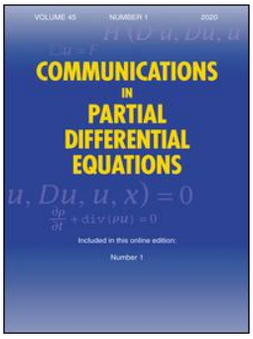

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The uniqueness of hierarchically extended backward solutions of the Wright–Fisher model

Julian Hofrichter, Tat Dat Tran, and Jürgen Jost

Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany

ABSTRACT
The diffusion approximation of the Wright-Fisher model of population genetics leads to partial differentiable equations, the Kolmogorov forward and backward equations, with a leading term that degenerates at the boundary. This degeneracy has the consequence that standard PDE tools do not apply, and solutions lack regularity properties. In this paper, we develop a regularizing blow-up scheme for the iteratively extended global solutions of the backward Kolmogorov equation presented in a previous paper, which are constructed from a known class of solutions, and establish their uniqueness for the stationary case. As the model describes the random genetic drift of several alleles at the same locus from a backward perspective, the occurring singularities result from the loss of an allele. While in an analytical approach, this provides substantial difficulties, from a biological or geometric perspective, this is a natural process that can be analyzed in detail. The presented scheme regularizes the solution via a carefully constructed iterative transformation of the domain.

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1. Introduction

The Wright-Fisher model [13, 39] models the most basic component of mathematical population genetics, i.e. genetic drift. In a finite population of fixed size, parents are randomly sampled and pass on the alleles they are carrying to the offspring generation. By repeating this process over many (non-overlapping) generations, the model describes the evolution of the probabilities of the different alleles in the population. In the basic setting, the model covers a single locus only. Extensions to several loci are possible, as is the inclusion of mutation, selection, or a spatial population structure. This has driven the research in mathematical population genetics ([4, 11]), inspired by the pioneering work of Kimura [23–25].

Nevertheless, the original model remains of considerable mathematical interest, in particular when we follow Kimura and consider the diffusion approximation. This diffusion approximation leads to a model with an infinite population size and continuous time. Its dynamics may then be described by the so-called forward and backward Kolmogorov equations. The forward equation is a partial differential equation of parabolic type and describes the evolution of the model over time. The backward equation, which is the adjoint of the former w. r. t. a suitable product, in contrast, models a process that runs backward in time as it describes the probability of ancestral states. According to this biological interpretation, the equation is not parabolic. Mathematically, however, we can easily convert it into a parabolic equation by

CONTACT Jürgen Jost jjost@mis.mpg.de Max Planck Institute for Mathematics in the Sciences, Inselstrasse 22, Leipzig 04103, Germany.

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simply replacing $-t$ by t. Putting it simply, a backward equation with a final condition can be converted into a forward equation with an initial condition. More serious mathematical difficulties arise from the fact that both equations become degenerate at the boundary.

This paper investigates solutions of the Kolmogorov backward equation for the relative frequencies $0 \le p^i \le 1$ of the alleles $i = 0, \dots, n$, that is

$$-\frac{\partial}{\partial t}u(p,t) = \frac{1}{2}\sum_{i,j=1}^{n} p^i(\delta^i_j - p^j)\frac{\partial}{\partial p^i}\partial p^j u(p,t) =: L^*_n u(p,t) \tag{1.1}$$

The frequency p^0 does not appear in (1.1) because of the normalization $\sum_{i=0}^n p^i = 1$. When one of the frequencies p^i becomes 0, the corresponding coefficient also becomes 0. Thus, the differential operator in (1.9) becomes degenerate at the boundary of our domain, the probability simplex $\Delta_n = \{(p^1, \dots, p^n) : p^i > 0, \sum_{j=1}^n p^j < 1\}$. In fact, a suitable extension of the solution of (1.1) to the boundary of Δ_n and the investigation of its properties will be our main concern and achievement.

There have been two lines of research on these Kolmogorov equations, one with tools from the theory of stochastic processes, see for instance [7, 9, 10, 22], as well as with tools from the theory of partial differential equations [5, 6]. By its general nature, this approach is capable of certain existence, uniqueness and regularity results, but cannot come up with explicit formulas, for instance for the expected time of loss of an allele. Therefore, the second line of research uses less general tools, but makes detailed use of the specific and explicit structure of the model. This has also included the global aspect, that is, connecting the solutions in the interior of the simplex and on its boundary faces, and a number of representation formulas has been derived. This aspect is also covered to some extent in Section 5.10 of [11] as well as in [4], but we wish to illustrate certain results in more detail and with a different focus.

In the literature, using an observation of [31], one usually writes the Kolmogorov backward operator in the form

$$\Lambda^*_n u(x,t) := \frac{1}{2}\sum_{i,j=0}^{n} x^i(\delta^i_j - x^j)\frac{\partial}{\partial x^i}\partial x^j u(x,t), \tag{1.2}$$

using the variables $(x^0, x^1, \dots, x^n)$ with $\sum_{j=0}^n x^j = 1$ in place of $L^*_n u(p,t)$ (cf. equation (1.1)) with $(p^1, \dots, p^n)$ and $p^0 = 1 - \sum_{i=1}^n p^i$ implicitly determined (for our notation, see Section 2.1, in particular (2.2) and (1.11). That is, one includes the variable x^0 and works on the simplex $\{x^0 + x^1 + \dots x^n = 1, x^i \ge 0\}$. This formulation has the advantage of being symmetric w. r. t. all x^i, but the downside is that the operator invokes more independent variables than the dimension of the space on which it is defined. Thus, the elliptic operator becomes degenerate. Here, we have opted to work with L^*_n, but for the comparison with the literature, we shall utilize the version (1.2).

Much of the literature to be referenced here is based on the observation of Wright [40] that the degeneracy at the boundary may be removed if one includes mutation. More precisely, let the mutation rate m_{ij} be the probability that when allele i is selected for offspring, the offspring carries the mutant j instead of i; furthermore, one defines $m_{ii} = -\sum_{j\neq i} m_{ij}$. The corresponding Kolmogorov backward operator then becomes

$$\Lambda^*_n u(x,t) := \frac{1}{2}\sum_{i,j=0}^{n} x^i(\delta^i_j - x^j)\frac{\partial}{\partial x^i}\partial x^j u(x,t) + \sum_{j=0}^{n}\sum_{i=0}^{n} m_{ij}x^i\frac{\partial}{\partial x^j}. \tag{1.3}$$

Wright [40] discovered that calculations may be considerably simplified by assuming

$$m_{ij} = \frac{1}{2}\mu_j > 0 \quad \text{for } i \neq j, \tag{1.4}$$

that is, the mutation rates depend only on the target gene (the factor $\frac{1}{2}$ is inserted solely for purposes of normalization) and are positive. With (1.4), (1.3) becomes

$$\Lambda_n^* u(x,t) := \frac{1}{2}\sum_{i,j=0}^{n} x^i(\delta_j^i - x^j)\frac{\partial}{\partial x^i}\partial x^j u(x,t) + \frac{1}{2}\sum_{j=0}^{n}\left(\mu_j - \sum_{i=0}^{n}\mu_i x^j\right)\frac{\partial}{\partial x^j}. \tag{1.5}$$

In this case, one obtains a unique stationary distribution for the Wright–Fisher diffusion, given by the Dirichlet distribution with parameters $\mu_0, \ldots, \mu_n$. A further simplification occurs when

$$\mu_0 = \cdots = \mu_n =: \mu > 0, \tag{1.6}$$

i.e., when all mutation rates are identical. The assumption (1.4) that the mutation rates only depend on the target gene is not very plausible from the biological perspective (the mutation rate should rather depend on the initial instead of the target gene, but (1.6) remedies that deficit in a certain sense), but in the present context the more crucial issue is the assumption of positivity.

Several papers have studied this model and derived explicit formulas for the transition density of the process with generator (1.5) including [3, 8, 14–16, 28, 32–34]; these, however, were rather of a local nature, as they did not connect solutions in the interior and the boundary strata of the domain. Furthermore, Kingman's coalescent [26] has proven to be a very useful tool in this line of research, that is, the method of tracing lines of descent back into the past and analyzing their merging patterns (for a quick introduction to that theory, see also [21]). In particular, some of these formulas likewise extend to the limiting case $\mu = 0$ in (1.6); Ethier and Griffiths [8] showed that the following formula for the transition density

$$P(t,x,dy) = \sum_{M\geq 1} d_M^0(t) \sum_{|\alpha|=M,\alpha\in\mathbb{Z}_+^n} \binom{|\alpha|}{\alpha} x^\alpha \operatorname{Dir}(\alpha, dy), \tag{1.7}$$

which had previously been derived under the assumption $\mu > 0$, also applies to the case $\mu = 0$. Here, Dir is the Dirichlet distribution, and $d_M^0(t)$ is the number of equivalence classes of lines of descent of length M at time t in Kingman's coalescent for which analytical formulas have been derived in [34]. (1.7) has been studied further in many subsequent papers, for instance [16]. However, the Dirichlet distribution in (1.7) becomes singular when y approaches the boundary of K.

Shimakura in [33] came up with the somewhat less explicit formula

$$\begin{aligned} P(t,x,dy) &= \sum_{m\geq 1} e^{-\lambda_m t} E_m(x,dy) \\ &= \sum_{K\in\Pi} P(t,x,y)\,dS_K(y) \\ &= \sum_{K\in\Pi} e^{-\lambda_m t} E_{m,K}(x,y)\,dS_K(y). \end{aligned} \tag{1.8}$$

Here, the λ_m are the eigenvalues of the elliptic operator, and E_m is the projection onto the corresponding eigenspace, and the index K enumerates the faces of the simplex. This solution is defined on the entire simplex, and it matches all (independent) data on different boundary strata as t tends to 0. However, the transitions from a face into one of its boundary faces are not accounted for in this scheme, which considers the solutions on the individual faces separately. Thus, (1.8) is simply a decomposition into the various modes of the solutions of a linear PDE, summed over all faces of the simplex. In particular, Shimakura's solution satisfies corresponding regularity properties. Altogether, this illustrates the rather local character of the solution scheme.

In the present paper, we want to get a more detailed analytical picture of the behavior at the boundary and investigate global solutions, specifically their uniqueness, on the entire state space including its stratified boundary. In an important recent work, Epstein and Mazzeo [5, 6] have developed PDE techniques to tackle the issue of solving PDEs on a manifold with corners that degenerate at the boundary with the same leading terms as the Kolmogorov backward equation for the Wright-Fisher model (1.1) in the closure of the probability simplex in $(\overline{\Delta}_n)_{-\infty} = \overline{\Delta}_n \times (-\infty, 0)$. A crucial ingredient of their analysis is the construction of appropriate function spaces. In our context, their spaces $C^{k,\gamma}_{WF}(\overline{\Delta}_n)$ would consist of k times continuously differentiable functions whose kth derivatives are Hölder continuous with exponent γ w. r. t. the Fisher metric. In terms of the Euclidean metric on the simplex, this means that a weaker Hölder exponent (essentially $\frac{\gamma}{2}$) is required in the normal than in the tangential directions at the boundary. Using this framework, they then show that if the initial values are of class $C^{k,\gamma}_{WF}(\overline{\Delta}_n)$, then there exists a unique solution in that class. This result is very satisfactory from the perspective of PDE theory (see e.g. [20]). In the situation that we are facing in this paper, however, the data and the solutions are not even continuous, let alone of some class $C^{0,\gamma}(\overline{\Delta}_n)$, as we want to study the boundary transitions. Likewise, the (stationary) uniqueness assertion does not apply, which Epstein and Mazzeo have established for largely regular (in particular, globally continuous) solutions by a modified version the Hopf boundary point Lemma and some maximum principle (yielding a similar, but more general result as Proposition 10.2 in [19]).

The same also holds for other works which treat uniqueness issues in the context of degenerate PDEs, but are not adapted to the very specific class of solutions at hand. This includes the extensive work by Feehan [12] where – amongst other issues – the uniqueness of solutions of elliptic PDE whose differential operator degenerates along a certain portion of the boundary $\partial_0\Omega$ of the domain Ω is established: for a problem with a partial Dirichlet boundary condition, where the boundary data are only given on $\partial\Omega\backslash\partial_0\Omega$, a so-called second-order boundary condition is applied for the degenerate boundary area; this condition says that a solution needs to be such that the leading terms of the differential operator continuously vanishes towards $\partial_0\Omega$, while the solution itself is also of class C^1 up to $\partial_0\Omega$. Within this framework, Feehan than shows that – under certain technical assumptions – degenerate operators satisfy a corresponding maximum principle for the partial boundary condition, which assures the uniqueness of a solution. Although this in principle may also apply to solutions of Wright–Fisher diffusion equations, this does not entirely cover the situation at hand, since, if $n \geq 2$, L^* only partially degenerates towards the boundary (instances of codimension 1). More precisely, its degeneracy behaviour is stepwise, corresponding to the stratified boundary structure of the domain $\overline{\Delta}_n$, and hence does not satisfy the requirements

for Feehan's scenario. Furthermore, in the language of [12], the intersection of the regular and the degenerate boundary part $\partial\partial_0\Omega$, would encompass a hierarchically iterated boundary-degeneracy structure, which is beyond the scope of that work.

Therefore, in this paper, we continue the detailed investigation of the boundary behavior of solutions of the (extended) Kolmogorov backward equation (1.1) started in [19] (the concept of solution developed there expands a notion of solution which is well-known in the literature (cf. [27, 29])). In analytical terms, the issue is the regularity of solutions at singularities of the boundary, that is, where two or more faces of the simplex Δ_n meet. When considering particular extension paths from the boundary into the interior of the simplex (they have nothing to do, however, with Kingman's coalescent lines of descent as utilized in some of the literature discussed above), these may result in boundary singularities at certain strata of the boundary of the domain, and we are interested in the directions in which the singularities of the boundary of the simplex are approached from the interior, because we want to resolve these boundary singularities.

In contrast to the approaches discussed above that invoke strong tools from the theory of stochastic processes, our approach is not stochastic, but analytic and geometric in nature, which means that the spirit of our approach is rather related to that of [5, 6]. In contrast to that approach, however, we develop geometric constructions, within the framework of information geometry, that is, the geometry of probability distributions, see [1, 2], in order to have an approach that on one hand is naturally capable of studying such generalizations as indicated above, but on the other hand can still derive explicit formulas. This is part of a general research program, see [17–19, 35–38]. The biological interpretation provides a key to some of our technical arguments. Alleles can disappear from the population in different order. We work on the n-dimensional probability simplex, which represents the relative frequencies of $(n+1)$ alleles in a population. Its k-dimensional boundary faces F_1, F_2 represent population states with only $(k+1)$ alleles. When two such faces meet in a $(k-1)$-dimensional subface F_0, we can approach each point in F_0 from either F_1 or F_2, but this then corresponds to different orders of the loss events. Therefore, the resulting limits might *a priori* be different. Therefore, there arises the issue of continuity of the solution of our process on faces of codimension 2 or higher in the boundary of the probability simplex. And for such discontinuous solutions, the maximum principle does not apply to show uniqueness. For this reasons, we need to combine biologically correct continuity and extension assumptions with a careful blow-up process that resolves the remaining ambiguities. This constitutes the main technical achievement of this paper.

Let us now describe in more specific terms what we achieve in this paper. Based on the previous work [19], we continue the analysis of solutions of the *(extended) Kolmogorov backward equation* for the diffusion approximation of the Wright–Fisher model

$$\begin{cases} L^*U(p,t) = -\dfrac{\partial}{\partial t}U(p,t) & \text{in } \left(\overline{\Delta}_n\right)_{-\infty} = \overline{\Delta}_n \times (-\infty,0) \\ U(p,0) = f(p) & \text{in } \overline{\Delta}_n, f \in L^2\left(\bigcup_{k=0}^n \partial_k\Delta_n\right) \end{cases} \tag{1.9}$$

for $U(\,\cdot\,,t) \in C_p^2\left(\overline{\Delta}_n\right)$ for each fixed $t \in (-\infty,0)$ and $U(p,\,\cdot\,) \in C^1((-\infty,0))$ for each fixed $p \in \overline{\Delta}_n$ resp. the *stationary (extended) Kolmogorov backward equation*

$$\begin{cases} L^*U(p) = 0 & \text{in } \overline{\Delta}_n \backslash \partial_0\Delta_n \\ U(p) = f(p) & \text{in } \partial_0\Delta_n \end{cases} \tag{1.10}$$

for $U \in C_p^2(\overline{\Delta}_n)$ where

$$L^* u(p,t) := \frac{1}{2} \sum_{i,j=1}^{n} \left(p^i(\delta_j^i - p^j)\right) \frac{\partial}{\partial p^i} \partial p^j u(p,t). \tag{1.11}$$

is the corresponding *backward operator*.

Emerging solutions of the backward Kolmogorov equation may be interpreted as probability distributions over ancestral states yielding some given current state of allele frequencies with time running backward as indicated by the name. Such an ancestral state could have possessed more alleles than the current state, as on the path towards that latter state, some alleles that had been originally present in the population could have been lost. In analytical terms, one could assume that such a loss of allele event is continuous, in the sense that the relative frequency of the corresponding allele simply goes to 0. Geometrically, however, this means that the process from the interior of a probability simplex enters into some boundary stratum and henceforth stays there. Also, when two or more alleles got lost, they could have disappeared in different orders from the population. A corresponding global and hierarchical solution for the Kolmogorov backward equation that persists and stays regular across different such loss of allele events in the past was constructed in the preceding paper [19] (Propositions 8.1 f.), which was technically rather involved:

Proposition (pathwise extension of solutions, informal version of Proposition 3.2). *Let $k, n \in \mathbb{N}$ with $0 \le k < n$, and let u_{I_k} be a proper solution of the Kolmogorov backward equation (1.9) restricted to $\Delta_k^{(I_k)}$ for some final condition $f \in \mathcal{L}^2(\Delta_k^{(I_k)})$. For $d = k+1, \dots, n$, there exist extensions $\bar{u}_{I_k}^{i_k,\dots,i_d} := \left(\bar{u}_{I_k}^{i_k,\dots,i_{d-1}}\right)^{i_{d-1},i_d}$ in $\left(\Delta_d^{(I_d)}\right)_{-\infty}$ of $\bar{u}_{I_k}^{i_k,\dots,i_{d-1}}$ (starting with $u_{I_k}^{i_k} \equiv u_{I_k}$) with*

$$\bar{u}_{I_k}^{i_k,\dots,i_d}(p,t) = u_{I_k}(\pi^{i_k,\dots,i_d}(p),t) \prod_{j=k}^{d-1} \frac{p^{i_j}}{\sum_{l=j}^{d} p^{i_l}}, \quad (p,t) \in \left(\Delta_d^{(I_d)}\right)_{-\infty} \tag{1.12}$$

and a global extension $\overline{U}_{I_k}^{i_k,\dots,i_n}$ in $\left(\bigcup_{k \le d \le n} \Delta_d^{(I_d)}\right)_{-\infty}$ by putting

$$\begin{aligned} \overline{U}_{I_k}^{i_k,\dots,i_n}(p,t) &:= u_{I_k}(p,t)\chi_{\Delta_k^{(I_k)}}(p) + \sum_{k+1 \le d \le n} \bar{u}_{I_k}^{i_k,\dots,i_d}(p,t)\chi_{\Delta_d^{(I_d)}}(p) \\ &= u_{I_k}(p,t)\chi_{\Delta_k^{(I_k)}}(p) + \sum_{k+1 \le d \le n} u_{I_k}(\pi^{i_k,\dots,i_d}(p),t) \prod_{j=k}^{d-1} \frac{p^{i_j}}{\sum_{l=j}^{d} p^{i_l}} \chi_{\Delta_d^{(I_d)}}(p) \end{aligned} \tag{1.13}$$

and we have

$$\begin{cases} L^* \overline{U}_{I_k}^{i_k,\dots,i_n} = -\dfrac{\partial}{\partial t} \overline{U}_{I_k}^{i_k,\dots,i_n} & \text{in } \left(\bigcup_{k \le d \le n} \Delta_d^{(I_d)}\right)_{-\infty} \\ \overline{U}_{I_k}^{i_k,\dots,i_n}(\,\cdot\,,0) = \overline{F}_{I_k}^{i_k,\dots,i_n} & \text{in } \bigcup_{k \le d \le n} \Delta_d^{(I_d)} \end{cases} \tag{1.14}$$

with $\overline{F}_{I_k}^{i_k,\dots,i_n} \in \mathcal{L}^2\left(\bigcup_{k \le d \le n} \Delta_d^{(I_d)}\right)$ being an analogous extension of the final condition $f = f_{I_k}$ in $\Delta_k^{(I_k)}$; in particular, we have $\overline{U}_{I_k}^{i_k,\dots,i_n}\big|_{\Delta_k^{(I_k)}}(\,\cdot\,,0) = f$ in $\Delta_k^{(I_k)}$.

