappa n \log(n)$$

(where κ is a positive constant). Hence we arrive at

$$\lambda_1 \geq (1-\gamma)\left[\kappa n \log(n)\right]^{-1}. \tag{8}$$

In the same way, if (6) is not fulfilled, we obtain for y satisfying $f(y) = \min_{v \in X} f(v)$

$$f(y) - E_x\left(f\left(X_{T_M}\right)\right) \quad \geq \quad \lambda_1 E_x\left(T_M\right) f(y).$$

This together with

$$E_x\left(f\left(X_{T_M}\right)\right) \geq f(y)\gamma$$

and the fact that $f(y) < 0$ again yields

$$\lambda_1 \geq (1-\gamma)\left[\kappa n \log(n)\right]^{-1}.$$

Hence, if one of (5) or (6) are violated we obtain a polynomial estimate for the spectral gap. More precisely we get

$$\lambda_1 \geq \mathcal{O}([n \log(n)]^{-1}).$$

□

The rest of the proof relies on a rather new technique, we call the *distance method*, for estimating the eigenvalues of a Markov chain, the idea of which is amazingly simple. It might be expedient to briefly illustrate this technique before bringing it into action.

Let $\beta \neq 1$ be an eigenvalue of Q with corresponding eigenfunction f. Assume that there exists a function $d : X \to \mathbb{R}_+$ such that for the L^2-operator $[\mathcal{Q}\cdot]$ associated with Q, $[\mathcal{Q}d](x) \leq \alpha d(x)$ for all $x \in X$ and some $\alpha \leq 1$. Let

$$m := \max\left\{\frac{|f(x)|}{d(x)} \;:\; x \in X\right\}.$$

Choose $x \in X$ such that $|f(x)|/d(x) = m$. By irreducibility we may assume that $m \neq 0$ and therefore also $f(x) \neq 0$. Then we have

$$\begin{aligned} |\beta f(x)| &= |[\mathcal{Q}f](x)| = \left| \sum_{y \in X} Q(x,y) f(y) \right| \\ &\leq \sum_{y \in X} Q(x,y) |f(y)| = \sum_{y \in X} Q(x,y) \frac{|f(y)|}{d(y)} d(y) \\ &\leq \frac{|f(x)|}{d(x)} [\mathcal{Q}d](x) \leq \alpha |f(x)|. \end{aligned}$$

Dividing by $|f(x)|$ we conclude $|\beta| \leq \alpha$.

A similar result can be obtained by using couplings, more precisely by coupling Q with itself. So, let $d : X \times X \to \mathbb{R}_+$ be a function, such that for some coupling $\widetilde{Q}$ of (Q, Q) the inequality $[\widetilde{\mathcal{Q}}d](x,y) \leq \alpha d(x,y)$ for all $x \neq y$ and some $\alpha \leq 1$ holds true (again $[\widetilde{\mathcal{Q}}\cdot]$ the L^2-operator associated with $\widetilde{Q}$). Then any eigenvalue $\beta \neq 1$ of Q satisfies, $|\beta| \leq \alpha$. Indeed, defining

$$m := \max \left\{ \frac{(f(y) - f(x))^+}{d(x,y)} \ : \ x \neq y \in X \right\}$$

(where for some number x we define x^+ to be the supremum of x with 0) and choosing (x, y) such that $|g(x,y)|/d(x,y) = m$ (where $g(x,y) = (f(y) - f(x))^+$) we can conclude that

$$|\beta g(x,y)| = \left| \left[\widetilde{\mathcal{Q}} g \right] (x,y) \right| \leq m \left[\widetilde{\mathcal{Q}} d \right] (x,y) \leq m\alpha d(x,y).$$

Hence $|\beta| \leq \alpha$. Note that this technique also works if we let

$$m := \max \left\{ \frac{(f(y) - f(x))^+}{d(x,y)} \ : \ (x,y) \in S \subset X \times X \right\}$$

for some set $S \subset X \times X$ which is invariant under the coupling $\widetilde{Q}$, that is for some set $S \subset X \times X$ with the property that

$$\sum_{(x',y') \in S} \widetilde{Q}((x,y),(x',y')) = 1$$

whenever $(x, y) \in S$.

