References

These notes are drawn from the following source:

- Karl Oelschläger, On the Derivation of Reaction-Diffusion Equations as Limit Dynamics of Systems of Moderately Interacting Stochastic Processes. Probability Theory & Related Fields (1989). 82. pg. 565-586.

On the Derivation of Reaction-Diffusion Equations as Limit Dynamics of Systems of Moderately Interacting Stochastic Processes **by Karl Oelschläger (1989)**

Notation & Set-Up

Group Meeting
November 2015

Set-up:

- System of $\approx N \in \mathbb{N}$ particles interacting in $\mathbb{R}^d$
- $K =$ number of different types of particles (different subpopulations in the total population)
- Particles interact by movement, birth, death, and transitions between subpopulations
- Particles are numbered $1, 2, ...$
- Newly-born particles are given new numbers
- The dynamics of each particle depend on the density of particles in its surrounding neighborhood

Notation + Equations:

- $M(N, r, t) =$ set of all particles living in subpopulation r at time t
- $M(N, t) =$ set of all particles living in the total population at time t
- $P_N^k(t) =$ position $\in \mathbb{R}^d$ of the kth particle at time t (here $k \in M(N, r, t)$)
- $S_{N,r}(t) = \frac{1}{N}\sum_{k\in M(N,r,t)} \delta_{P_N^k(t)}$ (measure-valued empirical process)
- $S_N(t) = \frac{1}{N}\sum_{k\in M(N,t)} \delta_{P_N^k(t)}$ (measure-valued empirical process)
- $s_{N,r}(x, t) = (S_{N,r}(t) * V_N)(x)$ (represents density of subpopulation r near position x at time t,)
- $\hat{s}_{N,r}(x, t) = (S_{N,r}(t) * \hat{V}_N)(x)$ (introduced for technical reasons, different scaling in N than for $s_{N,r}$)
- $dP_N^k(t) = F_{N,r}(P_N^k(t), t)dt + \sigma_r dW_k(t)$ (SDE for particle movement)
- $F_{N,r}(x, t) = G_{N,r}(x, t) - \sum_{q=1}^{K} D_{N,qr}(x, t)\nabla s_{N,q}(x, t)$

Scaling:

- $V_N(x) = \alpha_N^d V_1(\alpha_N x)$ (note that V_1 is fixed and sufficiently smooth)
- $\alpha_N = N^{\beta/d}$
- $0 < \beta < \frac{d}{d+2}$
- $\hat{V}_N(x) = \hat{\alpha}_N^d V_1(\hat{\alpha}_N x)$
- $\hat{\alpha}_N = N^{\hat{\beta}/d}$
- $0 < \hat{\beta} < \frac{\beta}{d+2}$
- As $N \to \infty$, the space element selected by V_N is macroscopically small but microscopically large.

Derivation of RD equations as the limit of moderately-interacting many-particle systems: Presentation of Oelschläger (1989)

$\boxed{\text{Outline}}$

1. N-particle system
   - 1a density, set-up, scalings in N
   - 1b particle movement
   - 1c particle birth, death, and transitions
2. Ito's formula to express the impact of movement, birth, death, and transitions on the population structure
3. Heuristic argument for RD system as $N \to \infty$
4. Assuptions & theorem statements
5. Extensions

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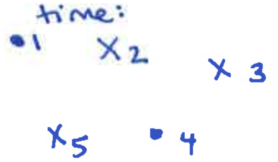
1 N-particle system

1a Set-up:

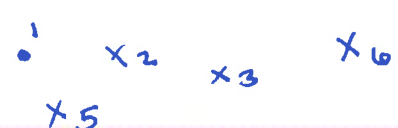
- Consider a system of $\approx N \in \mathbb{N}$ particles interacting in $\mathbb{R}^d$
- Particles can be of K different types (belong to K different subpopulations)
- Particles interact by movement, birth, death, and transitions between subpopulations
- Number particles as 1, 2, ...
- When a new particle is born, give it a new number

Example: If x's = subpopulation 1 and •'s = subpopulation 2, we could have

Initial time:



Later time: (after birth of new x, death of particle 4)



Define:

- $M(N,r,t)$ = set of all particles living in subpopulation r at time t
  (in our example, $M(5,1,0) = \{2,3,5\}$)