This result allows us to extend any solution of the Kolmogorov backward equation that lives on a certain stratum ("proper solution") to all corresponding strata of higher dimension of some larger domain. The obtained extension then solves the analogous problem in the entire larger domain, for a final condition which is likewise an extension of the original final condition. In terms of the Wright–Fisher model, where a proper solution models ancestral states of a certain set of alleles over time, this scheme yields corresponding ancestral states on all those sets from which the original set can be reached by a (multiple) loss of alleles. These states are again modelled over time; the final condition which is met by the solution corresponds to an analogous extension of the original target set which spans all relevant higher-dimensional strata. The scheme is versatile and can be applied for all potential losses of alleles.

The result improves results in the literature (cf. [27, 29], and is indispensable for a complete understanding and a rigorous solution of the Kolmogorov backward equation. The present paper completes this approach by establishing the uniqueness for this class of solution in the stationary case.

The key is the degeneracy at the boundary of the Kolmogorov equations. While from an analytical perspective, this presents a profound difficulty for obtaining boundary regularity of the solutions of the equations, from a biological or geometric perspective, this is very natural because it corresponds to the loss of some alleles from the population in finite time by random drift. And from a stochastic perspective, this has to happen almost surely. For this reason, the above equations are not accessible by standard theory (cf. e.g. [30]), because the square root of the coefficients of the second order terms of L^* is not Lipschitz continuous up to the boundary. As a consequence, in particular the uniqueness of solutions to the above Kolmogorov backward equations may not be derived from standard results. Instead, such degenerate equations arising from population biology have been analyzed by Epstein and Mazzeo (cf. [5, 6]) only recently. While their aim was to develop a general and widely applicable theory, we rather focus on the specific properties of the Wright-Fisher model to obtain results that do not readily follow from the general theory. We shall derive the regularity and uniqueness of a certain class of solutions that are the hierarchically extended solutions of the Kolmogorov backward equation developed in [19].

Our aim is the global regularity in the closure of the domain, and this will be achieved by resolving any incompatibilities between different boundary strata. For that purpose, we shall construct an appropriate transformation of the relevant part of the domain (i.e. the simplex Δ_n, cf. below). As a result, we can work on a domain that is a product of a simplex and a cube. Thereby, the iteratively extended solutions are turned into corresponding solutions of the transformed equation, which are then of sufficient global regularity; in particular, they are globally continuous. For generic iteratively extended solutions this does not yet yield a corresponding regularity. However, the transformation scheme is still applicable, and the transformation image may be extended that way as well (see 7.3 (iii)). In any case, before such a transformation, a solution may be highly irregular, and certainly not globally continuous on the closed simplex.

In the stationary case, such transformed solutions are uniquely defined by their values on the vertices of the domain (analogously to a globally continuous solution of the original problem in Δ_n, cf. Section 6). It just needs to be shown that a complete set of boundary data

on the simplex generates sufficient boundary data on the larger domain which is produced by the blow-up.

Theorem (informal version of Theorem 7.3 on p. 481). *Let $n \in \mathbb{N}_+$, $i_0 \in \{0, \dots, n\}$ and a solution $u_{\{i_0\}} \colon \Delta_0^{(\{i_0\})} \longrightarrow \mathbb{R}$ be given. Then an extension $\overline{U}$ of $u_{\{i_0\}}$ to the entire simplex (cf. Proposition 3.2) is unique within the class of all extensions U which satisfy certain 'extension constraints' and additional boundary regularity of the blow-up image if $n \geq 2$.*

2. Notation

2.1. The simplex

We want to consider relative frequencies (of alleles) in a population, and therefore, we shall use the probability simplex as the corresponding state space. In this subsection, we shall introduce a suitable simplex notation as well as the appropriate function spaces (see also [18]).

Let $p^0, p^1, \dots, p^n$ denote the relative frequencies of alleles $0, 1, \dots, n$. As we have $\sum_{j=0}^n p^j = 1 \Leftrightarrow p^0 = 1 - \sum_{i=1}^n p^i$, this leads to an n-dimensional state space

$$\Delta_n = \left\{ (p^0, \dots, p^n) \in \mathbb{R}^{n+1} \middle| p^j > 0 \text{ for } j = 0, 1, \dots, n \text{ and } \sum_{j=0}^n p^j = 1 \right\} \tag{2.1}$$

or equivalently

$$\Delta_n := \left\{ (p^1, \dots, p^n) \in \mathbb{R}^n \middle| p^i > 0 \quad \text{for } i = 1, \dots, n \text{ and } \sum_{i=1}^n p^i < 1 \right\}, \tag{2.2}$$

which is the (open) *n-dimensional standard orthogonal simplex*

The closure of this simplex is

$$\overline{\Delta}_n = \left\{ (p^1, \dots, p^n) \in \mathbb{R}^n \middle| p^i \geq 0 \text{ for } i = 1, \dots, n \text{ and } \sum_{i=1}^n p^i \leq 1 \right\}. \tag{2.3}$$

In order to include the time parameter $t \in (-\infty, 0]$, we also write

$$(\Delta_n)_{-\infty} := \Delta_n \times (-\infty, 0).$$

The boundary of the simplex $\partial \Delta_n = \overline{\Delta}_n \backslash \Delta_n$ consists of boundary strata, the *faces*, which are (sub-)simplices themselves, from the $(n-1)$-dimensional *facets* down to the 0-dimensional *vertices*. Each subsimplex of dimension $k \leq n-1$ is isomorphic to the k-dimensional standard orthogonal simplex Δ_k. To denote a particular subsimplex, we introduce index sets[1] $I_k = \{i_0, i_1, \dots, i_k\} \subset \{0, \dots, n\}$ with $i_j \neq i_l$ for $j \neq l$ and put

$$\Delta_k^{(I_k)} := \left\{ (p^1, \dots, p^n) \in \overline{\Delta}_n \middle| p^i > 0 \text{ for } i \in I_k; p^i = 0 \text{ for } i \in I_n \backslash I_k \right\}. \tag{2.4}$$

[1] In fact, any such ordering is just a relabeling of the standard set with standard ordering $\{0, \dots, n\}$ and consequently, one could just work with $I_k = \{0, \dots, k\}$ for $k = 0, \dots, n$. However, by the choice of notation, we wish to emphasize some combinatorial aspect, which is based on the underlying model: Different orderings correspond to different modes of allele extinction (which are all present in the model) and hence, a full description needs to account for all of them simultaneously (cf. also [19]).

The index set I_n may be omitted, thus $\Delta_n = \Delta_n^{(I_n)}$. The index 0 corresponding to p^0 plays an important role: On $\Delta_k^{(I_k)}$ we have

$$p^0 = \begin{cases} 1 - \sum_{i \in I_k \setminus \{0\}} p^i & \text{if } 0 \in I_k, \\ 0 & \text{if } 0 \notin I_k. \end{cases} \tag{2.5}$$

So, if $0 \in I_k$, we require $\sum_{i \in I_k \setminus \{0\}} p^i < 1$, otherwise $\sum_{i \in I_k \setminus \{0\}} p^i = 1$.

Each of the $\binom{n+1}{k+1}$ subsets I_k of I_n corresponds to a boundary face $\Delta_k^{(I_k)}$ ($k \leq n-1$). The *k-dimensional part of the boundary* $\partial_k \Delta_n$ *of* Δ_n is therefore

$$\partial_k \Delta_n^{(I_n)} := \bigcup_{I_k \subset I_n} \Delta_k^{(I_k)} \subset \partial \Delta_n^{(I_n)} \quad \text{for } 0 \leq k \leq n-1. \tag{2.6}$$

For notational consistency, we also put $\partial_n \Delta_n = \Delta_n$. This boundary concept can iteratively be applied to simplices in the boundary of some $\Delta_l^{(I_l)}$, $I_l \subset I_n$ for $0 \leq k < l \leq n$. We thus have

$$\partial_k \Delta_l^{(I_l)} = \bigcup_{I_k \subset I_l} \Delta_k^{(I_k)} \subset \partial \Delta_l^{(I_l)}. \tag{2.7}$$

Regarding the Wright–Fisher model, the simplex $\Delta_k^{(\{i_0,\ldots,i_k\})}$ corresponds to the state where precisely the $k+1$ alleles $i_0, \ldots, i_k$ are present in the population. The boundary $\partial_k \Delta_n$, i.e. the union of all corresponding subsimplices, represents the state with any $k+1$ alleles. In the set of alleles $i_0, \ldots, i_k$ corresponding to $\Delta_k^{(\{i_0,\ldots,i_k\})}$, the elimination of one of the alleles corresponds to a transition to $\partial_{k-1} \Delta_k^{(\{i_0,\ldots,i_k\})}$, and the particular component in that boundary then indicates which of the alleles got eliminated.

We also introduce spaces of square integrable functions for our subsequent integral products on Δ_n and its faces (which will mainly be used implicitly, for details cf. [37])[2],

$$L^2\left(\bigcup_{k=0}^{n} \partial_k \Delta_n\right) := \Big\{ f \colon \overline{\Delta}_n \longrightarrow \mathbb{R} \,\Big|\, f|_{\partial_k \Delta_n} \text{ is } \lambda_k\text{-measurable and} \\ \int_{\partial_k \Delta_n} |f(p)|^2 \, \lambda_k(dp) < \infty \text{ for all } k = 0, \ldots, n \Big\}. \tag{2.8}$$

In order to define an extended solution on Δ_n and its faces (indicated by a capitalized U), we shall in addition need appropriate spaces of *pathwise regular* functions. Such a solution needs to be at least of class C^2 in every boundary stratum (actually, a solution typically always is of class C^∞, which likewise applies to each boundary stratum). Moreover, it should stay regular at boundary transitions that reduce the dimension by one, i.e. for $\Delta_k^{(I_k)}$ and a boundary face $\Delta_{k-1} \subset \partial_{k-1} \Delta_k^{(I_k)}$. Thus, derivatives in the interior which are tangential towards the face under consideration have to smoothly connect with derivatives in that stratum, whereas for the normal derivatives, there is a smooth extension on the stratum.

[2]Here, λ_k stands for the k-dimensional Lebesgue measure, but when integrating over some $\Delta_k^{(I_k)}$ with $0 \notin I_k$, the measure needs to be replaced with the one induced on $\Delta_k^{(I_k)}$ by the Lebesgue measure of the containing $\mathbb{R}^{k+1}$ – this measure, however, will still be denoted by λ_k as it is clear from the domain of integration $\Delta_k^{(I_k)}$ with either $0 \in I_k$ or $0 \notin I_k$ which version is actually used.

Turning from some specific boundary transition to the entire simplex, we may require that a corresponding property applies to all possible boundary transitions within $\overline{\Delta}_n$ that reduce the dimension by one, thus formally for $\Delta_d^{(I_d)}$ and its boundary of codimension 1 $\partial_{d-1}\Delta_d^{(I_d)}$ for all $I_d \subset I_n$, $1 \le d \le n$. Globally, this raises the issue of incompatibilities, as a $\Delta_{d-1}^{(I_{d-1})}$ may represent a boundary stratum of both some $\Delta_d^{(I_d)}$ and some $\Delta_d^{(\widetilde{I}_d)}$; still, a solution needs to be well-defined everywhere. However, the class of solutions, which comply with such pathwise regularity even on the (entire) stratification of the domain, is certainly larger than that of plain globally smooth solutions.

Correspondingly, we define for $l \in \mathbb{N} \cup \{\infty\}$

$$U \in C_p^l(\overline{\Delta}_n) \;:\Leftrightarrow\; U|_{\Delta_d^{(I_d)} \cup \partial_{d-1}\Delta_d^{(I_d)}} \in C^l(\Delta_d^{(I_d)} \cup \partial_{d-1}\Delta_d^{(I_d)}) \quad \text{for all } I_d \subset I_n, 1 \le d \le n \tag{2.9}$$

with respect to the spatial variables. Likewise, for ascending chains of (sub-)simplices with a more specific boundary condition, we put for index sets $I_k \subset \cdots \subset I_n$ and again for $l \in \mathbb{N} \cup \{\infty\}$

$$U \in C_{p_0}^l\left(\bigcup_{d=k}^{n} \Delta_d^{(I_d)}\right) :\Leftrightarrow \begin{cases} U|_{\Delta_d^{(I_d)}} \text{ is extendable to } \overline{U} \in C^l(\Delta_d^{(I_d)} \cup \partial_{d-1}\Delta_d^{(I_d)}) \text{ with} \\ \overline{U}|_{\partial_{d-1}\Delta_d^{(I_d)}} = U\chi_{\Delta_{d-1}^{(I_{d-1})}}\chi_{\{d>k\}} \text{ for all } \max(1,k) \le d \le n \end{cases} \tag{2.10}$$

with respect to the spatial variables; χ denotes the characteristic function of a set, i.e. $= 1$ there and 0 elsewhere.

2.2. The cube

We next introduce some notation for cubes and their boundary instances and define for $n \in \mathbb{N}$ an *n-dimensional cube* $\square_n$ as

$$\square_n := \left\{(p^1, \ldots, p^n) \middle| p^i \in (0,1) \text{ for } i = 1, \ldots, n\right\}. \tag{2.11}$$

Analogous to Δ_n, if we wish to denote the corresponding coordinate indices explicitly, this may be done by providing the coordinate index set $I'_n := \{i_1, \ldots, i_n\} \subset \{1, \ldots, n\}$, $i_j \neq i_l$ for $j \neq l$ as upper index of $\square_n$, thus

$$\square_n^{(I'_n)} = \left\{(p^1, \ldots, p^n) \middle| p^i \in (0,1) \text{ for } i \in I'_n\right\}. \tag{2.12}$$

This is particularly useful for boundary instances of the cube (cf. below) or if for other purposes a certain ordering $(i_j)_{j=0,\ldots,n}$ of the coordinate indices is needed. For $\square_n$ itself and if no ordering is needed, the index set may be omitted (in such a case it may be assumed $I'_n \equiv \{1, \ldots, n\}$ as in equation (2.11)). Please note that a primed index set is always assumed to not contain the index 0 (resp. $i_0 = 0$, which we usually stipulate in case of orderings) as in (2.11), we do not have the coordinate index 0.

In the standard topology on $\mathbb{R}^n$, $\square_n$ is open (which we always assume when writing $\square_n$), and its closure $\overline{\square}_n$ is given by (again using the index set notation)

$$\overline{\square_n^{(I'_n)}} = \left\{(p^1, \ldots, p^n) \middle| p^i \in [0,1] \text{ for } i \in I'_n\right\}. \tag{2.13}$$

As in the case of the simplex, the boundary $\partial\square_n$ of $\square_n$ consists of various subcubes (faces) of descending dimensions, starting from the $(n-1)$-dimensional facets down to the vertices (which represent 0-dimensional cubes). All appearing subcubes of dimension $0 \le k \le n-1$ are isomorphic to the k-dimensional standard cube $\square_k$ and hence will be denoted by $\square_k$ if it is irrelevant or clear from the context which particular subcube we consider. We also put

$$\square_k^{(I'_k)} := \left\{(p^1,\dots,p^n)\middle| p^i \in (0,1) \text{ for } i \in I'_k; p^i = 0 \text{ for } i \in I'_n \backslash I'_k\right\} \tag{2.14}$$

down until $\square_0^{(\varnothing)} := (0,\dots,0)$ for $k=0$.

If necessary, we may also identify a certain boundary face $\square_k$ of $\partial\square_n$ for $0 \le k \le n-1$ by only giving the values of the $n-k$ fixed coordinates, i.e. with indices in $I'_n \backslash I'_k$, which may be either 0 or 1, hence

$$\square_k = \left\{p^{j_1} = b_1,\dots,p^{j_{n-k}} = b_{n-k}\right\} \tag{2.15}$$

with $j_1,\dots,j_{n-k} \in I'_n$, $i_r \neq i_s$ for $r \neq s$ and $b_1,\dots,b_{n-k} \in \{0,1\}$ chosen accordingly. If we wish to indicate the total *k-dimensional boundary of* $\square_n$, i.e. the union of all k-dimensional faces belonging to $\overline{\square}_n$, we may write $\partial_k\square_n$ for $k=0,\dots,n$ with $\partial_n\square_n := \square_n$.

Finally, when writing products of simplices and cubes which do not span all considered dimensions, we indicate the value of the missing coordinates by curly brackets marked with the corresponding coordinate index, i.e. for $I_n = \{i_0, i_1,\dots,i_n\}$ and $I_k \subset I_n$ with $i_{k+1} \notin I_k$ we have e.g.

$$\begin{aligned}&\Delta_k^{(I_k)} \times \{1\}^{(\{i_{k+1}\})} \times \square_{n-k-1}^{(I'_n\backslash(I'_k\cup\{i_{k+1}\}))}\\ &\quad := \left\{(p^{i_1},\dots,p^{i_n})\middle| p^i > 0 \text{ for } i \in I_k, p^{i_{k+1}} = 1, p^j \in (0,1) \text{ for } j \in I'_n\backslash(I'_k \cup \{i_{k+1}\})\right\}\end{aligned} \tag{2.16}$$

with $p^{i_0} = p^0 = 1 - \sum_{j=1}^k p^{i_j}$. If coordinates are fixed at 0, the corresponding entry may be omitted, e.g. we may just write $\Delta_k^{(I_k)}$ for $\Delta_k^{(I_k)} \times \{0\}^{(I_n\backslash I_k)}$.