Of course, this idea is in no way restricted to the situation of X being the knapsack and Q being the specific Markov chain (and indeed in [10],[8] has been applied to the analysis of other random walks).
In short the idea of the distance method can be described as comparing the landscape given by the eigenfunction f (resp. g) to an easier distance, for which the coupling still is contractive.

Proof of Theorem 1.3. :
A central argument in the proof will rely on the coupling technique introduced above where the random walk induced by Q starting in some point x will be coupled to another random walk induced by Q starting in some other point y. The idea of such a coupling technique is to let those random walks collide in short time.

Of course for the analysis of this so-called coupling time the indices i where x_i and y_i are different (or agree) are essential. To this end, for $x, y \in X$ such that $|x| = |y|$ define

$$\begin{aligned} C_1(x,y) &= \{ i \,:\, x_i = 1 = y_i \}, \\ C_0(x,y) &= \{ i \,:\, x_i = 0 = y_i \}, \\ D_1(x,y) &= \{ i \,:\, x_i = 1,\ y_i = 0 \}, \end{aligned}$$

and

$$D_0(x,y) = \{ i \,:\, x_i = 0,\ y_i = 1 \}.$$

Note that $|D_0(x,y)| = |D_1(x,y)| = d_H(x,y)/2$ since $|x| = |y|$.
In order to bring the above ideas into play and to continue the proof we need to consider the following coupling $\widetilde{Q}$ of Q (with itself), which we only need to define properly for $|x| = |y|$, since we will see that the coupling never leaves the set $\{(x,y) : |x| = |y|\}$.

$$\begin{aligned} \widetilde{Q}((x,y),(x+e_i, y+e_i)) &= \frac{1}{2n} \quad \text{for } i \in C_1(x,y) \cup C_0(x,y), &(9)\\ \widetilde{Q}((x,y),(x+e_i, y+e_j)) &= \frac{1}{2n\,|D_0(x,y)|} &(10) \end{aligned}$$

for $(i,j) \in D_1(x,y) \times D_0(x,y) \cup D_0(x,y) \times D_1(x,y)$. Here we implicitly have taken the convention $x + e_i = x$ if $x + e_i \notin X$.
For the other pairs of states $x, y \in X$ take an arbitrary coupling $\widetilde{Q}$ (e.g. the classical coupling). Intuitively speaking this coupling describes that we will only really couple random walks which contain the same number of items. In this case, if the first walk chooses an item which is contained in both knapsack, resp. is missing in both, the second walk will choose the same item. If the first walk selects another item, e.g. one which is contained in the first knapsack but not in the second, the second walk will try to do "the opposite", i.e. in this case will choose an item which is contained in the second knapsack but not in the first. This will bring the walks closer together in the Hamming distance.

Observe that the coupling $\widetilde{Q}$ respects the difference $|x|-|y|$ if $|x| = |y|$ and $\{x,y\} \cap B = \emptyset$.

From now on, for the rest of the paper let

$$g(x,y) := f(x) - f(y).$$

(where for some number x we define x^+ to be the supremum of x with 0).
As explained above we will be interested in the pair (x_1, y_1) given by

$$\frac{g(x_1,y_1)}{d(x_1,y_1)} = \max \left\{ \frac{g(v,w)}{d(v,w)} \,:\, v, w \in X,\ |v| = |w| \right\}. \tag{11}$$

First observe that by (5) and (6) (or the simple fact that by irreducibility f cannot be constant) the above maximum is not zero, such that later on we will be able to divide by it.