- $M(N,t) = \bigcup_{r=1}^{K} M(N,r,t)$
  = set of all living particles at time t
  (in our example, $M(5,t) = \{1,2,3,5,6\}$)

- $P_N^k(t)$ = position $\in \mathbb{R}^d$ of the kth particle at time t
  (here $k \in M(N,t)$)

Because no distinction between specific particles is needed when we talk about the full population or a specific subpopulation, Oelschläger introduces 2 measure-valued empirical processes, namely:

$$t \to S_{N,r}(t) = \frac{1}{N} \sum_{k \in M(N,r,t)} \delta_{P_N^k(t)} \qquad r = 1, \dots, K$$

(Dirac measures mark the positions of the living particles in subpopulation r at time t)

$$t \to S_N(t) = \frac{1}{N} \sum_{k \in M(N,t)} \delta_{P_N^k(t)}$$

$$= \sum_{r=1}^{K} S_{N,r}(t)$$

(Dirac measures mark the positions of all living particles at time t)

Density & Scalings in N:

Oelschläger assumes that the dynamics of each particle (birth, death, transitions, and movement) depend on the particles in its neighborhood.

Mathematically, he represents this assumption by smoothing out the empirical process $S_{N,r}(t)$ as:

$$s_{N,r}(x,t) = \left(S_{N,r}(t) * V_N \right)(x)$$

probability density function that smooths out $S_{N,r}$ in a neighborhood

convolution

represents density of subpopulation r near position x at time t

measure-valued empirical process marking positions of living particles in subpopulation r at time t

Here V_N is given by:

$$V_N(x) = \alpha_N^d \, V_1(\alpha_N x)$$

$$\alpha_N = N^{\beta/d}$$

- V_1 is a fixed, sufficiently smooth function

- β is a fixed scaling exponent satisfying $0 < \beta < \frac{d}{d+2}$

Aside: for example, if we are in $\mathbb{R}^2$, we would have

$$0 < \beta < \frac{1}{2},$$

$$\alpha_N = N^{\beta/2},$$

and

$$V_N(x) = N^{\beta} V_1(N^{\beta/2} x)$$

For technical reasons, Oelschläger introduces a second version of $s_{N,r}$ with a slightly different scaling:

$$\hat{s}_{N,r}(x,t) = \left(S_{N,r}(t) * \hat{V}_N \right)(x)$$

$$\hat{V}_N(x) = \hat{\alpha}_N^d \, V_1(\hat{\alpha}_N x)$$

$$\hat{\alpha}_N = N^{\hat{\beta}/d}$$

$$0 < \hat{\beta} < \frac{\beta}{d+1}$$

(Two forms of $s_{N,r}$ are needed to handle density-dependent cross-diffusion terms in the particle movement equations.)

Illustrative Example:

As an illustrative example (that does not satisfy the smoothness assumptions on V_1 stated earlier), Oelschläger considers

$$V_1(x) = \mathbb{1}_{B(1,0)}(x)$$

= indicator function of a ball with volume 1 and center 0

Then
$$V_N(x) = \alpha_N^d V_1(\alpha_N x)$$
$$= \alpha_N^d \mathbb{1}_{B(1,0)}(\alpha_N x)$$
$$= \alpha_N^d \mathbb{1}_{B(\alpha_N^{-d},0)}(x)$$

and

$$s_{N,r}(x,t) = (S_{N,r}(t) * V_N)(x)$$
$$= \int_{\mathbb{R}^d} \frac{1}{N} \sum_{k\in M(N,r,t)} \delta_{p_N^k(t)}(y)\, V_N(x-y)\, dy$$

$= \frac{1}{N}\alpha_N^d \times$ # of particles of subpopulation r in the ball $B(\alpha_N^{-d}, x)$ at time t

$$= \frac{\#\text{ of particles of } M(N,r,t) \text{ in } B(\alpha_N^{-d}, x)}{N\alpha_N^{-d}}$$

$$= \frac{\#\text{ of particles of } M(N,r,t) \text{ in } B(\alpha_N^{-d}, x)}{\text{Volume of } B(\alpha_N^{-d}, x)} \times \frac{1}{\text{size of total population}}$$

Note on "Moderate scaling": The space element $\Delta x = B(\alpha_N^{-d}, x)$ is macroscopically small, since its volume, $\alpha_N^{-d} = N^{-\beta}$, $\to 0$ as $N \to \infty$, but microscopically large, since the total # of particles in $B(\alpha_N^{-d}, x)$ is $O(N \times \text{volume } B(\alpha_d^{-N}, x)) = O(N \alpha_d^{-N}) = O(N^{1-\beta})$, which $\to \infty$ as $N \to \infty$ (assuming the particles are distributed reasonably evenly).