Furthermore, we also introduce a (closed) cube $\overline{\square_k^{(I'_k)}}$ with a removed base vertex $\square_0^{(\varnothing)}$ somewhat sloppily denoted by $\overline{\boxtimes_k^{(I'_k)}}$, i.e.

$$\overline{\boxtimes_k^{(I'_k)}} := \overline{\square_k^{(I'_k)}}\backslash\square_0^{(\varnothing)} = \left\{p^{i_1},\dots,p^{i_k} \in [0,1]\middle| \sum_{j=1}^k p^{i_j} > 0\right\}. \tag{2.17}$$

For functions defined on the cube, the pathwise smoothness required for an application of the corresponding Kolmogorov backward operator (cf. p. 463) may be defined as with the simplex in equality (2.9) in [19]; hence, we put

$$\tilde{u} \in C_p^l(\overline{\square}_n) \;:\Leftrightarrow\; \tilde{u}|_{\square_d\cup\partial_{d-1}\square_d} \in C^l(\square_d \cup \partial_{d-1}\square_d) \text{ for every } \square_d \subset \overline{\square}_n \tag{2.18}$$

with respect to the spatial variables, implying that the operator is continuous at all boundary transitions within $\overline{\square}_n$. This concept likewise applies to subsets of $\overline{\square}_n$ where needed.

3. Hierarchical extended solutions of the Kolmogorov backward equation

In this section, we recall the main results from [19]; for details please see also there. We define a class of extensions by imposing extension constraints (definition 6.1 in [18]); more precisely,

an extension is required to be smooth and constrained to vanish towards certain boundary strata:

Definition 3.1 (extension constraints). Let I_d be an index set with $|I_d| = d+1 \geq 2, 0, s \in I_d$ and $\Delta_d^{(I_d)} = \{(p^i)_{i\in I_d\setminus\{0\}} | p^i > 0 \text{ for } i \in I_d\}$ with $p^0 := 1 - \sum_{i\in I_d\setminus\{0\}} p^i$. For $d \geq 2$ and a solution $u\colon \big(\Delta_{d-1}^{(I_d\setminus\{s\})}\big)_{-\infty} \longrightarrow \mathbb{R}$ of the correspondingly restricted Kolmogorov backward equation (1.9), i.e. $u(\,\cdot\,,t) \in C^\infty\big(\Delta_{d-1}^{(I_d\setminus\{s\})}\big)$ for $t < 0$, $u(p,\,\cdot\,) \in C^\infty((-\infty,0))$ for $p \in \Delta_{d-1}^{(I_d\setminus\{s\})}$ and

$$-\frac{\partial}{\partial t}u = L^*u \quad \text{in } \big(\Delta_{d-1}^{(I_d\setminus\{s\})}\big)_{-\infty}, \tag{3.1}$$

a function $\bar{u}\colon \big(\Delta_d^{(I_d)}\big)_{-\infty} \longrightarrow \mathbb{R}$ with $\bar{u}(\,\cdot\,,t) \in C^\infty\big(\Delta_d^{(I_d)}\big)$ for $t < 0$ and $\bar{u}(p,\,\cdot\,) \in C^\infty((-\infty,0))$ for $p \in \Delta_d^{(I_d)}$ is said to be an extension of u satisfying the *extension constraints* if

(i) for $t < 0\bar{u}(\,\cdot\,,t)$ is continuously extendable to the boundary $\partial_{d-1}\Delta_d^{(I_d)}$ such that it coincides with $u(\,\cdot\,,t)$ in $\Delta_{d-1}^{(I_d\setminus\{s\})}$ resp. vanishes on the remainder of $\partial_{d-1}\Delta_d^{(I_d)}$ and is of class C^∞ with respect to the spatial variables in $\Delta_d^{(I_d)} \cup \partial_{d-1}\Delta_d^{(I_d)}$,

(ii) it is a solution of the corresponding Kolmogorov backward equation in $\big(\Delta_d^{(I_d)}\big)_{-\infty}$, i.e. $-\frac{\partial}{\partial t}\bar{u} = L^*\bar{u}$ in $\big(\Delta_d^{(I_d)}\big)_{-\infty}$.

For $d = 1$, this analogously applies to functions u with $-\frac{\partial}{\partial t}u = 0$ (in accordance with $L_0^* \equiv 0$), and consequently the equation in condition (ii) is replaced with $L^*\bar{u} = 0$. Furthermore, an extension which encompasses multiple extension steps satisfies the extension constraints if this holds for every extension step.

The presented extension scheme then first yields the existence of simple extensions of solutions from a boundary instance of the considered domain to the interior (Proposition 6.4 in [19]), from which one can advance to the existence of pathwise extensions (Propositions 8.1 in [19]):

Proposition 3.2 (pathwise extension of solutions). *Let $k, n \in \mathbb{N}$ with $0 \leq k < n$, $\{i_k, i_{k+1}, \ldots, i_n\} \subset I_n := \{0, 1, \ldots, n\}$ with $i_i \neq i_j$ for $i \neq j$ and $I_k := I_n\setminus\{i_{k+1}, \ldots, i_n\}$, and let u_{I_k} be a proper solution of the Kolmogorov backward equation (1.9) restricted to $\Delta_k^{(I_k)}$ for some final condition $f \in \mathcal{L}^2\big(\Delta_k^{(I_k)}\big)$. For $d = k+1, \ldots, n$ and $I_d := I_k \cup \{i_{k+1}, \ldots i_d\}$, an extension of $\bar{u}_{I_k}^{i_k,\ldots,i_{d-1}}$ in $\big(\Delta_{d-1}^{(I_{d-1})}\big)_{-\infty}$ to $\bar{u}_{I_k}^{i_k,\ldots,i_d} := \big(\bar{u}_{I_k}^{i_k,\ldots,i_{d-1}}\big)^{i_{d-1},i_d}$ in $\big(\Delta_d^{(I_d)}\big)_{-\infty}$ as by Proposition 6.4 in [19] satisfies the extension constraints 3.1 if (and for $d \geq k+2$ and $[f] \neq 0$ in $L^2\big(\Delta_k^{(I_k)}\big)$ also only if) putting $r(d) = i_{d-1}$ for the extension target face index, and we respectively have*

$$\bar{u}_{I_k}^{i_k,\ldots,i_d}(p,t) = u_{I_k}(\pi^{i_k,\ldots,i_d}(p),t)\prod_{j=k}^{d-1}\frac{p^{i_j}}{\sum_{l=j}^{d} p^{i_l}}, \quad (p,t) \in \big(\Delta_d^{(I_d)}\big)_{-\infty} \tag{3.2}$$

with $p^0 = 1 - \sum_{i\in I_d\setminus\{0\}} p^i$ and $\pi^{i_k,\ldots,i_d}(p) = (\tilde{p}^1, \ldots, \tilde{p}^n)$ such that $\tilde{p}^{i_k} = p^{i_k} + \ldots + p^{i_d}$, $\tilde{p}^{i_{k+1}} = \ldots = \tilde{p}^{i_d} = 0$ and $\tilde{p}^j = p^j$ for $j \in I_d\setminus\{i_k, \ldots, i_d\}$.

We combine all extensions into a function $\overline{U}_{I_k}^{i_k,\dots,i_n}$ *in* $\left(\bigcup_{k\le d\le n}\Delta_d^{(I_d)}\right)_{-\infty}$ *by putting*

$$\begin{aligned}\overline{U}_{I_k}^{i_k,\dots,i_n}(p,t) &:= u_{I_k}(p,t)\chi_{\Delta_k^{(I_k)}}(p) + \sum_{k+1\le d\le n}\bar{u}_{I_k}^{i_k,\dots,i_d}(p,t)\chi_{\Delta_d^{(I_d)}}(p)\\ &= u_{I_k}(p,t)\chi_{\Delta_k^{(I_k)}}(p) + \sum_{k+1\le d\le n} u_{I_k}(\pi^{i_k,\dots,i_d}(p),t)\prod_{j=k}^{d-1}\frac{p^{i_j}}{\sum_{l=j}^{d}p^{i_l}}\chi_{\Delta_d^{(I_d)}}(p) \qquad (3.3)\end{aligned}$$

with $p^0 = 1-\sum_{i\in I_n\setminus\{0\}}p^i$ *is in* $C^\infty_{p_0}\left(\bigcup_{k\le d\le n}\Delta_d^{(I_d)}\right)$ *with respect to the spatial variables for* $t<0$ *as well as in* $C^\infty((-\infty,0))$ *with respect to* t*, and we have*

$$\begin{cases} L^*\overline{U}_{I_k}^{i_k,\dots,i_n} = -\dfrac{\partial}{\partial t}\overline{U}_{I_k}^{i_k,\dots,i_n} & \text{in } \left(\bigcup_{k\le d\le n}\Delta_d^{(I_d)}\right)_{-\infty}\\ \overline{U}_{I_k}^{i_k,\dots,i_n}(\,\cdot\,,0) = \overline{F}_{I_k}^{i_k,\dots,i_n} & \text{in } \bigcup_{k\le d\le n}\Delta_d^{(I_d)}\end{cases} \qquad (3.4)$$

with $\overline{F}_{I_k}^{i_k,\dots,i_n}\in\mathcal{L}^2\left(\bigcup_{k\le d\le n}\Delta_d^{(I_d)}\right)$ *being an analogous extension of the final condition* $f=f_{I_k}$ *in* $\Delta_k^{(I_k)}$*; in particular, we have* $\overline{U}_{I_k}^{i_k,\dots,i_n}\big|_{\Delta_k^{(I_k)}}(\,\cdot\,,0)=f$ *in* $\Delta_k^{(I_k)}$.

This scheme already allows us to recover the existence result by Littler [29]. Assembling all pathwise extensions eventually yields the existence of the global extensions (Proposition 8.4 in [19]). By global iterative extensions, we obtain the following existence result (Theorem 9.1 in [19]):

Theorem 3.3. *For a given final condition* $f\in\mathcal{L}^2\left(\bigcup_{d=0}^n\partial_d\Delta_n\right)$*, the extended Kolmogorov backward equation*(1.9) *corresponding to the n-dimensional Wright–Fisher model in diffusion approximation always allows a solution* $\overline{U}\colon\left(\overline{\Delta}_n\right)_{-\infty}\longrightarrow\mathbb{R}$ *with* $\overline{U}(\,\cdot\,,t)\in C^\infty_p\left(\overline{\Delta}_n\right)$ *for each fixed* $t\in(-\infty,0)$ *and* $\overline{U}(p,\,\cdot\,)\in C^\infty((-\infty,0))$ *for each fixed* $p\in\overline{\Delta}_n$.

4. Motivation

To motivate the regularization scheme, we use the example of $\overline{U}_{I_k}^{i_k,\dots,i_n}$ in $\overline{\Delta_n^{(I_n)}}$ as in equation (3.3). We can see the incompatibilities in geometric terms. For every $t<0$, for the top-dimensional component $\bar{u}_{I_k}^{i_k,\dots,i_n}$ incompatibilities may arise in the domain where we have $p^{i_n}+p^{i_{n-1}}=0$, hence $\overline{\Delta_{n-2}^{(I_{n-2})}}$ (whereas for the next component this is the set given by $p^{i_n}+p^{i_{n-1}}+p^{i_{n-2}}=0$, hence $\overline{\Delta_{n-3}^{(I_{n-3})}}$, and so forth). On all other boundary strata of arbitrary (lower) dimension, $\bar{u}_{I_k}^{i_k,\dots,i_n}$ and the other component as in equation (3.2) respectively are continuously extendable and of class C^∞ with respect to the spatial variables there. Thus, we have to address one stratum of the boundary gap for each component of the solution.

Altogether, the full hierarchical solution $\overline{U}_{I_k}^{i_k,\dots,i_n}$ this way comprises a nested incompatibility in $\overline{\Delta_{n-2}^{(I_{n-2})}}$ in the sense that each $\bar{u}_{I_k}^{i_k,\dots,i_d}$ does not extend continuously to $\overline{\Delta_{d-2}^{(I_{d-2})}}$ for $d=n,\dots,k+2$. This implies that the desired transformation needs to affect all relevant dimensions in an iterative manner. In each step, one dimension from the simplex is removed and converted into a dimension of the corresponding cube component, i.e. the corresponding

coordinate is released from the simplex property $\sum_i p^i \leq 1$. In doing so, with each iteration, the relevant component of the solution gains the required regularity at the corresponding level while all other components remain unaffected; eventually, the entire solution resp. all its components are transformed such that they extend smoothly to the boundary.

Altogether, after $n-k-1$ of these steps, the relevant component of $\overline{\Delta_n^{(I_n)}}$ is converted into a cube of dimension $n-k-1$, and the transformed solution is sufficiently regularized; in particular, it will then smoothly extend to the full boundary.

4.1. Analysis of a simple example

A crucial aspect of our procedure is the resolution of the singularities that appear with those iteratively extended solutions. This will be done by suitable blow-up transformations. To give an example, we use a solution for $n=2$ (cf. Proposition 3.2): we then have e.g.

$$\overline{U}_{\{0\}}^{0,1,2} = u_{\{0\}}\chi_{\Delta_0^{(\{0\})}} + \bar{u}_{\{0\}}^{0,1}\chi_{\Delta_1^{(\{0,1\})}} + \bar{u}_{\{0\}}^{0,1,2}\chi_{\Delta_2^{(\{0,1,2\})}} \quad \text{in} \bigcup_{d=0}^{2} \Delta_d^{(\{0,\ldots,d\})}, \tag{4.1}$$

and of course only the top-dimensional component

$$\bar{u}_{\{0\}}^{0,1,2}(p) = p^0 \cdot \frac{p^1}{1-p^0} \quad \text{in } \Delta_2^{(\{0,1,2\})} \tag{4.2}$$

(with $p^0 = 1-p_1-p_2$) resp. its continuous extension yields incompatibilities. Hence, we may transform[3] it via $\tilde{p}^1 := p^1 + p^2$ and $\tilde{p}^2 := \frac{p^2}{p^1+p^2}$ into[4]

$$\tilde{u}_{\{0\}}^{0,1;2}(\tilde{p}) = (1-\tilde{p}^1)(1-\tilde{p}^2), \tag{4.3}$$

which smoothly extends to $\overline{\square_2^{(\{1,2\})}}$ (as then also $\widetilde{U}_{\{0\}}^{0,1;2} = u_{\{0\}}\chi_{\square_0} + \bar{u}_{\{0\}}^{0,1}\chi_{\square_1^{(\{1\})}} + \tilde{u}_{\{0\}}^{0,1;2}\chi_{\square_2^{(\{1,2\})}}$). This observed smooth extendability of $\tilde{u}_{\{0\}}^{0,1;2}$ in particular applies to the additional 1-dimensional face $N_1 := \{0\}^{(\{1\})} \times \overline{\boxtimes_1^{(\{2\})}}$ of $\overline{\square_2^{(\{1,2\})}}$, which is produced during the transformation (cf. below). As pointed out above, for greater n, we have to recursively apply such transformations in order to resolve all appearing singularities.

5. The blow-up transformation and its iteration

We shall now present the details of the blow-up transformation and derive all necessary results. We start with the basic transformation (cf. also Figure 1) and proceed to the results for a suitably iterated application of this blow-up transformation, by which we can resolve all singularities of our solution.

Lemma 5.1 (Blow-up transformation). *Let $I_d = \{0,1,\ldots,d\}$. A blow-up transformation Φ_s^r with $r,s \in I_d \backslash \{0\}$ mapping*

$$\overline{\Delta_d^{(I_d)}} \backslash \overline{\Delta_{d-2}^{(I_d\backslash\{r,s\})}} = \left\{(p^1,\ldots,p^d) \middle| p^i \geq 0 \textit{ for } i \in I_d, p^r + p^s > 0\right\} \tag{5.1}$$

[3]This corresponds to the choices $s=1, r=2$ in Lemma 5.1.
[4]Here, already the notation of Proposition 5.8 is applied.

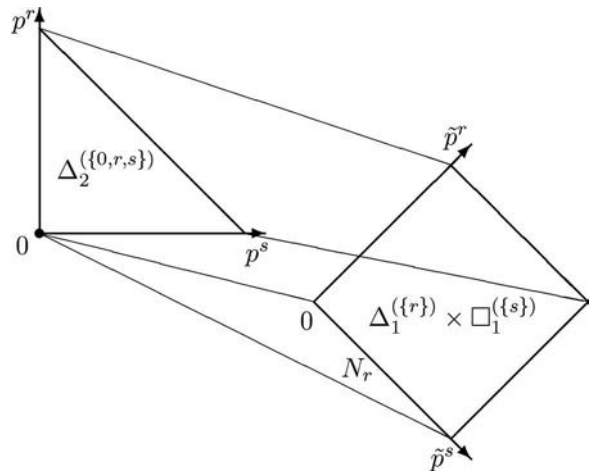

Figure 1. An illustration of the blow-up transformation for $d = 2$.

with $p^0 := 1 - \sum_{i \in I_d \setminus \{0\}} p^i$ C^∞*-diffeomorphically onto*

$$\left(\overline{\Delta_{d-1}^{(I_d \setminus \{s\})}} \setminus \overline{\Delta_{d-2}^{(I_d \setminus \{r,s\})}}\right) \times \overline{\square_1^{(\{s\})}}$$
$$= \left\{(\tilde{p}^1, \ldots, \tilde{p}^d) \middle| \tilde{p}^i \geq 0 \text{ for } i \in I_d \setminus \{s\}, \tilde{p}^r > 0; \tilde{p}^s \in [0,1]\right\} \tag{5.2}$$

with $\tilde{p}^0 := 1 - \sum_{i \in I_d \setminus \{0,s\}} \tilde{p}^i$ *and altogether*

$$\overline{\Delta_d^{(I_d)}} \longmapsto \left(\overline{\Delta_{d-1}^{(I_d \setminus \{s\})}} \times \overline{\square_1^{(\{s\})}}\right) \setminus N_r \tag{5.3}$$

with

$$N_r := \overline{\Delta_{d-2}^{(I_d \setminus \{r,s\})}} \times \{0\}^{(\{r\})} \times \overline{\boxtimes_1^{(\{s\})}}, \tag{5.4}$$

as an additional $(d-1)$*-dimensional face of* $\overline{\Delta_{d-1}^{(I_d \setminus \{s\})}} \times \overline{\square_1^{(\{s\})}}$*, is given by*

$$\tilde{p}^i := p^i \quad \text{for } i \neq r, s, \tag{5.5}$$
$$\tilde{p}^r := p^r + p^s, \tag{5.6}$$
$$\tilde{p}^s := \begin{cases} \dfrac{p^s}{p^r + p^s} & \text{for } p^r + p^s > 0 \\ 0 & \text{for } p^r + p^s = 0. \end{cases} \tag{5.7}$$

Corollary 5.2. *While we obtain* $N_r = \overline{\Delta_{d-2}^{(I_d \setminus \{r,s\})}} \times \overline{\boxtimes_1^{(\{s\})}}$ *as an additional* $(d-1)$*-dimensional face with* Φ_s^r*, the existing* $(d-1)$*-dimensional faces of* $\overline{\Delta_d^{(I_d)}}$ *including their boundaries are mapped as follows:*

$$\overline{\Delta_{d-1}^{(I_d \setminus \{s\})}} \longmapsto \overline{\Delta_{d-1}^{(I_d \setminus \{s\})}} \times \{0\}^{(\{s\})}, \tag{5.8}$$
$$\overline{\Delta_{d-1}^{(I_d \setminus \{r\})}} \setminus \overline{\Delta_{d-2}^{(I_d \setminus \{r,s\})}} \longmapsto \left(\overline{\Delta_{d-1}^{(I_d \setminus \{s\})}} \setminus \overline{\Delta_{d-2}^{(I_d \setminus \{r,s\})}}\right) \times \{1\}^{(\{s\})} \tag{5.9}$$

and

$$\overline{\Delta_{d-1}^{(I_d\setminus\{i\})}}\setminus\overline{\Delta_{d-3}^{(I_d\setminus\{i,r,s\})}} \longmapsto \left(\overline{\Delta_{d-2}^{(I_d\setminus\{i,s\})}}\setminus\overline{\Delta_{d-3}^{(I_d\setminus\{i,r,s\})}}\right)\times\overline{\square_1^{(\{s\})}} \quad \textit{for } i\in I_d\setminus\{r,s\}. \tag{5.10}$$

Remark 5.3. If the $\tilde{p}^s$ in Lemma 5.1 is chosen differently with

$$\tilde{p}^s := \frac{p^r}{p^r+p^s}, \tag{5.11}$$

this flips the orientation of the $\tilde{p}^s$-coordinate in $\square_1^{(\{s\})}$ as $\tilde{p}^s$ now has to be replaced by $1-\tilde{p}^s$ wherever it occurs. This, however, does not affect the statements of Lemma 5.1, whereas in Corollary 5.2 the images of $\overline{\Delta_{d-1}^{(I_d\setminus\{r\})}}\setminus\overline{\Delta_{d-2}^{(I_d\setminus\{r,s\})}}$ and $\overline{\Delta_{d-1}^{(I_d\setminus\{s\})}}\setminus\overline{\Delta_{d-2}^{(I_d\setminus\{r,s\})}}$ are interchanged. Thus, unless stated otherwise, in the following we shall always assume that the $\tilde{p}^s$-coordinate is chosen with an orientation as given in Lemma 5.1.