The quotient $\frac{g(x_1,y_1)}{d(x_1,y_1)}$ can be bounded from below by taking the maximum only over the middle level M. By (5) and (6) we the arrive at

$$\begin{aligned}\frac{g(x_1,y_1)}{d(x_1,y_1)} &\geq \|g\|_\infty \gamma \frac{1}{d_H(x_1,y_1)^{1/2}+cn^{-1}} \\ &\geq \|g\|_\infty \gamma \frac{1}{n^{1/2}+cn^{-1}}. \end{aligned} \tag{12}$$

If one of v or w is in B (without loss in generality $v \in B$) we obtain

$$\frac{g(v,w)}{d(v,w)} \leq \|g\|_\infty \frac{1}{2^{1/2}+c(\alpha-1/2)^2 n}. \tag{13}$$

Comparing the right hand side of (13) to the right hand side of (12) we see that

$$\gamma \frac{1}{n^{1/2}+cn^{-1}} > \frac{1}{2^{1/2}+c(\alpha-1/2)^2 n}.$$

if and only if

$$\gamma\left(2^{1/2}+c(\alpha-1/2)^2 n\right) > n^{1/2}+cn^{-1}. \tag{14}$$

Now obviously for large n the left side of (14) is growing faster than $n^{1/2}$ on the right side. This yields that in fact for n large enough the relation

$$\frac{g(x_1,y_1)}{d(x_1,y_1)} > \frac{g(v,w)}{d(v,w)},$$

holds true for every pair (v,w) with $\{v,w\} \cap B \neq \emptyset$. This means that for large n we can assume that neither x_1 nor y_1 is in B (where x_1 and y_1 are given by the characterisation (11)).

Now we are prepared to indeed apply the distance method as discussed above. To this end note that for the distance $\sqrt{d_H}$ the following equality holds true.

$$\begin{aligned} &\left[\widetilde{\mathcal{Q}}\sqrt{d_H}\right](x,y) && (15)\\ &= 1/2 d_H(x,y)^{1/2} + \frac{d_H(x,y)}{2n}(d_H(x,y)-2)^{1/2} + \frac{n-d_H(x,y)}{2n} d_H(x,y)^{1/2} \\ &= d_H(x,y)^{1/2}\left[1+\frac{d_H(x,y)^{1/2}(d_H(x,y)-2)^{1/2}}{2n} - \frac{d_H(x,y)}{2n}\right] && (16)\end{aligned}$$

Note that the expression $(\sqrt{t(t-2)}-t)/(2n)$ is smaller than $-1/(2n)$ for all $t \in [2,n]$, so that we finally obtain

$$\left[\widetilde{\mathcal{Q}}\sqrt{d_H}\right](x,y) \leq \sqrt{d_H(x,y)}\left(1-\frac{1}{2n}\right). \tag{17}$$

Now we are ready to apply the distance method. The points x_1, y_1 satisfying (11) can either be both in L or in M or in $X \setminus (L \cup M \cup B)$.

Case a) Suppose that both points x_1, y_1 satisfying (11) are in L. According to (17)

$$\left[\widetilde{\mathcal{Q}}\sqrt{d_H}\right](x_1,y_1) \leq \sqrt{d_H(x_1,y_1)}\left(1-\frac{1}{2n}\right). \tag{18}$$

and since d' is constant on $L \cup M$ and points in L can "at most" reach M

$$[\widetilde{\mathcal{Q}}d'](x_1,y_1) = d'(x_1,y_1) = \frac{c}{n}.$$

So, we are looking for $\kappa > 0$ such that for n large enough

$$d_H(x_1,y_1)^{1/2}\left(1-\frac{1}{2n}\right)+d'(x_1,y_1)\leq\left[d_H(x_1,y_1)^{1/2}+d'(x_1,y_1)\right]\left(1-\frac{\kappa}{n}\right) \tag{19}$$

holds. As (in Case a) $d'(x_1,y_1)=\frac{c}{n}$, (19) holds if

$$0\leq d_H(x_1,y_1)^{1/2}(\frac{1}{2}-\kappa)-\frac{\kappa c}{n}$$

is true. Since $d_H(x_1,y_1)\geq 2$, this is valid for every $\kappa<1/2$, any c and n large enough. Therefore, by choosing for example $\kappa=\frac{1}{3}$ and following the ideas explained above, in Case a) we get a lower bound on the spectral gap of Q of the form

$$\lambda_1\geq\frac{1}{3n}.$$

Case b) Suppose that both points x_1,y_1 satisfying (11) are in M.
Again, for the Hamming distance we have

$$\left[\widetilde{\mathcal{Q}}d_H^{1/2}\right](x_1,y_1)\leq d_H(x_1,y_1)^{1/2}\left(1-\frac{1}{2n}\right). \tag{20}$$