Remark: $S_{N,r}(x,t)$ is related to the concept of a "one-particle distribution function" in stat physics.

(1b) N-particle system: particle Migration

An SDE describes the motion of each particle:

$$dP_N^k(t) = F_{N,r}(P_N^k(t), t)\, dt + \sigma_r\, dW^k(t)$$

for $k \in M(N,r,t)$. Here $W^k(\cdot)$ = independent $\mathbb{R}^d$-valued standard Brownian motions.

Furthermore,

σ_r = a fixed matrix for each subpopulation r

$F_{N,r}(x,t)$ = $\mathbb{R}^d$-valued functions $(r = 1, \ldots, K)$ dependent on position x and the subpopulation densities $S_{N,q}(x,t)$, $\hat{S}_{N,q}(x,t)$ for $q = 1, \ldots, K$ at that position (so the time dependence is only through these densities)

The function $F_{N,r}(x,t)$ is broken into 2 terms, namely

$$F_{N,r}(x,t) = \underbrace{G_{N,r}(x,t)}_{\substack{\mathbb{R}^d\text{-valued,}\\ \text{represents local}\\ \text{contributions at}\\ (x,t)}} - \underbrace{\sum_{q=1}^{K}}_{\substack{\text{sum across}\\ \text{all subpopulations}}} \underbrace{D_{N,qr}(x,t)}_{\substack{\mathbb{R}^d \otimes \mathbb{R}^d\\ \text{valued}}} \underbrace{\nabla s_{N,q}(x,t)}_{\substack{\text{gradient of the}\\ \text{density of}\\ \text{subpopulation } q\\ \text{at } x}}$$

The functions $G_{N,r}$ & $D_{N,qr}$ depend on the densities at position x and time t as:

$$G_{N,r}(x,t) = \breve{G}_r\left(x, \hat{s}_1(x,t), \dots, \hat{s}_K(x,t)\right)$$

$$D_{N,qr}(x,t) = \breve{D}_{qr}\left(x, \hat{s}_1(x,t), \dots, \hat{s}_K(x,t)\right)$$

Remark: Oelschläger notes that the 2nd term in $F_{N,r}$ should be mainly repulsive to ensure the system does not collapse due to too strong of attraction.

(1c) Birth, death, and subpopulation transitions

An individual $k \in M(N,r,t)$ located at $y = P_N^k(t)$ can alter the population structure discontinuously in 3 different ways:

Transition: particle k can leave $M(N,r,t)$ and join $M(N,q,t)$ $q \neq r$ with intensity $t_{N,rq}(y,t)$

Birth: particle k can give birth to a new individual $k^* \in M(N,q,t)$ at position y with intensity $b_{N,rq}(y,t)$

Death: particle k can die with intensity $d_{N,r}(y,t)$

Aside: The intensity is like a rate — in particular,
$Pr\left(N(x, x+h] > 0 \right) = \lambda h + o(h)$.
The intuition is $dX = \lambda dt$

Just like the movement functions, Oelschläger assumes these intensities depend on the local particle configurations as:

$$t_{N,qr}(x,t) = \breve{t}_{qr}\left(x, \hat{s}_{N,1}(x,t), \ldots, \hat{s}_{N,K}(x,t)\right)$$

$$b_{N,qr}(x,t) = \breve{b}_{qr}\left(x, \hat{s}_{N,1}(x,t), \ldots, \hat{s}_{N,K}(x,t)\right)$$

$$d_{N,qr}(x,t) = \breve{d}_{qr}\left(x, \hat{s}_{N,1}(x,t), \ldots, \hat{s}_{N,K}(x,t)\right)$$

where $\breve{t}_{rr}(\ldots) = 0$ for $r = 1, \ldots, K$, so particles do not swap from their subpopulation into the same subpopulation.