That we put $\tilde{p}^s := 0$ where $p^r+p^s=0$ in Lemma 5.1 (cf. second line of equation 5.5) may appear somewhat surprising as the set $p^r+p^s=0$ lifts under the blow-up to the new boundary face, and the range of $\tilde{p}^s$ on that locus is what gives this subset a larger dimension. However, the main purpose is to be able to locate the set after the blow-up (which makes the blow-up well-defined). In the remainder, it will be crucial to identify all strata of the domain and the data/solution given on them after the blow-up.

Proof of Lemma 5.1. The transformation corresponds geometrically to a scaling of the domain into the $\tilde{p}^s$-direction with scaling factor $\frac{1}{\tilde{p}^r}$. The assertion about the transformation domains is straightforward since we have $0\le\frac{p^s}{p^r+p^s}\le 1$ on $\overline{\Delta_d^{(I_d)}}\setminus\overline{\Delta_{d-2}^{(I_d\setminus\{r,s\})}}$. Likewise, the C^∞-diffeomorphism property follows since Φ_s^r is smoothly differentiable as long as $\tilde{p}^r=p^r+p^s>0$ and the inverse transformation $(\Phi_s^r)^{-1}$ is likewise smooth. The latter is given by

$$p^r=\tilde{p}^r(1-\tilde{p}^s), \tag{5.12}$$
$$p^s=\tilde{p}^r\tilde{p}^s, \tag{5.13}$$
$$p^i=\tilde{p}^i \quad \text{for } i\neq r,s. \tag{5.14}$$

By this, it also becomes obvious that $(\Phi_s^r)^{-1}$ maps $\left(\overline{\Delta_{d-1}^{(I_d\setminus\{s\})}}\setminus\overline{\Delta_{d-2}^{(I_d\setminus\{r,s\})}}\right)\times\overline{\square_1^{(\{s\})}}$ onto $\overline{\Delta_d^{(I_d)}}\setminus\overline{\Delta_{d-2}^{(I_d\setminus\{r,s\})}}$. □

Consequently, we obtain for an iterated application of the blow-up transformation:

Proposition 5.4. *Let $k,n\in\mathbb{N}$ with $0\le k\le n-2$, $\{i_k,i_{k+1},\dots,i_n\}\subset I_n:=\{0,1,\dots,n\}$ with $i_i\neq i_j$ for $i\neq j$ and $I_d:=I_n\setminus\{i_{d+1},\dots,i_n\}$ for $d=k,\dots,n-1$. A repeated blow-up transformation $\Phi_{s_{n-k-1}}^{r_{n-k-1}}\circ\dots\circ\Phi_{s_1}^{r_1}$ with $\Phi_{s_m}^{r_m}$ as in Lemma 5.1 with $r_m=i_{n-m}$ and $s_m=i_{n-m+1}$ for $m=1,\dots,n-k-1$ maps $\overline{\Delta_{k+1}^{(I_{k+1})}}$ onto itself and*

$$\Delta_d^{(I_d)}\longmapsto\Delta_{k+1}^{(I_{k+1})}\times\square_{d-k-1}^{(I_d\setminus I_{k+1})} \quad \textit{for } d=k+2,\dots,n \tag{5.15}$$

and altogether

$$\overline{\Delta_n^{(I_n)}} \longmapsto \left(\overline{\Delta_{k+1}^{(I_{k+1})}} \times \overline{\square_{n-k-1}^{(I_n \setminus I_{k+1})}}\right) \setminus \bigcup_{j=k+1}^{n-1} N_j. \tag{5.16}$$

The $n-k-1$ additional $(n-1)$-dimensional faces $N_{k+1}, \dots, N_{n-1}$ of $\overline{\Delta_{k+1}^{(I_{k+1})}} \times \overline{\square_{n-k-1}^{(I_n \setminus I_{k+1})}}$ are given by

$$N_{k+1} = \overline{\Delta_k^{(I_k)}} \times \{0\}^{(\{i_{k+1}\})} \times \overline{\boxtimes_{n-k-1}^{(I_n \setminus I_{k+1})}} \tag{5.17}$$

and

$$N_j = \overline{\Delta_{k+1}^{(I_{k+1})}} \times \overline{\square_{j-k-2}^{(I_{j-1} \setminus I_{k+1})}} \times \{0\}^{(\{i_j\})} \times \overline{\boxtimes_{n-j}^{(I_n \setminus I_j)}} \tag{5.18}$$

for $j = k+2, \dots, n-1$.

Explicitly, $\Phi_{s_{n-k-1}}^{r_{n-k-1}} \circ \dots \circ \Phi_{s_1}^{r_1}$ is given by

$$\tilde{p}^{i_1} := p^{i_1} + \dots + p^{i_n}, \tag{5.19}$$

$$\tilde{p}^{i_2} := \begin{cases} \dfrac{p^{i_2} + \dots + p^{i_n}}{p^{i_1} + p^{i_2} + \dots + p^{i_n}} & \text{for } p^{i_1} + \dots + p^{i_n} > 0 \\ 0 & \text{for } p^{i_1} + \dots + p^{i_n} = 0, \end{cases} \tag{5.20}$$

$$\vdots$$

$$\tilde{p}^{i_j} := \begin{cases} \dfrac{p^{i_j} + \dots + p^{i_n}}{p^{i_{j-1}} + p^{i_j} + \dots + p^{i_n}} & \text{for } p^{i_{j-1}} + \dots + p^{i_n} > 0 \\ 0 & \text{for } p^{i_{j-1}} + \dots + p^{i_n} = 0, \end{cases} \tag{5.21}$$

$$\vdots$$

$$\tilde{p}^{i_n} := \begin{cases} \dfrac{p^{i_n}}{p^{i_{n-1}} + p^{i_n}} & \text{for } p^{i_{n-1}} + p^{i_n} > 0 \\ 0 & \text{for } p^{i_{n-1}} + p^{i_n} = 0 \end{cases} \tag{5.22}$$

for $p \in \bigcup_{d=0}^{n} \Delta_d^{(I_d)}$. If in any step the coordinate $\tilde{p}^{s_j}$ is chosen with alternative orientation (cf. remark 5.3), $\tilde{p}^{s_j}$ needs to be replaced by $(1 - \tilde{p}^{s_j})$.

Proof. The Proposition will be proven in parallel with Propositions 5.7 and 5.8, cf. below. □

The next Lemma is concerned with the transformation behaviour of the operator L_n^*, at first for a single blow-up step. All considerations apply to L_n^* in its domain Δ_n as well as, taking the restriction property of L_n^* (cf. [19]) into account, in the closure $\overline{\Delta}_n$ resp. to the transformed operator $\widetilde{L}_n^*$ in the subsequent transformed images of the domain (the domain in question may not be stated explicitly – this will be done in Proposition 5.7):

Lemma 5.5. *Let $I'_n := \{1, \dots, n\}$ be an index set with $r, s \in I'_n$ and let $\{i_1, \dots, i_n\}$ be an ordering of I'_n such that $r, s \in \{i_1, \dots, i_m\}$ for some $m \leq n$. When changing coordinates*

$(p^i)_{i\in I'_n} \mapsto (\tilde{p}^i)_{i\in I'_n}$ *by* Φ^r_s*, the operator*

$$L^*_n = \frac{1}{2}\sum_{i,j=1}^{n} a^{ij}(p)\frac{\partial}{\partial p^i}\frac{\partial}{\partial p^j} \tag{5.23}$$

with $a^{ij}(p) = p^i(\delta^i_j - p^j)$ *for* $i,j \in \{i_1,\dots,i_m\}$, $a^{ij} = 0$ *else for* $i \neq j$ *is transformed into*

$$\widetilde{L}^*_n = \frac{1}{2}\sum_{k,l=1}^{k} \tilde{a}^{kl}(\tilde{p})\frac{\partial}{\partial \tilde{p}^k}\frac{\partial}{\partial \tilde{p}^l} \tag{5.24}$$

with $\tilde{a}^{kl}(\tilde{p}) = \tilde{p}^k(\delta^k_l - \tilde{p}^l)$ *for* $k,l \in \{i_1,\dots,i_m\}\backslash\{s\}$, $\tilde{a}^{ss}(\tilde{p}) = \frac{\tilde{p}^s(1-\tilde{p}^s)}{\tilde{p}^r}$, $\tilde{a}^{sl} = \tilde{a}^{ls} = 0$ *for* $l \neq s$ *and* $\tilde{a}^{kl}(\tilde{p}) = a^{kl}(p)$ *(with the coordinates yet to be replaced) for all remaining indices. This also holds if the* $\tilde{p}^s$*-coordinate is chosen with opposite orientation (cf. remark 5.3).*

For the proof, we need the following lemma:

Lemma 5.6. *A partial differential operator*

$$\sum_{i,j=1}^{n} a^{ij}(p)\frac{\partial}{\partial p^i}\partial p^j u(p) + \sum_{i=1}^{n} b^i(p)\frac{\partial}{\partial p^i}u(p) + c(p)u(p) \tag{5.25}$$

transforms under a change of the spatial coordinates $\Omega \longrightarrow \widetilde{\Omega}, p \longmapsto \tilde{p}$ *into*

$$\sum_{k,l=1}^{n} \tilde{a}^{kl}(\tilde{p})\frac{\partial^2}{\partial \tilde{p}^k \partial \tilde{p}^l}\tilde{u}(\tilde{p}) + \sum_{k=1}^{n} \tilde{b}^k(\tilde{p})\frac{\partial}{\partial \tilde{p}^k}\tilde{u}(\tilde{p}) + \tilde{c}(\tilde{p})\tilde{u}(\tilde{p}) \tag{5.26}$$

with $\tilde{u}\big(\tilde{p}(p)\big) = u(p)$ *and*

$$\tilde{a}^{kl}(\tilde{p}) = \sum_{i,j=1}^{n} a^{ij}(p)\frac{\partial \tilde{p}^k}{\partial p^i}\frac{\partial \tilde{p}^l}{\partial p^j} \quad \text{for } k,l = 1,\dots,n, \tag{5.27}$$

$$\tilde{b}^k(\tilde{p}) = \sum_{i=1}^{n} b^i(p)\frac{\partial \tilde{p}^k}{\partial p^i} + \sum_{i,j=1}^{n} a^{ij}(p)\frac{\partial^2 \tilde{p}^k}{\partial p^i \partial p^j} \quad \text{for } k = 1,\dots,n, \tag{5.28}$$

$$\tilde{c}(\tilde{p}) = c(p). \tag{5.29}$$

Proof. Let $\tilde{p}$ be a change of coordinates and $\tilde{u}$ such that $u(p) = \tilde{u}(\tilde{p}(p))$. Then we have by the chain rule

$$\begin{aligned}
\sum_{i,j=1}^{n} a^{ij}\frac{\partial}{\partial p^i}\partial p^j u &= \sum_{i,j=1}^{n}\sum_{k=1}^{n} a^{ij}\frac{\partial}{\partial p^i}\left(\frac{\partial \tilde{p}^k}{\partial p^j}\frac{\partial}{\partial \tilde{p}^k}\tilde{u}\right) \\
&= \sum_{i,j=1}^{n}\left(\sum_{l,k=1}^{n} a^{ij}\frac{\partial \tilde{p}^l}{\partial p^i}\frac{\partial \tilde{p}^k}{\partial p^j}\frac{\partial}{\partial \tilde{p}^l}\partial \tilde{p}^k\tilde{u} + \sum_{k=1}^{n} a^{ij}\frac{\partial^2 \tilde{p}^k}{\partial p^i \partial p^j}\frac{\partial}{\partial \tilde{p}^k}\tilde{u}\right) \\
&= \sum_{l,k=1}^{n}\sum_{i,j=1}^{n} a^{ij}\frac{\partial \tilde{p}^l}{\partial p^i}\frac{\partial \tilde{p}^k}{\partial p^j}\frac{\partial}{\partial \tilde{p}^l}\partial \tilde{p}^k\tilde{u} + \sum_{k=1}^{n}\sum_{i,j=1}^{n} a^{ij}\frac{\partial^2 \tilde{p}^k}{\partial p^i \partial p^j}\frac{\partial}{\partial \tilde{p}^k}\tilde{u}
\end{aligned} \tag{5.30}$$

and

$$\sum_{i=1}^{n} b^i \frac{\partial}{\partial p^i} u = \sum_{i=1}^{n}\sum_{k=1}^{n} b^i \frac{\partial \tilde{p}^k}{\partial p^i}\frac{\partial}{\partial \tilde{p}^k}\tilde{u} = \sum_{k=1}^{n}\sum_{i=1}^{n} b^i \frac{\partial \tilde{p}^k}{\partial p^i}\frac{\partial}{\partial \tilde{p}^k}\tilde{u}. \tag{5.31}$$

Now putting $\tilde{a}^{lk}$, $\tilde{b}^k$ and $\tilde{c}$ as in equation (5.27), we have

$$\sum_{i,j=1}^{n} a^{ij}\frac{\partial}{\partial p^i}\partial p^j u + \sum_{i=1}^{n} b^i \frac{\partial}{\partial p^i} u + cu = \sum_{l,k=1}^{n} \tilde{a}^{lk}\frac{\partial}{\partial \tilde{p}^l}\partial \tilde{p}^k \tilde{u} + \sum_{k=1}^{n} \tilde{b}^k \frac{\partial}{\partial \tilde{p}^k}\tilde{u} + \tilde{c}\tilde{u}. \qquad \square$$

Proof of Lemma 5.5. When changing coordinates $(p^i) \mapsto (\tilde{p}^i)$, the coefficients of the 2nd order derivatives a^{ij} transform as

$$\tilde{a}^{kl} = \sum_{i,j} a^{ij}\frac{\partial \tilde{p}^k}{\partial p^i}\frac{\partial \tilde{p}^l}{\partial p^j}, \tag{5.32}$$

while we may get additional first order terms with coefficients $\sum_{i,j} a^{ij}\frac{\partial^2 \tilde{p}^k}{\partial p^i \partial p^j}$ (cf. Lemma 5.6).

For the transformation at hand, we have (cf. equations (5.6) and (5.5))

$$\frac{\partial \tilde{p}^k}{\partial p^i} = \delta_i^k + \delta_r^k \delta_i^s \quad \text{for } k \neq s \tag{5.33}$$

and (cf. equation (5.7))

$$\frac{\partial \tilde{p}^s}{\partial p^i} = \frac{p^r}{(p^r+p^s)^2}\delta_i^s - \frac{p^s}{(p^r+p^s)^2}\delta_i^r = \frac{1-\tilde{p}^s}{\tilde{p}^r}\delta_i^s - \frac{\tilde{p}^s}{\tilde{p}^r}\delta_i^r. \tag{5.34}$$

Therefore, (5.32) yields

$$\tilde{a}^{kl}(\tilde{p}) = \sum_{i,j} a^{ij}(p)(\delta_i^k + \delta_r^k\delta_i^s)(\delta_j^l + \delta_r^l\delta_j^s) \tag{5.35}$$

for $k, l \neq s$, that is,

$$\begin{aligned}\tilde{a}^{kl}(\tilde{p}) &= a^{kl}(p) + a^{kt}(p)\delta_r^l + a^{sl}(p)\delta_r^k + a^{ss}(p)\delta_r^k\delta_r^l \\ &= p^k(\delta_l^k - p^l) - p^k p^s \delta_r^l - p^s p^l \delta_r^k + p^s(1-p^s)\delta_r^k\delta_r^l \\ &= \tilde{p}^k(\delta_l^k - \tilde{p}^l)\end{aligned} \tag{5.36}$$

for $k, l \in \{i_1, \ldots, i_m\}\backslash\{s\}$ using the given form of the a^{ij}, whereas for all other index pairs not containing the index s, we always have

$$a^{kt}(p)\delta_r^l = a^{sl}(p)\delta_r^k = a^{ss}(p)\delta_r^k\delta_r^l = 0 \tag{5.37}$$

and hence

$$\tilde{a}^{kl}(\tilde{p}) = \sum_{i,j} a^{ij}(p)\delta_i^k\delta_j^l = a^{kl}(p), \tag{5.38}$$

thus proving the last statement. Furthermore, we have for arbitrary $l \neq s$

$$\begin{aligned}
\tilde{a}^{sl}(\tilde{p}) &= \sum_{i,j} a^{ij}(p)\left(\frac{1-\tilde{p}^s}{\tilde{p}^r}\delta_i^s - \frac{\tilde{p}^s}{\tilde{p}^r}\delta_i^r\right)(\delta_j^l + \delta_r^l\delta_j^s) \\
&= \frac{1-\tilde{p}^s}{\tilde{p}^r}(a^{sl}(p) + a^{ss}(p)\delta_r^l) - \frac{\tilde{p}^s}{\tilde{p}^r}(a^{rl}(p) + a^{rt}(p)\delta_r^l) \\
&= \left(-\frac{1-\tilde{p}^s}{\tilde{p}^r}\tilde{p}^r\tilde{p}^s\tilde{p}^l + \frac{\tilde{p}^s}{\tilde{p}^r}(1-\tilde{p}^s)\tilde{p}^r\tilde{p}^l\right)\chi_{\{i_1,\ldots,i_m\}}(l) \\
&\quad -\frac{\tilde{p}^s}{\tilde{p}^r}\tilde{p}^r(1-\tilde{p}^s)\delta_r^l + \left(\frac{1-\tilde{p}^s}{\tilde{p}^r}\tilde{p}^r\tilde{p}^s(1-\tilde{p}^r\tilde{p}^s) + \frac{\tilde{p}^s}{\tilde{p}^r}\tilde{p}^r(1-\tilde{p}^s)\tilde{p}^r\tilde{p}^s\right)\delta_r^l = 0
\end{aligned} \tag{5.39}$$

as well as $\tilde{a}^{ls} = 0$ $(l \neq s)$ by symmetry and finally

$$\begin{aligned}
\tilde{a}^{ss}(\tilde{p}) &= \sum_{i,j} a^{ij}(p)\left(\frac{1-\tilde{p}^s}{\tilde{p}^r}\delta_i^s - \frac{\tilde{p}^s}{\tilde{p}^r}\delta_i^r\right)\left(\frac{1-\tilde{p}^s}{\tilde{p}^r}\delta_j^s - \frac{\tilde{p}^s}{\tilde{p}^r}\delta_j^r\right) \\
&= a^{ss}(p)\left(\frac{1-\tilde{p}^s}{\tilde{p}^r}\right)^2 + a^{rr}(p)\left(\frac{\tilde{p}^s}{\tilde{p}^r}\right)^2 - 2a^{sr}(p)\frac{\tilde{p}^s(1-\tilde{p}^s)}{(\tilde{p}^r)^2} \\
&= \tilde{p}^s(1-\tilde{p}^r\tilde{p}^s)\frac{(1-\tilde{p}^s)^2}{\tilde{p}^r} + (1-\tilde{p}^s)(1-\tilde{p}^r+\tilde{p}^r\tilde{p}^s)\frac{(\tilde{p}^s)^2}{\tilde{p}^r} \\
&\quad - 2\tilde{p}^r\tilde{p}^s(1-\tilde{p}^s)\frac{\tilde{p}^s(1-\tilde{p}^s)}{\tilde{p}^r} = \frac{\tilde{p}^s(1-\tilde{p}^s)}{\tilde{p}^r}.
\end{aligned} \tag{5.40}$$

Thus, all $\tilde{a}^{kl}$ have the desired expression.