For $d'(x_1,y_1)$ we calculate

$$\begin{aligned}\left[\widetilde{\mathcal{Q}}d'\right](x_1,y_1) &\leq \frac{1}{2}d'(x_1,y_1)+\frac{1}{4}\frac{2^2c}{n}+\frac{1}{4}\frac{c}{n}\\ &= d'(x_1,y_1)\left(1+\frac{3}{4}\right).\end{aligned}$$

Again we want to find $\kappa>0$ such that for sufficiently large n an inequality of the form

$$d_H(x_1,y_1)^{1/2}\left(1-\frac{1}{2n}\right)+d'(x_1,y_1)\frac{7}{4}\leq\left[d_H(x_1,y_1)^{1/2}+d'(x_1,y_1)\right]\left(1-\frac{\kappa}{n}\right) \tag{21}$$

holds.
Using $d'(x_1,y_1)=cn^{-1}$ we see that this is true if and only if

$$\frac{3c}{2}\leq(1-2\kappa)\,d_H(x_1,y_1)^{1/2}-2c\kappa n^{-1}. \tag{22}$$

Choosing for example $\kappa=1/4$ the right side becomes $\frac{1}{2}d_H(x_1,y_1)^{1/2}-\frac{c}{2n}$ which dominates $1/2$ for n sufficiently large, since $d_H(x_1,y_1)\geq 2$ and the last term on the right hand side converges to zero. Hence (22) holds true for $0<c<1/3$.
This shows that in Case b) we obtain a bound for the spectral gap of the form

$$\lambda_1\geq\frac{1}{4n},$$

where we have to choose $0<c<1/3$ in the definition of the metrics d in (4).

Case c) Suppose $x_1, y_1 \in X \setminus B$ such that $|x_1| = |y_1| > n/2$. Computing $\left[\widetilde{\mathcal{Q}}d'\right](x_1, y_1)$ gives

$$\begin{aligned}
&\left[\widetilde{\mathcal{Q}}d'\right](x_1, y_1) \\
= \;& \frac{1}{2}d'(x_1,y_1) + \frac{|x_1|}{2n}\frac{c\left(|x_1| - n/2\right)^2}{n} + \frac{n-|x_1|}{2n}\frac{c\left(|x_1| + 2 - n/2\right)^2}{n} &(23)\\
= \;& d'(x_1,y_1) + \frac{|x_1|}{2n}\frac{c(-1-2|x_1|+n)}{n} + \frac{n-|x_1|}{2n}\frac{c(3+2|x_1|-n)}{n} \\
= \;& d'(x_1,y_1) + c\frac{3n - 4|x_1|^2 + 4n|x_1| - n^2 - 4|x_1|}{2n^2} &(24)
\end{aligned}$$

We want to check whether we can find an appropriate $\kappa > 0$ such that for large n the inequality

$$\left[\widetilde{\mathcal{Q}}(d_H^{1/2} + d')\right](x_1, y_1) \leq \left(1 - \frac{\kappa}{n}\right)\left(d_H(x_1,y_1)^{1/2} + d'(x_1,y_1)\right) \tag{25}$$

holds. Using (20) and (24) we obtain that this is true if

$$-\frac{d_H(x_1,y_1)^{1/2}}{2n} + c\frac{3n - 4|x_1|^2 + 4n|x_1| - n^2 - 4|x_1|}{2n^2} \leq -\frac{\kappa}{n}(d_H(x_1,y_1)^{1/2} + d'(x_1,y_1)). \tag{26}$$

or equivalently

$$2\kappa d'(x_1,y_1) + c\frac{3n - 4|x_1|^2 + 4n|x_1| - n^2 - 4|x_1|}{n} \leq (1-2\kappa)d_H(x_1,y_1)^{1/2}. \tag{27}$$