To obtain a condensed form of the impact of birth, death, and transitions, Oelschläger introduces 3 point processes:

you can't jump from r to q if you are not already in r.

intensity to jump from r to q

$$t^{*,k}_{N,rq}(u) = \underbrace{\beta^{c,k}_{N,rq}\left(\int_0^u \mathbb{1}_{M(N,r,s)}^{(k)} t_{N,rq}\left(P^k_N(s), s\right) ds \right)}$$

u is a time with $0 \leq u < \infty$

Poisson process – think of $N(t, \lambda)$, only now λ, our rate parameter or intensity, is time-dependent, so we have a non-homogeneous Poisson process and the expected # of events in $[0, u]$ is

$$\int_0^u \mathbb{1}_{M(N,r,s)}^{(k)} t_{N,rq}\left(P^k_N(s), s\right) ds$$
$$= \int_0^u \lambda(s)\, ds$$

$\Longrightarrow$ The point process $t^{*,k}_{N,rq}(u)$ has intensity $\mathbb{1}_{M(N,r,u)}^{(k)} t_{N,rq}\left(P^k_N(u), u\right)$ for a jump of size $+1$ at time u.

Similarly, Oelschläger introduces the point processes

$$b^{*,k}_{N,rq}(u) = \beta^{b,k}_{N,rq}\left(\int_0^u \underbrace{\mathbb{1}_{M(N,r,s)}(k)\, b_{N,rq}(P^k_N(s),s)}\, ds \right)$$

$\Rightarrow$ $b^{*,k}_{N,rq}(u)$ has this intensity with $s=u$

and

$$d^{*,k}_{N,r}(u) = \beta^{d,k}_{N,r}\left(\int_0^u \underbrace{\mathbb{1}_{M(N,r,s)}(k)\, d_{N,r}(P^k_N(s),s)}\, ds \right)$$

$\Rightarrow$ $d^{*,k}_{N,r}(u)$ has this intensity with $s=u$

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(2) <u>Ito's formula to collect all changes to population structure: movement, birth, death, & transitions</u>

<u>Aside on Ito's formula:</u>

The intuition behind Ito's formula is Taylor expansion.

Consider an SDE

$$dX(\omega,t) = \mu(\omega,t)\,dt + \sigma\, dW_t$$

Then given a function $f(\omega,t)$, we can Taylor expand as:

$$df = \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial x} dx + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}(dx)^2 + \ldots$$

Substituting $X(\omega,t)$ for x and $dX(\omega,t) = \mu(\omega,t)\,dt + \sigma\, dW_t$ for dx, we obtain:

$$\begin{aligned}
df &= \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial X} dX + \frac{1}{2}\frac{\partial^2 f}{\partial X^2}(dX)^2 + \ldots \\
&= \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial x}\left(\mu(\omega,t)\,dt + \sigma\, dW_t\right) + \frac{1}{2}\frac{\partial^2 f}{\partial X^2}\left(\mu(\omega,t)\,dt + \sigma\, dW_t\right)^2 + \ldots \\
&= \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial x}\mu(\omega,t)\,dt + \sigma\frac{\partial f}{\partial x} dW_t + \frac{1}{2}\frac{\partial^2 f}{\partial X^2}\left(\mu(\omega,t)\,dt\right)^2 \\
&\quad + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}(\sigma\, dW_t)^2 + \frac{\partial^2 f}{\partial x^2}\mu(\omega,t)\sigma\, dt\, dW_t + \ldots
\end{aligned}$$

Keeping terms of $O(dt)$ and noting that $(dW_t)^2 = O(dt)$, we obtain:

$$df = \frac{\partial f}{\partial t} dt + \mu(\omega,t) \frac{\partial f}{\partial x} dt + \frac{1}{2}\sigma^2 \frac{\partial^2 f}{\partial x^2} dt + \sigma \frac{\partial f}{\partial x} dW_t$$

$$+ \text{ higher order terms}$$

In integral form, this is written as

$$f(X(\omega,t),t) = \overset{①}{f(X(\omega,0),0)} + \overset{②}{\int_0^t \frac{\partial f}{\partial t}(X(\omega,s),s)\,ds}$$

$$+ \int_0^t \mu(\omega,s) \frac{\partial f}{\partial x}(X(\omega,s),s)\,ds \qquad ③$$

$$+ \int_0^t \frac{1}{2}\sigma^2 \frac{\partial^2 f}{\partial x^2}(X(\omega,s),s)\,ds \qquad ④$$

$$+ \int_0^t \frac{\partial f}{\partial x}(X(\omega,s),s)\,dW_s. \qquad ⑤$$

With Ito's formula in mind, we are ready to proceed.