Possible additional first order terms would have to contain second derivatives of $\tilde{p}$. the only component for which they do not obviously vanish is $\tilde{p}^s$. But we have (cf. equation (5.34))

$$\frac{\partial}{\partial p^j}\frac{\partial}{\partial p^i}\tilde{p}^s = \frac{2}{(p^r+p^s)^3}(p^s\delta_i^r - p^r\delta_i^s)(\delta_j^r + \delta_j^s) + \frac{1}{(p^r+p^s)^2}(\delta_i^s\delta_j^r - \delta_i^r\delta_j^s) \tag{5.41}$$

and subsequently

$$\begin{aligned}
\sum_{i,j} a^{ij}\frac{\partial}{\partial p^i}\frac{\partial}{\partial p^j}\tilde{p}^s &= \frac{2}{(p^r+p^s)^3}\big(p^s(a^{rr}+a^{rs}) - p^r(a^{sr}+a^{ss})\big) + \frac{1}{(p^r+p^s)^2}(a^{sr}-a^{rs}) \\
&= \frac{2}{(p^r+p^s)^3}\big(p^sp^r(1-p^r-p^s) + p^rp^s(p^r-1+p^s)\big) = 0,
\end{aligned} \tag{5.42}$$

for which again the particular expression for the a^{ij} is needed.

If $\tilde{p}^s$ is chosen with different orientation as in remark 5.3, instead of equation (5.34) we then have

$$\frac{\partial\tilde{p}^s}{\partial p^i} = \frac{\tilde{p}^s}{\tilde{p}^r}\delta_i^s - \frac{1-\tilde{p}^s}{\tilde{p}^r}\delta_i^r. \tag{5.43}$$

This means that in the respective formulae the indices r and s are swapped, which in turn is matched by the corresponding inverse transformation which now yields $p^r = \tilde{p}^r\tilde{p}^s$ and $p^s = \tilde{p}^r(1-\tilde{p}^s)$. □

For an iterated application of the blow-up transformation, we obtain thus:

Proposition 5.7. *In the setting of a full blow-up transformation as in Proposition 5.4, the operator* $L^* = \sum p^i(\delta^i_j - p^j)\frac{\partial}{\partial p^i}\frac{\partial}{\partial p^j}$ *in* $\overline{\Delta_n^{(I_n)}}$ *is transformed into* [5]

$$\widetilde{L}^* = \frac{1}{2}\sum_{j,l=1}^{k+1}\tilde{p}^{i_j}(\delta^j_l - \tilde{p}^{i_l})\frac{\partial}{\partial\tilde{p}^{i_j}}\frac{\partial}{\partial\tilde{p}^{i_l}} + \frac{1}{2}\sum_{j=k+2}^{n}\frac{\tilde{p}^{i_j}(1-\tilde{p}^{i_j})}{\prod_{l=k+1}^{j-1}\tilde{p}^{i_l}}\frac{\partial^2}{(\partial\tilde{p}^{i_j})^2} \tag{5.44}$$

in $\left(\overline{\Delta_{k+1}^{(I_{k+1})}} \times \overline{\square_{n-k-1}^{(I_n\setminus I_{k+1})}}\right)\setminus\bigcup_{j=k+1}^{n-1}N_j$.

If in any step the coordinate $\tilde{p}^{s_j}$ *is chosen with alternative orientation (cf. remark 5.3),* $\tilde{p}^{s_j}$*, whenever it appears in the above formulae, is replaced by* $(1-\tilde{p}^{s_j})$.

Thus, the iterated blow-up translates the (extended) Kolmogorov backward equation in $\overline{\Delta}_n$ into a corresponding differential equation in $\left(\overline{\Delta_{k+1}^{(I_{k+1})}} \times \overline{\square_{n-k-1}^{(I_n\setminus I_{k+1})}}\right)\setminus\bigcup_{j=k+1}^{n-1}N_j$. For the iteratively extended solutions of the Kolmogorov backward equation introduced in the preceding chapter, the transformation behaviour is as follows:

Proposition 5.8. *Let* $k, n \in \mathbb{N}$ *with* $0 \le k \le n-2$, $\{i_k, i_{k+1}, \dots, i_n\} \subset I_n := \{0, 1, \dots, n\}$ *with* $i_i \neq i_j$ *for* $i \neq j$ *and* $I_d := I_n\setminus\{i_{d+1}, \dots, i_n\}$ *for* $d = k, \dots, n-1$*, and let* u_{I_k} *in* $\left(\Delta_k^{(I_k)}\right)_{-\infty}$ *and* $\overline{U}_{I_k}^{i_k,\dots,i_n}$ *in* $\left(\bigcup_{k\le d\le n}\Delta_d^{(I_d)}\right)_{-\infty}$ *as in Proposition 3.2. Then a repeated blow-up transformation* $\Phi_{s_{n-k-1}}^{r_{n-k-1}} \circ \dots \circ \Phi_{s_1}^{r_1}$ *with* $\Phi_{s_m}^{r_m}$ *as in Lemma 5.1 with* $r_m = i_{n-m}$ *and* $s_m = i_{n-m+1}$ *for* $m = 1, \dots, n-k-1$ *converts*

$$\begin{aligned}\overline{U}_{I_k}^{i_k,\dots,i_n}(p,t) &:= u_{I_k}(p,t)\chi_{\Delta_k^{(I_k)}}(p) + \sum_{k+1\le d\le n}\bar{u}_{I_k}^{i_k,\dots,i_d}(p,t)\chi_{\Delta_d^{(I_d)}}(p)\\ &= u_{I_k}(p,t)\chi_{\Delta_k^{(I_k)}}(p) + \sum_{k+1\le d\le n}u_{I_k}(\pi^{i_k,\dots,i_d}(p),t)\prod_{j=k}^{d-1}\frac{p^{i_j}}{\sum_{l=j}^{d}p^{i_l}}\chi_{\Delta_d^{(I_d)}}(p)\end{aligned} \tag{5.45}$$

on $\left(\bigcup_{k\le d\le n}\Delta_d^{(I_d)}\right)_{-\infty}$ *into*

$$\begin{aligned}\widetilde{U}_{I_k}^{i_k,i_{k+1};i_{k+2},\dots,i_n}(\tilde{p},t) &:= u_{I_k}(\tilde{p},t)\chi_{\Delta_k^{(I_k)}}(\tilde{p})\\ &\quad + \sum_{k+1\le d\le n}\tilde{u}_{I_k}^{i_k,i_{k+1};i_{k+2},\dots,i_d}(\tilde{p},t)\chi_{\Delta_{k+1}^{(I_{k+1})}\times\square_{d-k-1}^{(I_d\setminus I_{k+1})}}(\tilde{p})\end{aligned} \tag{5.46}$$

on $\left(\bigcup_{k\le d\le n}\Delta_{k+1}^{(I_{k+1})} \times \square_{n-k-1}^{(I_n\setminus I_{k+1})}\right)_{-\infty}$ *with*

$$\tilde{u}_{I_k}^{i_k,i_{k+1};i_{k+2},\dots,i_d}(\tilde{p},t) := \bar{u}_{I_k}^{i_k,i_{k+1}}(\tilde{\pi}^{i_{k+1}}(\tilde{p}),t)\prod_{j=k+2}^{d}(1-\tilde{p}^{i_j}) \quad \text{for } d = k+2, \dots, n \tag{5.47}$$

[5] Please note that on boundary instances of $\square_{n-k-1}^{(I_n\setminus I_{k+1})}$, i.e. $\tilde{p}^{i_l} = 0$ for some $l \in I_n\setminus I_{k+1}$, the corresponding summands are assumed not to appear in the right sum in equation (5.44), which may be interpreted as a result of a successive restriction. The given domain is the maximal domain for the operator as it is not defined on the exception set $\bigcup_{j=k+1}^{n-1}N_j$ (however, cf. also Lemma 7.1 for the stationary case).

with $\tilde{\pi}^{i_{k+1}}(\tilde{p}^{i_j}) := \tilde{p}^{i_j}$ *for* $i_j \in I_{k+1}$, $\tilde{\pi}^{i_{k-1}}(\tilde{p}^{i_j}) := 0$ *else. The transformed functions* $\tilde{u}_{I_k}^{i_k,i_{k+1};i_{k+2},\dots,i_d}$ *smoothly extend to* $\left(\overline{\Delta_{k+1}^{(I_{k+1})}} \times \overline{\square_{d-k-1}^{(I_d\setminus I_{k+1})}}\right)_{-\infty}$ *respectively; consequently also* $\widetilde{U}_{I_k}^{i_k,i_{k+1};i_{k+2},\dots,i_n}$ *smoothly extends to* $\left(\overline{\Delta_{k+1}^{(I_{k+1})}} \times \overline{\square_{n-k-1}^{(I_n\setminus I_{k+1})}}\right)_{-\infty}$. *Furthermore, it may be simplified to*

$$\widetilde{U}_{I_k}^{i_k,i_{k+1};i_{k+2},\dots,i_n}(\tilde{p},t) \equiv \tilde{u}_{I_k}^{i_k,i_{k+1};i_{k+2},\dots,i_n}(\tilde{p},t) \quad \text{in } \left(\overline{\Delta_{k+1}^{(I_{k+1})}} \times \overline{\square_{n-k-1}^{(I_n\setminus I_{k+1})}}\right)_{-\infty}. \tag{5.48}$$

If in any step the coordinate $\tilde{p}^{s_j}$ *is chosen with alternative orientation (cf. remark 5.3),* $\tilde{p}^{s_j}$ *in the above formulae needs to be replaced by* $(1-\tilde{p}^{s_j})$.

For the stationary components, we have in particular:

Corollary 5.9. *For* $k=0$ *and w. l. o. g.* $i_0=0$, *the transformed function of Proposition 5.8 in equation (5.48) simplifies to*

$$\widetilde{U}_{\{i_0\}}^{i_0,i_1;i_2,\dots,i_n}(\tilde{p}) = u_{\{i_0\}}(1)\cdot\prod_{j=1}^{n}(1-\tilde{p}^{i_j}) \quad \text{in } \overline{\square_n^{(I'_n)}}, \tag{5.49}$$

while in accordance with Proposition 5.4 the domain is mapped

$$\Delta_d^{(I_d)} \longmapsto \square_d^{(I'_d)} \quad \text{for } d=0,\dots,n \tag{5.50}$$

and altogether

$$\overline{\Delta_n^{(I_n)}} \longmapsto \overline{\square_n^{(I'_n)}}\setminus\bigcup_{j=1}^{n-1} N_j. \tag{5.51}$$

The $n-1$ *additional* $(n-1)$*-dimensional faces* $N_1,\dots,N_{n-1}$ *of* $\partial\square_n^{(I'_n)}$ *are given by*

$$N_1 = \{0\}^{(\{i_1\})} \times \overline{\boxtimes_{n-1}^{(I'_n\setminus I'_1)}} \tag{5.52}$$

and

$$N_j = \overline{\square_{j-1}^{(I'_{j-1})}} \times \{0\}^{(\{i_j\})} \times \overline{\boxtimes_{n-j}^{(I'_n\setminus I'_j)}} \tag{5.53}$$

for $j=2,\dots,n-1$, *whereas the operator* $L^* = \sum p^i(\delta_j^i - p^j)\frac{\partial}{\partial p^i}\frac{\partial}{\partial p^j}$ *in* $\overline{\Delta_n^{(I_n)}}$ *is transformed into*

$$\widetilde{L}^* = \frac{1}{2}\sum_{j=1}^{n}\frac{\tilde{p}^{i_j}(1-\tilde{p}^{i_j})}{\prod_{l=1}^{j-1}\tilde{p}^{i_l}}\frac{\partial^2}{(\partial\tilde{p}^{i_j})^2} \quad \text{in } \overline{\square_n^{(I'_n)}}\setminus\bigcup_{j=1}^{n-1} N_j. \tag{5.54}$$

Proof of Propositions 5.4–5.8. We prove the assertions of the three Propositions in parallel: Our aim is to transform $\overline{U}_{I_k}^{i_k,\dots,i_n}$ into a function that does not feature any incompatibilities and hence is sufficiently regular with respect to the entire closure of the (transformed) domain. For that purpose, we shall show that the full blow-up via a repeated application of the coordinate transformation Φ_s^r of Lemma 5.1 with the indices r and s to be picked as shown in each step yields the desired result for $\widetilde{U}_{I_k}^{i_k,i_{k+1};i_{k+2},\dots,i_n}$, while the transformation behaviour of the

domain and the operator is as stated in Proposition 5.4. For notational simplicity, we will usually suppress the t-component in the notation for our domains throughout this proof; for instance, we shall write $\Delta_n^{(I_n)}$ instead of $\left(\Delta_n^{(I_n)}\right)_{-\infty}$.

Starting with the top-dimensional component of $\overline{U}_{I_k}^{i_k,\dots,i_n}$, which is

$$\begin{aligned}\bar{u}_{I_k}^{i_k,\dots,i_n}(p,t) &= \bar{u}_{I_k}^{i_k,\dots,i_{n-1}}(\pi^{i_{n-1},i_n}(p),t)\cdot\frac{p^{i_{n-1}}}{p^{i_{n-1}}+p^{i_n}}\\ &= u_{I_k}(\pi^{i_k,\dots,i_{n-1}}(\pi^{i_{n-1},i_n}(p)),t)\prod_{j=k}^{n-2}\frac{p^{i_j}}{\sum_{l=j}^n p^{i_l}}\cdot\frac{p^{i_{n-1}}}{p^{i_{n-1}}+p^{i_n}}\quad\text{in }\Delta_n^{(I_n)}\end{aligned}\tag{5.55}$$

with $p^{i_0}\equiv p^0 = 1-\sum_{j=1}^n p^{i_j}$ (if $i_0\neq 0$, one may change the coordinates, i.e. permute the vertices correspondingly), we initially put [6] $r_1 := i_{n-1}$ and $s_1 := i_n$. Changing coordinates $(p^i)\mapsto(\tilde{p}^i)$ by $\Phi_{s_1}^{r_1}$ maps $\Delta_n^{(I_n)}$ onto $\Delta_{n-1}^{(I_{n-1})}\times\square_1^{(\{i_n\})}$ and $\overline{\Delta_{n-1}^{(I_{n-1})}}$ onto $\overline{\Delta_{n-1}^{(I_{n-1})}}\times\{0\}^{(\{i_n\})}$, whereas the entire domain $\overline{\Delta_n^{(I_n)}}$ is transformed into $\left(\overline{\Delta_{n-1}^{(I_{n-1})}}\times\overline{\square_1^{(\{i_n\})}}\right)\backslash N_{n-1}$ with

$$N_{n-1} := \overline{\Delta_{n-2}^{(I_{n-2})}}\times\{0\}^{(\{i_{n-1}\})}\times\overline{\boxtimes_1^{(\{i_n\})}}\tag{5.56}$$

being an additional $(n-1)$-dimensional face of $\overline{\Delta_{n-1}^{(I_{n-1})}}\times\overline{\square_1^{(\{i_n\})}}$ (cf. Lemma 5.1). At the same time, the $(n-2)$-dimensional incompatibility at $\overline{\Delta_{n-2}^{(I_{n-2})}}$ of the continuous extension of $\bar{u}_{I_k}^{i_k,\dots,i_n}$ to $\partial_{n-1}\Delta_n^{(I_n)}$ is removed as the transformation yields

$$\begin{aligned}\tilde{u}_{I_k}^{i_k,\dots,i_{n-1};i_n}(\tilde{p},t) &:= \bar{u}_{I_k}^{i_k,\dots,i_{n-1}}(\tilde{\pi}^{i_{n-1}}(\tilde{p}),t)\cdot(1-\tilde{p}^{i_n})\\ &= u_{I_k}(\pi^{i_k,\dots,i_{n-1}}(\tilde{\pi}^{i_{n-1}}(\tilde{p})),t)\prod_{j=k}^{n-2}\frac{\tilde{p}^{i_j}}{\sum_{l=j}^n\tilde{p}^{i_l}}\cdot(1-\tilde{p}^{i_n})\\ &\qquad\text{in }\Delta_{n-1}^{(I_{n-1})}\times\square_1^{(\{i_n\})}\end{aligned}\tag{5.57}$$

by equation (5.12) et seq. (note $\tilde{\pi}^{i_{n-1}}(\tilde{p}) = \pi^{i_{n-1},i_n}(p)$). Hence, the complete function $\overline{U}_{I_k}^{i_k,\dots,i_n}$ is transformed into

$$\begin{aligned}\widetilde{U}_{I_k}^{i_k,\dots,i_{n-1};i_n}(p,t) := &\sum_{k\le d\le n-1}\bar{u}_{I_k}^{i_k,\dots,i_d}(p,t)\chi_{\Delta_d^{(I_d)}}(p)\\ &+\tilde{u}_{I_k}^{i_k,\dots,i_{n-1};i_n}(p,t)\chi_{\Delta_{n-1}^{(I_{n-1})}\times\square_1^{(I_n\backslash I_{n-1})}}(p)\end{aligned}\tag{5.58}$$

with the transformed top-dimensional component $\tilde{u}_{I_k}^{i_k,\dots,i_{n-1};i_n}(\tilde{p},t)$ smoothly extending to $\Delta_{n-1}^{(I_{n-1})}\times\overline{\square_1^{(\{i_n\})}}$ with

$$\tilde{u}_{I_k}^{i_k,\dots,i_{n-1};i_n}(\tilde{p},t)\big|_{\Delta_{n-1}^{(I_{n-1})}\times\{0\}^{(\{i_n\})}}\equiv\bar{u}_{I_k}^{i_k,\dots,i_{n-1}}(\tilde{p},t)\quad\text{in }\Delta_{n-1}^{(I_{n-1})}\times\{0\}^{(\{i_n\})}.\tag{5.59}$$

[6] Alternatively, one could also put $r_1 := i_n$ and $s_1 := i_{n-1}$, which would correspond to inverting the orientation of the $\tilde{p}^{s_1}$-coordinate as in remark 5.3 (cf. also below) plus subsequently swapping the coordinate indices i_n and i_{n-1}, thus $\tilde{p}^{i_n}$ would get replaced by $1-\tilde{p}^{i_{n-1}}$ and $\tilde{p}^{i_{n-1}}$ with $\tilde{p}^{i_n}$.