Now note that

$$\begin{aligned}
& 2\kappa d'(x_1,y_1) + c\frac{3n - 4|x_1|^2 + 4n|x_1| - n^2 - 4|x_1|}{n} \\
= \;& \frac{c}{n}(2\kappa(|x_1| - n/2 + 1)^2 + 3n - 4|x_1|^2 + 4n|x_1| - n^2 - 4|x_1|)
\end{aligned}$$

and that for $\kappa < 2$ the function

$$h(y) := 2\kappa(y - n/2 + 1)^2 + 3n - 4y^2 + 4ny - n^2 - 4y)$$

becomes maximal for $y = \frac{n}{2} + \frac{1-\kappa}{\kappa-2}$. In this case the value is

$$f\left(\frac{n}{2} + \frac{1-\kappa}{\kappa-2}\right) = n + \frac{2}{2-\kappa}.$$

Hence we can show (27) if we can find a $\kappa < 2$ such that

$$c + \frac{c\frac{2}{2-\kappa}}{n} \leq (1-2\kappa)\, d_H(x_1,y_1)^{1/2}.$$

As the second term on the left hand side goes to zero and $(1-2\kappa)\, d_H(x_1,y_1)^{1/2}$ is at least $(1-2\kappa)\sqrt{2}$, we obtain that (27) is for example satisfied if we choose $c = 1/4$ and $\kappa = \frac{1}{3}$ in which case we then obtain the estimate

$$\lambda_1 \geq \frac{1}{3n}$$

for the spectral gap of Q.
Summarizing the results of cases a) through c) we obtain that $\lambda_1 \geq \frac{1}{4n}$ for n sufficiently large.

This finishes the proof of the case where the number n of items is even. For the case of an odd number of items one could in principle try to mimic the proof for even n by replacing the middle level by the two middle levels and then try to obtain similar estimates.

Instead of this we apply a rather elegant comparison technique, the idea of which is to be credited to Diaconis and Saloff-Coste (cf. [4], e.g.). The principle idea behind this technique is the variational characterisation of the second largest eigenvalue (resp. the spectral gap) as

$$\lambda_1 = \inf \left\{ \frac{\mathcal{E}(f,f)}{Var_\pi(f)}, f \text{ non-constant} \right\}$$

(cf [6], e.g.). Here $Var_\pi(f)$ denotes the variance of f with respect to the measure π and

$$\begin{aligned} \mathcal{E}(f,f) &= \langle \Gamma f, f\rangle_\pi \\ &= \frac{1}{2}\sum_{x,y}(f(x)-f(y))^2 Q(x,y)\pi(x) \end{aligned}$$

is the discrete Dirichlet form associated with $\Gamma = Id - Q$.

The idea of the comparison technique is now to compare the Dirichlet form and the variance associated to the knapsack Markov chain with an odd number of items to that of a knapsack Markov chain with an even number of items for which we already know an appropriate bound on the spectral gap.

So, let α be defined as in Assumption 1.1 and take $\varepsilon > 0$ such that $\alpha - \varepsilon > 1/2$. Choose $N = \alpha/\varepsilon - 1$ such that $(\alpha-\varepsilon)(n+1) \le \alpha n$ for all $n \ge N$. Consider the set $X' = \{0,1\} \times X$ which is again a knapsack obtained by adding another object with weight $a_0 = 0$ (and if for X the number n of items was odd, it is even for X'). Note that X' also satisfies (1.1) for all $n \ge N$ with the parameter α replaced by $\alpha - \varepsilon$. Given $f \in L^2(X,\pi)$ we define $\widetilde{f} \in L^2(X',\pi')$ by

$$\widetilde{f}(x_0, x_1, \dots, x_n) = f(x_1, \dots, x_n)$$

for any choice of x_0. We now can associate to any $x' = (x_0, x_1, \dots, x_n) \in X'$ an $x = (x_1, \dots, x_n) \in X$ by removing its first coordinate. Thus we obtain $|X'| = 2|X|$, $\pi'(x') = \frac{1}{2}\pi(x)$ and $\frac{Q'(x',y')}{Q(x,y)} = \frac{n}{n+1}$ (where x resp. y is associated to x' resp. y' in the above manner). This yields