As $\bar{u}_{I_k}^{i_k,\dots,i_{n-1}}$ itself smoothly extends to $\partial_{n-2}\Delta_{n-1}^{(I_{n-1})}$, thus $\tilde{u}_{I_k}^{i_k,\dots,i_{n-1};i_n}$ now smoothly extends to the entire $(\partial_{n-2}\Delta_{n-1}^{(I_{n-1})})\times\overline{\square_1^{(\{i_n\})}}$, in particular to $\Delta_{n-2}^{(I_{n-2})}\times\overline{\square_1^{(\{i_n\})}}\subset\overline{N}_{n-1}$ (however, $\bar{u}_{I_k}^{i_k,\dots,i_{n-1}}$ resp. its continuous extension to $\partial_{n-2}\Delta_{n-1}^{(I_{n-1})}$ still has an incompatibility at $\overline{\Delta_{n-3}^{(I_{n-3})}}$).

The operator $L^* = \frac{1}{2}\sum_{i,j=1}^n p^i(\delta_j^i - p^j)\frac{\partial}{\partial p^i}\frac{\partial}{\partial p^j}$ in $\overline{\Delta_n^{(I_n)}}$ transforms into (cf. Lemma 5.5)

$$\widetilde{L}^* = \frac{1}{2}\sum_{j,l\neq n}\tilde{p}^{i_j}(\delta_l^j - \tilde{p}^{i_l})\frac{\partial}{\partial\tilde{p}^{i_j}}\frac{\partial}{\partial\tilde{p}^{i_l}} + \frac{1}{2}\frac{\tilde{p}^{i_n}(1-\tilde{p}^{i_n})}{\tilde{p}^{i_{n-1}}}\frac{\partial}{\partial\tilde{p}^{i_n}}\frac{\partial}{\partial\tilde{p}^{i_n}} \tag{5.60}$$

on $\left(\overline{\Delta_{n-1}^{(I_{n-1})}}\times\overline{\square_1^{(\{i_n\})}}\right)\backslash N_{n-1}$ since we have $\tilde{a}^{kl}(\tilde{p}) = p^k(\delta_l^k - p^l) = \tilde{p}^k(\delta_l^k - \tilde{p}^l)$ for $k,l\neq i_{n-1},i_n$. If $\tilde{p}^{i_n}$ is chosen with alternative orientation (cf. remark 5.3), then $\tilde{p}^{i_n}$ needs to be replaced by $(1-\tilde{p}^{i_n})$ everywhere.

As already indicated, the transformed solution is still not smoothly extendable to the full boundary of the transformed domain: its $(n-2)$-dimensional incompatibility is resolved, but its lower-dimensional incompatibilities persist. Thus, the highest-dimensional incompatibility now is of dimension $n-3$, and hence the situation is ready for another application of the blow-up transformation.

Thus, we need an iterative procedure to resolve all incompatibilities. For this purpose, we assume that after the m-th step ($m = 1,\dots,n-k-2$) an already transformed function $\widetilde{U}_{I_k}^{i_k,\dots,i_{n-m};i_{n-m+1},\dots,i_n}$ with (note that we again associate coordinates p resp. $\tilde{p}$ etc. to the domain before/after the $(m+1)$-th transition; furthermore, we will use the convention $\bar{u}_{I_k}^{i_k} \equiv u_{I_k}$ to simplify the notation)

$$\begin{aligned}\widetilde{U}_{I_k}^{i_k,\dots,i_{n-m};i_{n-m+1},\dots,i_n}(p,t) = &\sum_{k\le d\le n-m}\bar{u}_{I_k}^{i_k,\dots,i_d}(p,t)\chi_{\Delta_d^{(I_d)}}(p)\\ &+\sum_{n-m+1\le d\le n}\tilde{u}_{I_k}^{i_k,\dots,i_{n-m};i_{n-m+1},\dots,i_d}(p,t)\chi_{\Delta_{n-m}^{(I_{n-m})}\times\square_{d-n+m}^{(I_d\backslash I_{n-m})}}(p)\end{aligned} \tag{5.61}$$

with

$$\tilde{u}_{I_k}^{i_k,\dots,i_{n-m};i_{n-m+1},\dots,i_d}(p,t) = \bar{u}_{I_k}^{i_k,\dots,i_{n-m}}(\tilde{\pi}^{i_{n-m}}(p),t)\prod_{j=n-m+1}^{d}(1-p^{i_j}) \tag{5.62}$$

for $d = n-m+1,\dots,n$ and

$$\begin{aligned}\bar{u}_{I_k}^{i_k,\dots,i_{n-m}}(p,t) &= \bar{u}_{I_k}^{i_k,\dots,i_{n-m-1}}(\pi^{i_{n-m-1},i_{n-m}}(p),t)\cdot\frac{p^{i_{n-m-1}}}{p^{i_{n-m-1}}+p^{i_{n-m}}}\\ &= u_{I_k}(\pi^{i_k,\dots,i_{n-m-1}}(\pi^{i_{n-m-1},i_{n-m}}(p)),t)\prod_{j=k}^{n-m-2}\frac{p^{i_j}}{\sum_{l=j}^n p^{i_l}}\cdot\frac{p^{i_{n-m-1}}}{p^{i_{n-m-1}}+p^{i_{n-m}}}\end{aligned} \tag{5.63}$$

in $\Delta_{n-m}^{(I_{n-m})}$. The corresponding total domain as an image of $\overline{\Delta_n^{(I_n)}}$ is given by

$$\left(\overline{\Delta_{n-m}^{(I_{n-m})}}\times\overline{\square_m^{(I_n\backslash I_{n-m})}}\right)\backslash\bigcup_{j=n-m}^{n-1}N_j \tag{5.64}$$

with additional $(n-1)$-dimensional faces from previous steps

$$N_{n-m} = \overline{\Delta_{n-m-1}^{(I_{n-m-1})}} \times \{0\}^{(\{i_{n-m}\})} \times \overline{\boxtimes_m^{(I_n \setminus I_{n-m})}} \tag{5.65}$$

and

$$N_j = \overline{\Delta_{n-m}^{(I_{n-m})}} \times \overline{\square_{j-n+m-1}^{(I_{j-1} \setminus I_{n-m})}} \times \{0\}^{(\{i_j\})} \times \overline{\boxtimes_{n-j}^{(I_n \setminus I_j)}} \tag{5.66}$$

for $j = n-m+1, \dots, n-1$.

The functions $\tilde{u}_{I_k}^{i_k,\dots,i_{n-m};i_{n-m+1},\dots,i_d}$ smoothly extend each to $\Delta_{n-m}^{(I_{n-m})} \times \overline{\square_{d-n+m}^{(I_d \setminus I_{n-m})}}$, and we have

$$\tilde{u}_{I_k}^{i_k,\dots,i_{n-m};i_{n-m+1},\dots,i_d}\big|_{\Delta_{n-m}^{(I_{n-m})} \times \square_m^{(I_{d-1} \setminus I_{n-m})}} = \tilde{u}_{I_k}^{i_k,\dots,i_{n-m};i_{n-m+1},\dots,i_{d-1}} \tag{5.67}$$

for $d = n-m+2, \dots, n$ and

$$\tilde{u}_{I_k}^{i_k,\dots,i_{n-m};i_{n-m+1}}\big|_{\Delta_{n-m}^{(I_{n-m})}} = \bar{u}_{I_k}^{i_k,\dots,i_{n-m}}. \tag{5.68}$$

With $\bar{u}_{I_k}^{i_k,\dots,i_{n-m}}$ being smoothly extendable to $\partial_{n-m-1}\Delta_{n-m}^{(I_{n-m})}$, also the functions $\tilde{u}_{I_k}^{i_k,\dots,i_{n-m};i_{n-m+1},\dots,i_d}$ smoothly extend to $\left(\partial_{n-m-1}\Delta_{n-m}^{(I_{n-m})}\right) \times \overline{\square_{d-n+m}^{(I_d \setminus I_{n-m})}}$, in particular all additional faces are covered.

Furthermore, we assume that the operator L^* has the corresponding form

$$L^* = \frac{1}{2}\sum_{j,l=1}^{n-m} p^{i_j}(\delta_l^j - p^{i_l})\frac{\partial}{\partial p^{i_j}}\frac{\partial}{\partial p^{i_l}} + \frac{1}{2}\sum_{j=n-m+1}^{n} \frac{p^{i_j}(1-p^{i_j})}{\prod_{l=n-m}^{j-1} p^{i_l}}\frac{\partial^2}{(\partial p^{i_j})^2} \tag{5.69}$$

on $\left(\overline{\Delta_{n-m}^{(I_{n-m})}} \times \overline{\square_m^{(I_n \setminus I_{n-m})}}\right) \setminus \bigcup_{j=n-m}^{n-1} N_j$.

For the $(m+1)$-th blow-up step going to be applied now, we first notice that $\bar{u}_{I_k}^{i_k,\dots,i_{n-m}}$ resp. its continuous extension to $\partial_{n-m-1}\Delta_{n-m}^{(I_{n-m})}$ still has an incompatibility at $\overline{\Delta_{n-m-2}^{(I_{n-m-2})}} \subset \Delta_{n-m}^{(I_{n-m})}$, corresponding to $p^{i_{n-m}} + p^{i_{n-m-1}} = 0$. Consequently, this may be resolved by a blow-up transformation $\Phi_{s_{m+1}}^{r_{m+1}}$ with $r_{m+1} = i_{n-m-1}$ and $s_{m+1} = i_{n-m}$ (note that, due to the stipulation $i_0 = 0$, we always have $r_{m+1}, s_{m+1} \neq 0$), mapping the simplex part of the domain (cf. Lemma 5.1)

$$\Delta_{n-m}^{(I_{n-m})} \longmapsto \Delta_{n-m-1}^{(I_{n-m-1})} \times \square_1^{(\{i_{n-m}\})} \tag{5.70}$$

resp.

$$\overline{\Delta_{n-m-1}^{(I_{n-m-1})}} \longmapsto \overline{\Delta_{n-m-1}^{(I_{n-m-1})}} \times \{0\}^{(\{i_{n-m}\})} \tag{5.71}$$

and altogether

$$\overline{\Delta_{n-m}^{(I_{n-m})}} \longmapsto \overline{\Delta_{n-m-1}^{(I_{n-m-1})}} \times \overline{\square_1^{(\{i_{n-m}\})}} \setminus N_{n-m-1} \tag{5.72}$$

with

$$N_{n-m-1} := \overline{\Delta_{n-m-2}^{(I_{n-m-2})}} \times \{0\}^{(\{i_{n-m-1}\})} \times \overline{\boxtimes_1^{(\{i_{n-m}\})}} \tag{5.73}$$

being an additional $(n-m-1)$-dimensional face of $\overline{\Delta_{n-m-1}^{(I_{n-m-1})}} \times \overline{\square_1^{(\{i_{n-m}\})}}$.

From this, when gradually adding the cube part $\square_m^{(I_n\setminus I_{n-m})}$ with coordinates $p^{i_{n-m+1}},\dots,p^{i_n}$, equation (5.70) turns into

$$\Delta_{n-m}^{(I_{n-m})}\times\square_{d-n+m}^{(I_d\setminus I_{n-m})}\longmapsto\Delta_{n-m-1}^{(I_{n-m-1})}\times\square_{d-n+m+1}^{(I_d\setminus I_{n-m-1})}\quad\text{for } d\geq n-m, \tag{5.74}$$

and by applying equation (5.72) to the previous image of the initial domain $\overline{\Delta_n^{(I_n)}}$ in equation (5.64), we obtain for the transformed total domain

$$\Big(\overline{\Delta_{n-m-1}^{(I_{n-m-1})}}\times\overline{\square_{m+1}^{(I_n\setminus I_{n-m-1})}}\Big)\setminus\bigcup_{j=n-m-1}^{n-1}\widetilde{N}_j \tag{5.75}$$

with $\widetilde{N}_{n-m},\dots,\widetilde{N}_{n-1}$ being the images of the previous additional faces: The faces $N_{n-m+1},\dots,N_{n-1}$ are only affected indirectly as they contain the full $\overline{\Delta_{n-m}^{(I_{n-m})}}$ as a factor, and hence only the i_{n-m}-th coordinate is moved from the simplex to the cube, thus

$$\widetilde{N}_j=\overline{\Delta_{n-m-1}^{(I_{n-m-1})}}\times\overline{\square_{j-n+m}^{(I_{j-1}\setminus I_{n-m-1})}}\times\{0\}^{(\{i_j\})}\times\overline{\boxtimes_{n-j}^{(I_n\setminus I_j)}} \tag{5.76}$$

for $j=n-m+1,\dots,n-1$, whereas $N_{n-m}\equiv\widetilde{N}_{n-m}$ is virtually not affected as only $p^{i_{n-m}}=0$ is transformed into $\tilde{p}^{i_{n-m}}=0$. For the 'new' additional $(n-1)$-dimensional face $\widetilde{N}_{n-m-1}$ (resulting from N_{n-m-1}), we may – having added the remaining dimensions – relax the condition $\tilde{p}^{i_{n-m}}>0$ in equation (5.73), which ensures $N_{n-m-1}\neq\overline{\Delta_{n-m-2}^{(I_{n-m-2})}}$, into $\sum_{j=n-m}^{n}\tilde{p}^{i_j}>0$ and hence obtain

$$\widetilde{N}_{n-m-1}:=\overline{\Delta_{n-m-2}^{(I_{n-m-2})}}\times\{0\}^{(\{i_{n-m-1}\})}\times\overline{\boxtimes_{m+1}^{(I_n\setminus I_{n-m-1})}}. \tag{5.77}$$

At the same time, $\bar{u}_{I_k}^{i_k,\dots,i_{n-m}}$ and $\tilde{u}_{I_k}^{i_k,\dots,i_{n-m};i_{n-m+1},\dots,i_d}$, $d=n-m+1,\dots,n$ get transformed into

$$\tilde{u}_{I_k}^{i_k,\dots,i_{n-m-1};i_{n-m},\dots,i_d}(\tilde{p},t)=\bar{u}_{I_k}^{i_k,\dots,i_{n-m-1}}(\tilde{\pi}^{i_{n-m-1}}(\tilde{p}),t)\prod_{j=n-m}^{d}(1-\tilde{p}^{i_j}) \tag{5.78}$$

in $\Delta_{n-m-1}^{(I_{n-m-1})}\times\square_{d-n+m+1}^{(I_d\setminus I_{n-m-1})}$ for $d\geq n-m$, and hence

$$\begin{aligned}\widetilde{U}_{I_k}^{i_k,\dots,i_{n-m-1};i_{n-m},\dots,i_n}(p,t):=&\sum_{k\leq d\leq n-m-1}\bar{u}_{I_k}^{i_k,\dots,i_d}(p,t)\chi_{\Delta_d^{(I_d)}}(p)\\&+\sum_{n-m\leq d\leq n}\tilde{u}_{I_k}^{i_k,\dots,i_{n-m-1};i_{n-m},\dots,i_d}(p,t)\chi_{\Delta_{n-m-1}^{(I_{n-m-1})}\times\square_{d-n+m+1}^{(I_d\setminus I_{n-m-1})}}(p).\end{aligned} \tag{5.79}$$

The transformed functions $\tilde{u}_{I_k}^{i_k,\dots,i_{n-m-1};i_{n-m},\dots,i_d}$ then each smoothly extend to $\Delta_{n-m-1}^{(I_{n-m-1})}\times\overline{\square_{d-n+m+1}^{(I_d\setminus I_{n-m-1})}}$, and we have

$$\tilde{u}_{I_k}^{i_k,\dots,i_{n-m-1};i_{n-m},\dots,i_d}\big|_{\Delta_{n-m-1}^{(I_{n-m-1})}\times\square_{m+1}^{(I_{d-1}\setminus I_{n-m-1})}}=\tilde{u}_{I_k}^{i_k,\dots,i_{n-m-1};i_{n-m},\dots,i_{d-1}} \tag{5.80}$$

for $d=n-m+1,\dots,n$ and

$$\tilde{u}_{I_k}^{i_k,\dots,i_{n-m-1};i_{n-m}}\big|_{\Delta_{n-m-1}^{(I_{n-m-1})}}=\bar{u}_{I_k}^{i_k,\dots,i_{n-m-1}}. \tag{5.81}$$

With $\bar{u}_{I_k}^{i_k,\dots,i_{n-m-1}}$ being smoothly extendable to $\partial_{n-m-2}\Delta_{n-m-1}^{(I_{n-m-1})}$, the functions $\tilde{u}_{I_k}^{i_k,\dots,i_{n-m-1};i_{n-m},\dots,i_d}$ also smoothly extend to $\left(\partial_{n-m-2}\Delta_{n-m-1}^{(I_{n-m-1})}\right) \times \overline{\square_{d-n+m+1}^{(I_d\setminus I_{n-m-1})}}$, by which all additional faces are covered; in particular, $\tilde{u}_{I_k}^{i_k,\dots,i_{n-m-1};i_{n-m}}$ smoothly extends to N_{n-m-1} resp. eventually $\tilde{u}_{I_k}^{i_k,\dots,i_{n-m-1};i_{n-m},\dots,i_n}$ extends to $\widetilde{N}_{n-m-1}$ (however, $\bar{u}_{I_k}^{i_k,\dots,i_{n-m-1}}$ resp. its continuous extension to $\partial_{n-m-2}\Delta_{n-m-1}^{(I_{n-m-1})}$ still has an incompatibility at $\overline{\Delta_{n-m-3}^{(I_{n-m-3})}}$).

To analyze the transformation behaviour of the operator, we first note that the requirements of Lemma 5.5 on a^{ij} are met as for $i,j \in \{i_1,\dots,i_{n-m}\}$ we have $a^{ij}(p) = p^i(\delta_j^i - p^j)$ by equation (5.69), while all other non-diagonal coefficients vanish. Hence, by the Lemma, we have for $i,j \in \{i_1,\dots,i_{n-m}\}$

$$\tilde{a}^{ij}(\tilde{p}) = \tilde{p}^i(\delta_j^i - \tilde{p}^j), \tag{5.82}$$

while for $\tilde{a}^{i_ji_j}$ with $j = n-m+1,\dots,n$ we obtain

$$\tilde{a}^{i_ji_j}(\tilde{p}) = a^{i_ji_j}(p) = \frac{p^{i_j}(1-p^{i_j})}{\prod_{l=n-m}^{j-1} p^{i_l}} = \frac{\tilde{p}^{i_j}(1-\tilde{p}^{i_j})}{\prod_{l=n-m-1}^{j-1} \tilde{p}^{i_l}}. \tag{5.83}$$

Likewise, $\tilde{a}^{i_{n-m}i_{n-m}}$ takes the form

$$\tilde{a}^{i_{n-m}i_{n-m}}(\tilde{p}) = \frac{\tilde{p}^{i_{n-m}}(1-\tilde{p}^{i_{n-m}})}{\tilde{p}^{i_{n-m-1}}}, \tag{5.84}$$

whereas all other coefficients vanish. Altogether, this yields

$$\widetilde{L}^* = \frac{1}{2}\sum_{j,l=1}^{n-m-1} \tilde{p}^{i_j}(\delta_l^j - \tilde{p}^{i_l})\frac{\partial}{\partial\tilde{p}^{i_j}}\frac{\partial}{\partial\tilde{p}^{i_l}} + \frac{1}{2}\sum_{j=n-m}^{n} \frac{\tilde{p}^{i_j}(1-\tilde{p}^{i_j})}{\prod_{l=n-m-1}^{j-1}\tilde{p}^{i_l}}\frac{\partial^2}{(\partial\tilde{p}^{i_j})^2} \tag{5.85}$$

on $\left(\overline{\Delta_{n-m-1}^{(I_{n-m-1})}} \times \overline{\square_{m+1}^{(I_n\setminus I_{n-m-1})}}\right)\setminus\bigcup_{j=n-m-1}^{n-1} N_j$. If $\tilde{p}^{i_{n-m}}$ is chosen with alternative orientation (cf. remark 5.3), then $\tilde{p}^{i_{n-m}}$ needs to be replaced by $(1-\tilde{p}^{i_{n-m}})$ everywhere.