$$\begin{aligned} \mathcal{E}'(\widetilde{f},\widetilde{f}) &= \frac{1}{2}\sum_{x',y'\in X'}(\widetilde{f}(x')-\widetilde{f}(y'))^2 Q'(x',y')\pi'(x') \\ &= \frac{1}{2}\sum_{x,y\in X}\left(f(x_1,\dots,x_n)-f(y_1,\dots,y_n)\right)^2 Q(x,y)\pi(x)\frac{n}{n+1} \\ &= \mathcal{E}(f,f)\frac{n}{n+1}, \end{aligned}$$

where for the second equality we used both, that $\pi'(x') = \frac{1}{2}\pi(x)$ as well as the fact that every summand in the sum over X' appears twice (with $x_0 = 0$ and with $x_0 = 1$, note that necessarily $x_0 = y_0$ since otherwise $Q(x',y') = 0$).

We compute the variance of f with respect to π using the following variational characterisation of the variance

$$Var_{\pi}(f) = \min_{c\in\mathbb{R}} \sum_{x\in X} |f(x)-c|^2 \pi(x).$$

This immediately yields

$$\begin{aligned} Var_{\pi}(f) &= \min_{c\in\mathbb{R}} \sum_{x\in X} |f(x)-c|^2 \pi(x) \\ &= \min_{c\in\mathbb{R}} \sum_{x'\in X'} \left|\widetilde{f}(x')-c\right|^2 \pi'(x') \\ &= Var_{\pi'}(\widetilde{f}). \end{aligned}$$

where we made use of the fact that $\pi(x) = 2\pi'(x')$ and that every summand in the first sum appears twice in the second sum.

Hence we obtain

$$\lambda_1 \geq \lambda_1' \frac{n+1}{n}.$$

Since we already bounded the spectral gap of λ_1' this finishes the proof of the theorem. □

Appendix A. Hitting Times for a random walk on the cube $\mathbb{Z}_2^d$

In this appendix we bound the mean entrance time into the middle level of the d-dimensional cube $\mathbb{Z}_2^d$ by a nearest neighbor random walk without holding (the generalisations to the case of positive holding probability are straight forward).
So, let us consider the nearest-neighbor random walk on the cube $\mathbb{Z}_2^d$ with holding probability zero.

Theorem A.1. *Let $E^x_{[\frac{d+1}{2}]}$ be the mean first hitting of the middle level*

$$N_{[\frac{d+1}{2}]} := \{x \in \mathbb{Z}_2^d : |x| = [\frac{d+1}{2}]\}$$

of a nearest-neighbor random walk on the cube $\mathbb{Z}_2^d$ with holding probability zero starting in $x \in \mathbb{Z}_2^d$. Here for $x \in \mathbb{R}$ we denote by $[x]$ the smallest integer less than or equal to x.
Then

$$E^x_{[\frac{d+1}{2}]} \leq \kappa d \log d$$

for some constant $\kappa > 0$.

Proof. Obviously, due to symmetry it suffices to prove the result for $|x| \leq [\frac{d+1}{2}]$.

So, for $i \in \{0, \dots, d\}$ introduce the sets $N_i := \{x \in \mathbb{Z}_2^d : |x| = i\}$. Let $k \in \{1, \dots, d\}$ be fixed. We denote by $E_{i,k}$ for $i \in \{0, \dots, k\}$ the mean hitting time of N_k, when starting in level N_i. Note that by a coupling argument $E_{i,k} \leq E_{0,k}$ and thus it suffices to bound $E_{0,k}$.

Obviously, the $E_{i,k}$ have to satisfy the following equations

$$\begin{aligned} E_{k,k} &= 0 \\ E_{0,k} &= E_{1,k} + 1 \\ E_{i,k} &= \frac{i}{d} E_{i-1,k} + \frac{d-i}{d} E_{i+1,k} + 1 \text{ for } i \in \{1, \dots, k-1\}. \end{aligned}$$

This system of equations is equivalent to

$$\begin{pmatrix} d & -d & 0 & \cdots & \cdots & 0 \\ -1 & d & -(d-1) & 0 & & \vdots \\ 0 & -2 & d & -(d-2) & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ & & 0 & -(k-2) & d & -(d-(k-2)) \\ 0 & \cdots & \cdots & 0 & -(k-1) & d \end{pmatrix} \begin{pmatrix} E_{0,k} \\ E_{1,k} \\ E_{2,k} \\ \vdots \\ E_{k-2,k} \\ E_{k-1,k} \end{pmatrix} = \begin{pmatrix} d \\ d \\ d \\ \vdots \\ d \\ d \end{pmatrix}$$

For $m \in \{0 \dots, k-1\}$ define

$$v_m := d \left(\sum_{i=0}^{m} \frac{\binom{d}{i}}{\binom{d}{m}} \right)$$

and let $v := (v_0, \dots, v_{k-1})^t$.
By induction one can show that the system above is equivalent to

$$\begin{pmatrix} d & -d & 0 & \cdots & \cdots & 0 \\ 0 & d-1 & -(d-1) & 0 & & \vdots \\ 0 & 0 & d-2 & -(d-2) & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ & & 0 & 0 & d-(k-2) & -(d-(k-2)) \\ 0 & \cdots & \cdots & 0 & 0 & d-(k-1) \end{pmatrix} \begin{pmatrix} E_{0,k} \\ E_{1,k} \\ E_{2,k} \\ \vdots \\ E_{k-2,k} \\ E_{k-1,k} \end{pmatrix} = v. \tag{28}$$

From this we obtain that

$$E_{k-1,k} = \frac{1}{d-(k-1)} v_{k-1} = \frac{d}{d-(k-1)} \sum_{i=0}^{k-1} \frac{\binom{d}{i}}{\binom{d}{k-1}}. \tag{29}$$

Now suppose $k \le [\frac{d+1}{2}]$. Then there is a drift from 0 to the set $N_k \cup \ldots \cup N_d$. This enables us to give an upper bound on $E_{k-1,k}$ by using Wald's identity.
Consider the following random walk on the set of integers. For $(X_i)_{i \ge 0}$ i.i.d. random variables we examine the process $S_n := \sum_{i=0}^{n} X_i$, where

$$P(X_i = +1) = \frac{d-(k-1)}{d} \quad \text{and} \quad P(X_i = -1) = \frac{k-1}{d}.$$

Let $T := \inf\{n \ge 0 : S_n = 1\}$. Since $\frac{d-(k-1)}{d} \ge \frac{d+1}{2d} > \frac{1}{2}$ we have $T < \infty$ almost surely. Hence by applying Wald's identity

$$E(S_T) = E(T) E(X_1).$$

Computing $E(X_1)$ and using that $E(S_T) = 1$ gives

$$E(T) = \frac{1}{E(X_1)} = \frac{d}{d-2(k-1)}.$$

It is obvious that $E_{k-1,k} \leq E(T)$ so that we get the following upper bound for the expression that has been calculated in (29):

$$\frac{d}{d-(k-1)} \sum_{i=0}^{k-1} \frac{\binom{d}{i}}{\binom{d}{k-1}} = E_{k-1,k} \leq E(T) = \frac{d}{d-2(k-1)}. \tag{30}$$

Our aim is to bound $E_{0,k}$ with $k = [\frac{d+1}{2}]$. By solving the system (28) recursively we obtain that

$$E_{0,k} = \sum_{i=0}^{k-1} \frac{1}{d-i} v_i.$$

Since the estimate (30) holds for all $i \in \{1, \dots, \frac{d+1}{2}\}$ we have $\frac{1}{d-i} v_i \leq \frac{d}{d-2i}$. Thus we get the following estimate for $E_{0,[\frac{d+1}{2}]}$.

$$\begin{aligned} E_{0,\frac{d+1}{2}} &= \sum_{i=0}^{[\frac{d-1}{2}]} \frac{1}{d-i} v_i \\ &\leq \sum_{i=0}^{\frac{d-1}{2}} \frac{d}{d-2i} \leq d\left(1 + \int_0^{[\frac{d-1}{2}]} \frac{1}{2x+1} dx\right) = d\left(1 + \frac{\ln(d)}{2}\right). \end{aligned}$$

□

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