Thus, after the $(m+1)$-st blow-up step, the structure of domain, solution and operator is the same as before, just with the index m replaced by $m+1$. Eventually, after $n-k-1$ blow-up steps domain, solution and operator have attained the asserted form of the corresponding statements. In particular, the remaining u_{I_k} as a proper solution smoothly extends to the entire boundary of $\Delta_k^{(I_k)}$, and hence so does $\bar{u}_{I_k}^{i_k,i_{k+1}}$ in $\Delta_{k+1}^{(I_k)}$, implying that each $\tilde{u}_{I_k}^{i_k,i_{k+1};i_{k+2},\dots,i_d}$ smoothly extends to $\overline{\Delta_{k+1}^{(I_{k+1})}} \times \overline{\square_{d-k-1}^{(I_d\setminus I_{k+1})}}$, and eventually $\widetilde{U}_{I_k}^{i_k,i_{k+1};i_{k+2},\dots,i_n}$ smoothly extends to $\overline{\Delta_{k+1}^{(I_{k+1})}} \times \overline{\square_{n-k-1}^{(I_n\setminus I_{k+1})}}$. Moreover, the restriction property in equations (5.80) and (5.81) yields equation (5.48). □

Proof of Corollary 5.9. In the given setting, we have $\bar{u}_{\{i_0\}}^{i_0,i_1}(\tilde{p}) = u_{\{i_0\}}(\tilde{p}^{i_0} + \tilde{p}^{i_1})\frac{\tilde{p}^{i_0}}{\tilde{p}^{i_0}+\tilde{p}^{i_1}} = u_{\{i_0\}}(1)(1-\tilde{p}^{i_1})$ in $\overline{\Delta_1^{(\{i_0,i_1\})}} = \overline{\square_1^{(\{i_1\})}}$ (and $\overline{\Delta_0^{(\{i_0\})}} = \{0\}^{(\{i_0\})}$), which proves the asserted form of the (simplified) solution, the domain and the additional faces. □

However, the global smoothness of the transformed solution of Proposition 3.2 observed in the preceding Corollary does not necessarily hold for other functions in question, i.e. arbitrary

iteratively extended solutions U satisfying the extension constraints 3.1 (this corresponds to U particularly being of class $C^\infty_{p_0}$). However, we still have a weaker global regularity assertion for the transformed function $\widetilde{U}$ on the entire image of the simplex (only formulated for the stationary component corresponding to the setting of Corollary 5.9):

Lemma 5.10. *Let $n \geq 2$, $I_d := \{i_0, i_1, \dots, i_d\} \subset \{0, 1, \dots, n\}$ for $d = 0, \dots, n$ with $i_i \neq i_j$ for $i \neq j$ and $u_{\{i_0\}} \colon \Delta_0^{(\{i_0\})} \longrightarrow \mathbb{R}$. Then an iterated extension $U = \sum_{d=0}^n u_d \in C^\infty_{p_0}\big(\bigcup_{d=0}^n \Delta_d^{(I_d)}\big)$ of $u_{\{i_0\}}$ obeying the extension constraints 3.1 is transformed by a successive blow-up transformation $\Phi_{s_{n-1}}^{r_{n-1}} \circ \dots \circ \Phi_{s_1}^{r_1}$ as in Proposition 5.4 into a function $\widetilde{U} = \sum_{d=0}^n \tilde{u}_d \colon \bigcup_{d=0}^n \square_d^{(I'_d)} \longrightarrow \mathbb{R}$ with extension to all faces $\{\tilde{p}^{i_1} = 1, \dots, \{\tilde{p}^{i_n} = 1\}$ (which can be considered as boundary instances of any $\square_d^{(I'_d)} \subset \overline{\square_n^{(I'_n)}}$) which is of class C^∞_p and vanishes on the mentioned faces.*

For the proof, we trace the extendability of $\widetilde{U}$ towards the additional faces back to that of U in $\overline{\Delta_n^{(I_n)}}$ for approaching the incompatibilities – which will be accomplished by the next lemma. Note that in the following we will use a disjoint formulation of the additional faces by putting

$$N_j = \square_{j-1}^{(I'_{j-1})} \times \{0\}^{(\{i_j\})} \times \overline{\boxtimes_{n-j}^{(I'_n \setminus I'_j)}}. \tag{5.86}$$

Lemma 5.11. *In the setting of a full blow-up transformation as in Proposition 5.4, for $d = 1, \dots, n$ the additional face $N_d = \square_{d-1}^{(I'_{d-1})} \times \{0\}^{(\{i_d\})} \times \overline{\boxtimes_{n-d}^{(I'_n \setminus I'_d)}} \subset \overline{\square_n^{(I'_n)}}$ corresponds to $\Delta_{d-1}^{(I_{d-1})} \subset \overline{\Delta_n^{(I_n)}}$ with additional values existing for $\frac{p^{i_{d+1}} + \dots + p^{i_n}}{p^{i_d} + p^{i_{d+1}} + \dots + p^{i_n}}, \dots, \frac{p^{i_n}}{p^{i_{n-1}} + p^{i_n}}$ (which can be considered as limits of corresponding sequences). Furthermore, for $j = 1, \dots, d-1$ the face $\{\tilde{p}^{i_j} = 1\} \subset \overline{\square_{d-1}^{(I'_{d-1})}}$ corresponds to $p^{i_{j-1}} = 0$ in $\overline{\Delta_{d-1}^{(I_{d-1})}}$, in particular its interior corresponds to $\Delta_{d-2}^{(I_{d-1} \setminus \{i_{j-1}\})}$.*

Proof. To take account of the 'additional' faces N_m of $\overline{\square_n^{(I'_n)}}$ produced during the blow-up transformations, we carry out the inverse of the full blow-up transformation of Proposition 5.4 (cf. equations (5.19)–(5.22)), yielding

$$\tilde{p}^{i_1} := p^{i_1} + \dots + p^{i_n}, \tag{5.87}$$

$$\tilde{p}^{i_2} := \begin{cases} \dfrac{p^{i_2} + \dots + p^{i_n}}{p^{i_1} + p^{i_2} + \dots + p^{i_n}} & \text{for } p^{i_1} + \dots + p^{i_n} > 0 \\ 0 & \text{for } p^{i_1} + \dots + p^{i_n} = 0, \end{cases} \tag{5.88}$$

$$\vdots$$

$$\tilde{p}^{i_j} := \begin{cases} \dfrac{p^{i_j} + \dots + p^{i_n}}{p^{i_{j-1}} + p^{i_j} + \dots + p^{i_n}} & \text{for } p^{i_{j-1}} + \dots + p^{i_n} > 0 \\ 0 & \text{for } p^{i_{j-1}} + \dots + p^{i_n} = 0, \end{cases} \tag{5.89}$$

$$\vdots$$

$$\tilde{p}^{i_n} := \begin{cases} \dfrac{p^{i_n}}{p^{i_{n-1}} + p^{i_n}} & \text{for } p^{i_{n-1}} + p^{i_n} > 0 \\ 0 & \text{for } p^{i_{n-1}} + p^{i_n} = 0 \end{cases} \tag{5.90}$$

for $p \in \bigcup_{d=0}^{n} \Delta_d^{(I_d)}$ and conversely

$$p^{i_1} = \tilde{p}^{i_1}(1 - \tilde{p}^{i_2}), \tag{5.91}$$

$$\vdots$$

$$p^{i_j} = \tilde{p}^{i_1} \cdots \tilde{p}^{i_j}(1 - \tilde{p}^{i_{j+1}}), \tag{5.92}$$

$$\vdots$$

$$p^{i_{n-1}} = \tilde{p}^{i_1} \cdots \tilde{p}^{i_{n-1}}(1 - \tilde{p}^{i_n}), \tag{5.93}$$

$$p^{i_n} = \tilde{p}^{i_1} \cdots \tilde{p}^{i_n} \tag{5.94}$$

for $\tilde{p} \in \bigcup_{d=0}^{n} \square_d^{(I'_d)}$ (note that we also have $p^{i_0} = 1 - \tilde{p}^{i_1}$); however, the given equations also smoothly extend to the entire $\overline{\square_n^{(I'_n)}}$. We can therefore also transform the $N_d \subset \overline{\square}_n$ back to $\overline{\Delta}_n$, i.e. $\tilde{p}^{i_d} = 0$ implies $p^{i_d}, \ldots, p^{i_n} = 0$, whereas $0 < \tilde{p}^{i_1}, \ldots, \tilde{p}^{i_{d-1}} < 1$ leads to $p^{i_1}, \ldots, p^{i_{d-1}} > 0$. If however $\tilde{p}^{i_j} = 1$, this corresponds to $p^{i_{j-1}} = 0$ (and $p^{i_1}, \ldots, p^{i_{j-1}}, p^{i_{j+1}} \ldots, p^{i_d} > 0$ if $0 < \tilde{p}^{i_1}, \ldots, \tilde{p}^{i_{j-1}}, \tilde{p}^{i_{j+1}}, \ldots, \tilde{p}^{i_d} < 1$ and $\tilde{p}^{i_{d+1}} = 0$). □

Proof of Lemma 5.10. By Lemma 5.1 and Proposition 5.4 and Corollary 5.9, the full blow-up transformation respectively maps

$$\bigcup_{d=0}^{n} \Delta_d^{(I_d)} \longmapsto \bigcup_{d=0}^{n} \square_d^{(I'_d)} \tag{5.95}$$

C^∞-diffeomorphically (cf. equation (5.50)). By the $C^\infty_{p_0}$-regularity of U, u_n in $\Delta_n^{(I_n)}$ smoothly connects with u_{n-1} in $\Delta_{n-1}^{(I_{n-1})}$, and consequently so does $\tilde{u}_n$ in $\square_n^{(I'_n)}$ with $\tilde{u}_{n-1}$ in $\square_{n-1}^{(I'_{n-1})}$; an analogous statement holds for all lower dimensions. Thus it remains to show that $\widetilde{U}$ extends those faces of $\overline{\square_n^{(I'_n)}}$ given by $\{\tilde{p}^{i_j} = 1\}$ for $j = 1, \ldots, n$ such that the extension is of class C^∞_p.

By Lemma 5.11, the interior of $\{\tilde{p}^{i_j} = 1\} \subset \overline{\square_n^{(I'_n)}}$ corresponds to $p^{i_{j-1}} = 0$ and $p^{i_l} > 0$ for $l \neq j - 1$ in $\overline{\Delta_n^{(I_n)}}$, thus to $\Delta_{n-1}^{(I_n \setminus \{i_{j-1}\})}$, which is a boundary face of $\Delta_n^{(I_n)}$ outside the assumed extension path defined by the (ordered) I_n. Hence by the $C^\infty_{p_0}$-regularity, the relevant continuous extension of U needs to be zero there, and this is attained smoothly when coming from the interior $\Delta_n^{(I_n)}$. Considering the diffeomorphism properties of the transformation, this also applies to the cube.

An analogous observation holds for subcubes $\square_{d-1}^{(I'_{d-1})} \subset \overline{\square}_n$, $d = 1, \ldots, n$: The interior of its face $\{\tilde{p}^{i_j} = 1\}$ corresponds to $\Delta_{d'-1}^{(I_{d-1} \setminus \{i_{j-1}\})} \subset \overline{\Delta_{d-1}^{(I_{d-1})}}$ when transformed back to the simplex (cf. equation (5.95) and Lemma 5.11). This is again outside the assumed extension path, in particular if starting in $\Delta_{d-1}^{(I_{d-1})}$, and hence the corresponding boundary extension of u_{d-1} needs to smoothly attain zero there by the $C^\infty_{p_0}$-regularity, which likewise applies analogously to the cube. □

6. The stationary Kolmogorov backward equation and uniqueness

When we ask for the long-term behaviour of the process, i.e. which alleles are eventually lost and in which order, we are lead to the stationary Kolmogorov backward equation. Solutions of this equation have already appeared implicitly in the preceding section as extensions of solutions in $\partial_0\Delta_n$ since the corresponding operator L_0^* has 0 as its only eigenvalue.

Although we have already developed the extended setting presented in Section 3, we start by considering some interior simplex Δ_n, (resp. the corresponding restriction of an extended solution). Then, for a solution in Δ_n, we may argue again that all eigenmodes of the solution corresponding to a positive eigenvalue vanish for $t \to -\infty$, while those corresponding to the eigenvalue zero are preserved. This implies that a solution of the Kolmogorov backward equation (1.9) in Δ_n converges uniformly to a solution of the corresponding *homogeneous* or *stationary Kolmogorov backward equation*

$$\begin{cases} L^*u(p) = 0 & \text{in } \Delta_n \\ u(p) = f(p) & \text{in } \partial\Delta_n \end{cases} \tag{6.1}$$

for $u \in C^2(\Delta_n)$ and with boundary condition f (which needs to be attained smoothly in a suitable sense).

At first sight, this looks like a boundary value problem (for some suitably chosen boundary function f, assuring the uniqueness of a solution). However, as may be expected from the previous considerations, the role of the boundary here is different from usual boundary value problems and again requires some extra care: On the one hand, a proper solution in Δ_n always converges to the trivial stationary solution ($\equiv 0$), whose (continuous) extension to the boundary also vanishes at all negative times. On the other hand, any solution which extends to $\partial\Delta_n$ is already strongly constrained by the degeneracy behaviour of the differential operator if suitable regularity assumptions on the solution in $\overline{\Delta}_n$ (cf. also (2.9)) apply:

Lemma 6.1 (Stem lemma). *For a solution $u \in C^\infty(\Delta_n)$ of equation (6.1) with extension $U \in C_p^\infty(\overline{\Delta}_n)$, we have*

$$L^*U = 0 \qquad \text{in } \overline{\Delta}_n. \tag{6.2}$$

Proof. We shall proceed iteratively: Assuming that $L_k^*U = 0$ for all $\Delta_k^{(I_k)} \subset \partial_k\Delta_n$, we show that this property extends to each $\Delta_{k-1}^{(I_{k-1})} \subset \partial_{k-1}\Delta_k^{(I_k)}$ for every $\Delta_k^{(I_k)}$, and hence we obtain $L_{k-1}^*U = 0$ on $\partial_{k-1}\Delta_n$. A repeated application then yields (6.2).

W. l. o. g. let $\Delta_k^{(I_k)}$ and $\Delta_{k-1}^{(I_{k-1})} \subset \partial_{k-1}\Delta_k^{(I_k)}$ with $I_k \backslash I_{k-1} = \{i_k\}$. Then for the operator L_k^* in $\Delta_k^{(I_k)}$, we have

$$L_k^* = L_{k-1}^* + p^{i_k}\left(\sum_{i_j \in I_k\backslash\{0\}} (\delta_{i_k}^{i_j} - p^{i_j})\frac{\partial}{\partial p^{i_j}}\frac{\partial}{\partial p^{i_k}}\right) \tag{6.3}$$

with L_{k-1}^* being the restriction of L_k^* to $\Delta_{k-1}^{(I_{k-1})}$.

We take some $p \in \Delta_{k-1}^{(I_{k-1})}$ and choose a sequence $(p_l)_{l\in\mathbb{N}}$ in $\Delta_k^{(I_k)}$ with $p_l \to p$ and apply this operator to U at $p_l \in \Delta_k^{(I_k)}$. The resulting expression inside the bracket is

controlled by $p_l^{i_k} \to 0$ while approaching p. Since the derivatives of U are bounded in the interior on a closed neighbourhood of p because of the regularity of U, the expression is continuous up to p. Likewise, all derivatives of U within $\Delta_{k-1}^{(I_{k-1})}$ are continuously matched by the corresponding ones in $\Delta_k^{(I_k)}$, thus $L_{k-1}^*(U(p_l))$ is also continuous up to the boundary in p (as the corresponding coefficients are, too). Hence, the whole expression is continuous up to the boundary in p with $L_{k-1}^* U(p) \equiv L_k^* U(p) = 0$, and since p was arbitrary, this applies to all of $\Delta_{k-1}^{(I_{k-1})}$. □

Assuming the stated pathwise regularity, this confines the boundary values of U resp. f on $\partial\Delta_n = \bigcup_{k=0}^{n-1} \partial_k \Delta_n$ and consequently, equation (6.1) is rather restated as an *extended homogeneous* or *extended stationary Kolmogorov backward equation*[7]

$$\begin{cases} L^* U(p) = 0 & \text{in } \overline{\Delta}_n \backslash \partial_0 \Delta_n \\ U(p) = f(p) & \text{in } \partial_0 \Delta_n \end{cases} \tag{6.4}$$

for $U \in C_p^2(\overline{\Delta}_n)$ with the only 'free' boundary values remaining the ones at the vertices $\partial_0 \Delta_n$. If we also assume global continuity of the solution, the values on $\partial_0 \Delta_n$, however, suffice as boundary information determining a solution uniquely. In such a case, a stationary solution and the stationary component of a global extension as in the preceding section also coincide:

Proposition 6.2. *A solution $U \in C_p^\infty(\overline{\Delta}_n) \cap C^0(\overline{\Delta}_n)$ of the extended stationary Kolmogorov backward equation (6.4) for some boundary condition $f_0 \colon \partial_0 \Delta_n \longrightarrow \mathbb{R}$ is uniquely defined and coincides with (the projection of) a solution of the extended Kolmogorov backward equation (1.9) in $(\overline{\Delta}_n)_{-\infty}$ to $\overline{\Delta}_n$ for a final condition $f \in \mathcal{L}^2(\bigcup_{d=0}^n \partial_d \Delta_n)$ with $f \equiv f_0 \chi_{\partial_0 \Delta_n}$ as in theorem 3.3. Furthermore, the space of solutions is spanned by $p^1, \ldots, p^n$ and 1.*

Proof. The first assertion may be shown by an iterative application of the maximum principle: On every face $\Delta_k^{(I_k)} \subset \partial_k \Delta_n$ for all $1 \le k \le n$, the operator L^* is locally uniformly elliptic, and hence, $U|_{\Delta_k^{(I_k)}}$ is uniquely defined by its values on $\partial \Delta_k^{(I_k)}$ by virtue of the maximum principle. Applying this consideration iteratively for $\partial_0 \Delta_n, \ldots, \partial_n \Delta_n = \Delta_n$ yields the desired global uniqueness.

Next, we will show that a final condition $f = \chi_{\Delta_0^{(\{i_0\})}}$ for some $i_0 \in I_n$ gives rise to an extended solution $\overline{U}(p,t) = \overline{U}(p) = p^{i_0}$ in $(\overline{\Delta}_n)_{-\infty}$ resp. $\overline{\Delta}_n$ proving the second assertion. With f as described, the extended solution (cf. theorem 3.3) is solely given by $\overline{U} \equiv \overline{U}_{i_0}$, i.e.

$$\begin{aligned} \overline{U}_{\{i_0\}}(p,t) = {} & u_{\{i_0\}}(p,t) \chi_{\Delta_0^{(\{i_0\})}}(p) \\ & + \sum_{1 \le d \le n} \sum_{i_1 \in I_n \backslash \{i_0\}} \cdots \sum_{i_d \in I_n \backslash \{i_0, \ldots, i_{d-1}\}} U_{\{i_0\}}^{i_0, \ldots, i_d}(p,t) \chi_{\Delta_d^{(\{i_0, \ldots, i_d\})}}(p) \end{aligned} \tag{6.5}$$

[7] As already stated, it does not matter whether $\partial_0 \Delta_n$ is added to the domain of definition of the differential equation or not. Although $\partial_0 \Delta_n$ has been included in equation (6.2), we omit this here for formal consistency.

(cf. equation (8.8) in [19]). Considering an arbitrary $\Delta_d^{(I_d)} \subset \overline{\Delta}_n$, $I_d \subset I_n$, we obtain for the restriction of $\overline{U}_{i_0}$ to $\Delta_d^{(I_d)}$ using equation (3.3)

$$\begin{aligned}\overline{U}_{\{i_0\}}(p,t)|_{\Delta_d^{(I_d)}} &= \sum_{i_1 \in I_d \setminus \{i_0\}} \cdots \sum_{\substack{i_d \in \\ I_d \setminus \{i_0,\ldots,i_{d-1}\}}} U_{\{i_0\}}^{i_0,\ldots,i_d}(p,t) \\ &= \sum_{i_1 \in I_d \setminus \{i_0\}} \cdots \sum_{\substack{i_d \in \\ I_d \setminus \{i_0,\ldots,i_{d-1}\}}} u_{\{i_0\}}(\pi^{i_0,\ldots,i_d}(p),t) \prod_{j=0}^{d-1} \frac{p^{i_j}}{\sum_{l=j}^d p^{i_l}} \end{aligned} \tag{6.6}$$

with $u_{\{i_0\}}(\pi^{i_0,\ldots,i_d}(p),t) \equiv 1$ as $\pi^{i_0,\ldots,i_d}(p) \in \Delta_0^{(\{i_0\})}$ for all $p \in \Delta_d^{(I_d)}$ and $u_{\{i_0\}} = f = 1$ in $\left(\Delta_0^{(\{i_0\})}\right)_{-\infty}$ by assumption. Since we have $\sum_{l=0}^d p^{i_l} = 1$ in $\Delta_d^{(I_d)}$, we may replace the expression $\sum_{l=j}^d p^{i_l}$ by $1 - \sum_{l=0}^{j-1} p^{i_l}$ and rearrange the sum (by also suppressing the last sum as the index i_d does no longer occur), which yields altogether

$$\begin{aligned}&\overline{U}_{\{i_0\}}(p,t)|_{\Delta_d^{(I_d)}} \\ &= p^{i_0}\left(\sum_{\substack{i_1 \in \\ I_d \setminus \{i_0\}}} \frac{p^{i_1}}{1-p^{i_0}} \cdots \left(\sum_{\substack{i_j \in \\ I_d \setminus \{i_0,\ldots,i_{j-1}\}}} \frac{p^{i_j}}{1-\sum_{l=0}^{j-1} p^{i_l}} \cdots \left(\sum_{\substack{i_{d-1} \in \\ I_d \setminus \{i_0,\ldots,i_{d-2}\}}} \frac{p^{i_{d-1}}}{1-\sum_{l=0}^{d-2} p^{i_l}}\right)\right)\right).\end{aligned} \tag{6.7}$$

As we have $\frac{p^{i_j}+\ldots+p^{i_d}}{1-\sum_{l=0}^{j-1} p^{i_l}} = 1$ for $j = d-1,\ldots,1$, the whole expression reduces to $\overline{U}_{\{i_0\}}(p,t)|_{\Delta_d^{(I_d)}} = p^{i_0}$. Since $\Delta_d^{(I_d)}$ was arbitrary, we obtain $\overline{U}_{\{i_0\}}(p,t) \equiv \overline{U}_{\{i_0\}}(p) = p^{i_0}$ in the entire $\overline{\Delta}_n$. □

In terms of the probabilistic interpretation, the extended setting (6.4) also matches the considerations of Section 3 as equation (6.4) may be viewed as the limit equation for $t \to -\infty$ of the extended Kolmogorov backward equation (1.9) (which may be shown as previously). This is also reflected in proposition 6.2: For $t \to -\infty$ and any solution, the only target sets that remain attractors for all time are of course the vertices (which correspond to configurations of the model where all but one allele are extinct), and hence the stationary solutions match the stationary components of the global extensions as in Theorem 3.3, which in turn result from a non-vanishing final condition in $\partial_0\Delta_n$. Then, every $\Delta_0^{(\{i\})} \subset \partial_0\Delta_n$ may give rise to a solution (component) p^i – in particular yielding a positive target hit probability on the entire Δ_n for all times. However, even the stationary component of solutions as in Theorem 3.3 may in principle be perceived as time-dependent and also describing the transitional attraction of target sets in the entire $\overline{\Delta}_n$ induced by a given ultimate target set in $\partial_0\Delta_n$.

Altogether, Proposition 6.2 under the given restrictions thus already yields a full description of the stationary model in the entire $\overline{\Delta}_n$. However, dropping the global continuity assumption, a much wider class of (stationary) solutions, i.e. iteratively extended solutions of the Kolmogorov backward equation obeying the extension constraints 3.1, may be obtained as described in the preceding section. To establish the uniqueness also for this bigger class, we may apply the blow-up scheme of Section 5 and demonstrate the uniqueness of solutions of the

correspondingly transformed stationary Kolmogorov backward equation on the cube (which is basically analogous to the simplex, cf. the preceding considerations). The eventual result will be obtained by applying the uniqueness result for the cube to the transformed iteratively extended solutions (assuming sufficient regularity if necessary). Again, this is limited to the stationary components.

7. The uniqueness of solutions of the stationary Kolmogorov backward equation

The main application of the blow-up scheme is the uniqueness proof for the iteratively extended solutions of the Kolmogorov backward equation that satisfy the extension constraints 3.1. In the present paper, this is limited to the stationary components. First, we will discuss the uniqueness of solutions of the correspondingly transformed stationary Kolmogorov backward equation on the cube (which is basically analogous to the simplex, cf. section 10 in [19]). After that, the main result will be stated by applying the uniqueness result for the cube to the transformed iteratively extended solutions (assuming sufficient regularity if necessary).

Regarding the uniqueness of stationary solutions on the cube with the transformed Kolmogorov backward operator given by equation (5.54), we have the cube version of the simplex result of Lemma 10.1 in [19]:

Lemma 7.1 (stem Lemma, cube version). *For a solution $u \in C^\infty(\square_n)$ of the stationary Kolmogorov backward equation $\widetilde{L}_n^* u = 0$ in $\square_n$ with*

$$\widetilde{L}_n^* := \frac{1}{2}\sum_{i=1}^{n} \frac{\tilde{p}^i(1-\tilde{p}^i)}{\prod_{j=1}^{i-1}\tilde{p}^j}\frac{\partial^2}{(\partial\tilde{p}^i)^2} \tag{7.1}$$

and with extension $U \in C_p^\infty(\overline{\square}_n)$, we have

$$\widetilde{L}^* U = 0 \quad \text{in } \overline{\square}_n, \tag{7.2}$$

i.e.

$$\widetilde{L}_d^* U = 0 \quad \text{with} \quad \widetilde{L}_d^* := \frac{1}{2}\sum_{\substack{i=\hat{\imath}(d)+1\\ i\neq i_m}}^{n} \frac{\tilde{p}^i(1-\tilde{p}^i)}{\prod\limits_{\substack{j=\hat{\imath}(d)+1\\ j\neq i_m}}^{i-1}\tilde{p}^j}\frac{\partial^2}{(\partial\tilde{p}^i)^2} \tag{7.3}$$

in $\square_d = \left\{\tilde{p}^{i_1} = b_{i_1}, \ldots, \tilde{p}^{i_{n-d}} = b_{i_{n-d}}\right\} \subset \partial_d\square_n$ for all $1 \le d \le n-1$ and all $i_1, \ldots, i_{n-d} \in \{1, \ldots, n\}$, $i_k \neq i_l$ for $k \neq l$ with $\hat{\imath} = \hat{\imath}(d) := \underset{i_1,\ldots,i_{n-d}}{\arg\max}\{b_{i_m} = 0\}$ resp. $\hat{\imath}(d) := 0$ if $b_{i_m} = 1$ for all i_m.

Proof. The statement is proven iteratively: Assuming that equation (7.3) holds in some (arbitrary) domain $\square_{d+1} \subset \partial_{d+1}\square_n$, we show that a corresponding formula also holds for any $\square_d \subset \partial_d\square_{d+1} \subset \partial_d\square_n$. A repeated application of the argument then yields the assertion.

Let $\square_{d+1} = \left\{\tilde{p}^{i_1} = b_1, \ldots, \tilde{p}^{i_{n-d-1}} = b_{n-d-1}\right\}$ and $\square_d = \left\{\tilde{p}^{i_1} = b_1, \ldots, \tilde{p}^{i_{n-d}} = b_{n-d}\right\}$ with $i_{n-d} \neq i_1, \ldots, i_{n-d-1}$ and $b_{n-d} \in \{0, 1\}$. If we have $i_{n-d} < \hat{\imath}(d+1)$, then as

$\tilde{p}^{i_{n-d}} \to 0$ resp. $\tilde{p}^{i_{n-d}} \to 1$, the value of the operator in equation (7.3) applied to U – with the occurring derivatives and the coefficients being continuous – depends continuously on $\tilde{p}$ up to the boundary. Thus equation (7.3), which already has the corresponding form for $\square_d$ (note $\hat{\imath}(d) \equiv \hat{\imath}(d+1)$), also holds on $\square_d$.

If we rather have $i_{n-d} > \hat{\imath}(d+1)$ and $b_{n-d} = 1$, then, when choosing some $\tilde{p} \in \square_d$ and a sequence $(\tilde{p}_l)_{l\in\mathbb{N}}$ in $\square_{d+1}$ with $\tilde{p}_l \to \tilde{p}$, the expression

$$\frac{1}{2}\frac{\tilde{p}_l^{i_{n-d}}(1-\tilde{p}_l^{i_{n-d}})}{\prod_{\substack{j=\hat{\imath}(d)+1\\ j\neq i_m}}^{i_{n-d}-1}\tilde{p}_l^j}\frac{\partial^2}{(\partial\tilde{p}_l^{i_{n-d}})^2}U(\tilde{p}_l) \tag{7.4}$$

is controlled by $(1-\tilde{p}_l^{i_{n-d}})$ while approaching $\tilde{p}$ and – with the derivatives of U being bounded on a closed neighbourhood of $\tilde{p}$ because of the regularity of U – is continuous up to $\tilde{p}$. Analogous to the previous case, all other summands of the operator in equation (7.3) are also continuous on the boundary, thus proving that the corresponding form of equation (7.3) (with the i_{n-d}-th summand deleted) holds in $\square_d$ (again $\hat{\imath}(d) \equiv \hat{\imath}(d+1)$).

If instead $i_{n-d} > \hat{\imath}(d+1)$ and $b_{n-d} = 0$, then we may multiply the whole equation (7.3) by $\tilde{p}^{i_{n-d}}$. If now $\tilde{p}^{i_{n-d}} \to 0$, then by a similar argument as above all derivatives of the operator that do not contain $\tilde{p}^{i_{n-d}}$ in the denominator of their coefficient continuously vanish, whereas the values of all other summands are also continuous up to the boundary. Thus, equation (7.3) holds on $\square_d$ with the index $\hat{\imath}(d+1)$ replaced by $\hat{\imath}(d) = i_{n-d}$. □

The obtained equation (7.2) may again be perceived as an extended version of the stationary Kolmogorov backward equation on the cube (cf. also equation (6.4), although the domains do not fully correspond), and we have (cf. Proposition 10.2 in [19]):

Proposition 7.2. *A solution $U \in C_p^\infty(\overline{\square}_n) \cap C^0(\overline{\square}_n)$ of the extended stationary Kolmogorov backward equation*

$$\widetilde{L}^* U = 0 \quad \text{in } \overline{\square}_n \tag{7.5}$$

with $\widetilde{L}^*$ as in equation (7.3) is uniquely determined by its values on $\partial_0\square_n$.

Proof. The uniqueness may be shown by a successive application of the maximum principle for strata of increasing dimension, starting from $\partial_0\square_n$. We shall first show that in every instance of the domain $\square_d \subset \partial_d\square_n$ for all $1 \le d \le n$, the solution $U|_{\square_d}$ is uniquely defined by its values on $\partial\square_d$: If equation (7.3) on $\square_d$ comprises d derivative terms, it is straightforward to see that the operator is locally uniformly elliptic on $\square_d$, hence satisfies the assumptions of Hopf's maximum principle. Since the solution is of class C^0 on $\overline{\square}_d$, this yields the desired uniqueness. If, in contrast, $\square_d$ is such that the operator on $\square_d$ comprises only $d' < d$ derivative terms, we first show the uniqueness on each d'-dimensional fibre of $\square_d$ (with corresponding boundary part), which follows from an analogous consideration: Clearly, on each fibre the operator is locally uniformly elliptic and the solution is continuous up to the respective boundary, thus the uniqueness likewise follows from Hopf's maximum principle. By assembling, the desired uniqueness is then obtain for the entire $\square_d$. Applying these considerations successively for $\partial_0\square_n, \ldots, \partial_n\square_n = \square_n$ yields the desired global uniqueness. □

With the blow-up scheme at hand, the preceding uniqueness result may also be conveyed to the simplex $\overline{\Delta}_n$, assuming some additional regularity for the transformation image (which still does not imply an analogous regularity for the pre-image). We finally arrive at:

Theorem 7.3. *Let $n \in \mathbb{N}_+$, $I_d := \{i_0, i_1, \dots, i_d\} \subset \{0, 1, \dots, n\}$ for $d = 0, \dots, n$ with $i_i \neq i_j$ for $i \neq j$ and $u_{\{i_0\}} \colon \Delta_0^{(\{i_0\})} \longrightarrow \mathbb{R}$ be given. Then an extension $\overline{U}_{\{i_0\}}^{i_0,\dots,i_n} \colon \bigcup_{0\le d\le n} \Delta_d^{(I_d)} \longrightarrow \mathbb{R}$ as in Proposition 3.2 is unique within the class of extensions U which satisfy the extension constraints 3.1, i.e.*

(i) *are of class $C_{p0}^\infty\big(\bigcup_{0\le d\le n} \Delta_d^{(I_d)}\big)$ with $U|_{\Delta_0^{(\{i_0\})}} = u_{\{i_0\}}$ and*

(ii) *solve the stationary Kolmogorov backward equation(6.4) in $\bigcup_{0\le d\le n} \Delta_d^{(I_d)}$,*

as well as, in case $n \ge 2$, whose

(iii) *transformation image $\widetilde{U} \colon \bigcup_{d=0}^n \square_d^{(I'_d)} \longrightarrow \mathbb{R}$ by a successive blow-up transformation $\Phi_{s_{n-1}}^{r_{n-1}} \circ \dots \circ \Phi_{s_1}^{r_1}$ as in Proposition 5.4 has an extension to the entire boundary $\partial\square_n^{(I'_n)}$ which is of class $C_p^\infty\big(\overline{\square_n^{(I'_n)}}\big) \cap C^0\big(\overline{\square_n^{(I'_n)}}\big)$.*

Consequently, also the global extension $\overline{U}_{\{i_0\}}$ as in Proposition 8.4 in [19] or in Theorem 3.3 is unique.

Proof. The assertion for the trivial case $n = 1$ directly follows, as $\overline{U}_{\{i_0\}}^{i_0,i_1}$ is already sufficiently regular in $\overline{\Delta_1^{(I_1)}} \equiv \overline{\square_1^{(I'_1)}}$ for an application of the maximum principle: In particular, it is globally continuous, and along with the locally uniform ellipticity of the Kolmogorov backward operator, the uniqueness follows. For $n \ge 2$, any function U which is a solution of the stationary Kolmogorov backward equation (6.4) in $\overline{\Delta_n^{(I_n)}}$ by a full blow-up transformation of the domain transforms into a function $\widetilde{U}$, which solves the stationary Kolmogorov backward equation (5.44) in $\bigcup_{d=0}^n \square_d^{(I'_d)}$ (cf. Proposition 5.4 resp. Corollary 5.9 and Lemma 5.10). Furthermore, with the assumed regularity after a full blow-up, it has an extension to $\overline{\square_n^{(I'_n)}}$ which is pathwise smooth as well as globally continuous and by Lemma 7.1 solves the stationary Kolmogorov backward equation $\widetilde{L}^*\widetilde{U} = 0$ in $\overline{\square_n^{(I'_n)}}$ with $\widetilde{L}^*$ as in equation (7.3). Hence, the uniqueness result of Proposition 7.2 applies and proves the uniqueness of the transformed function (and, in view of the injectivity of the blow-up, also the uniqueness of U) – for specified boundary data on the entire $\partial_0\square_n^{(I'_n)}$. Thus, we only need to show that these boundary data are uniquely determined by the assumptions made.

This is straightforward: In accordance with Lemma 5.10, $\widetilde{U}$ or its corresponding continuous extension vanishes on $\{\tilde{p}^{i_j} = 1\} \subset \partial\square_n^{(I'_n)}$, $j = 1, \dots, n$. As by assumption (iii) the continuous extendability applies to the entire $\overline{\square_n^{(I'_n)}}$, $\widetilde{U}$ resp. its extension even vanishes on

$$\overline{\{\tilde{p}^{i_1} = 1\}}, \dots, \overline{\{\tilde{p}^{i_n} = 1\}}. \tag{7.6}$$

In particular, this means that $\widetilde{U}$ or its extension vanishes on any vertex $\square_0 \subset \partial_0\square_n^{(I'_n)}$ – which may always be written as

$$\square_0 = \big\{\tilde{p}^{i_j} = b_j \quad \text{for } j = 1, \dots, n\big\} \quad \text{with } b_j \in \{0, 1\}- \tag{7.7}$$

except for the vertex $\square_0^{(\varnothing)} = \{(0, \dots, 0)\}$, where it attains the value $u_{\{i_0\}}$ as stated previously. Thus, the (transformed) boundary data given on all vertices are the same for any extension in question, and since $\overline{U}_{\{i_0\}}^{i_0,\dots,i_n} : \bigcup_{0\le d\le n} \Delta_d^{(I_d)} \longrightarrow \mathbb{R}$ as in Proposition 3.2 satisfies the extension constraints and has an extension to the entire boundary $\partial\square_n^{(I'_n)}$ which is in $C_p^\infty(\overline{\square_n^{(I'_n)}}) \cap C^0\big(\overline{\square_n^{(I'_n)}}\big)$ (this may be seen directly from equation (5.49)), it also is the unique extension. $\square$

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