Define $\langle \mu, f \rangle = \int_{\mathbb{R}^d} f(x)\,\mu(dx)$ for a measure μ and a function $f \in C_b^{2,1}(\mathbb{R}^d \times \mathbb{R}_+)$. Recall that $S_{N,r}(t) = \frac{1}{N}\sum_{k\in M(N,r,t)} \delta_{P^k_N(t)}$.

Then:

$$\langle S_{N,r}(t), f(\cdot,t) \rangle$$

$$= \frac{1}{N}\int_{\mathbb{R}^d} f(x,t) \sum_{k\in M(N,r,t)} \delta_{P^k_N(t)}(x)\,dx$$

$$= \frac{1}{N}\sum_{k\in M(N,r,t)} f(P^k_N(t),t)$$

$$\overset{\text{Using Ito}}{=} \frac{1}{N}\sum_{k\in M(N,r,t)} f(P^k_N(0),0) \qquad ①$$

$$3 \left[+ \frac{1}{N} \int_0^t \sum_{k \in M(N,r,s)} \left(G_{N,r}(p^k_N(s), s) - \sum_{q=1}^{K} D_{N,qr}(p^k_N(s), s) \nabla S_{N,q}(p^k_N(s), s) \right) \cdot \nabla f(p^k_N(s), s) \, ds \right.$$

$$+ \frac{1}{N} \int_0^t \sum_{k \in M(N,r,s)} \frac{1}{2} \sum_{m,n=1}^{d} \Big(\underbrace{A_{r,mn}}_{= \sigma_r \sigma_r^T} \nabla_m \nabla_n f(p^k_N(s), s) \Big) \, ds \qquad 4$$

$$+ \frac{1}{N} \int_0^t \sum_{k \in M(N,r,s)} \frac{\partial}{\partial s} f(p^k_N(s), s) \, ds \qquad 2$$

$$+ \frac{1}{N} \int_0^t \sum_{k \in M(N,r,s)} \nabla f(p^k_N(s), s) \cdot \sigma_r \, dW_k(s) \qquad 5$$

+ contributions due to birth, death, & transitions

Using that $\langle \mu, f \rangle = \int_{\mathbb{R}^d} f(x) \, \mu(dx)$, the contributions due to birth, death, & transitions are:

$$6 \quad \underbrace{-}_{\text{removal from subpopulation } r} \frac{1}{N} \int_0^t \sum_{k \in M(N,r,s)} f(p^k_N(s), s) \Big(\underbrace{d^{*,k}_{N,r}(ds)}_{\text{any particle can be removed by death}} + \underbrace{\sum_{q=1}^{K} t^{*,k}_{N,rq}(ds)}_{\text{or by transitioning into any of the } K \text{ subpopulations}} \Big)$$

$$7 \quad + \frac{1}{N} \int_0^t \sum_{k \in M(N,r,s)} f(p^k_N(s), s) \Big(\sum_{q=1}^{K} \big(\underbrace{t^{*,k}_{N,qr}(ds)}_{\text{a particle of type } r \text{ is added anytime a particle transitions}} + \underbrace{b^{*,k}_{N,qr}(ds)}_{\text{or anytime a particle of type } q \text{ births a particle}} \big) \Big)$$

Oelschläger then makes use of the notation $\langle \mu, f \rangle = \int_{\mathbb{R}^d} f(x)\,\mu(dx)$ to rewrite $\langle S_{N,r}(t), f(\cdot,t) \rangle$ as:

$\langle S_{N,r}(t), f(\cdot,t) \rangle =$

$$① \ \langle S_{N,r}(0), f(\cdot,0) \rangle$$

$$③ + \int_0^t \Big(\langle \overbrace{S_{N,r}(s)}^{\text{measure}}, \overbrace{\Big(G_{N,r}(\cdot,s) - \sum_{q=1}^{K} D_{N,qr}(\cdot,s)\nabla S_{N,q}(\cdot,s)\Big)\cdot \nabla f(\cdot,s)}^{\text{function}}$$

$$④ \quad + \frac{1}{2}\sum_{m,n=1}^{d} A_{r,mn} \nabla_m \nabla_n f(\cdot,s)$$

$$② \quad + \frac{\partial}{\partial s} f(\cdot,s)$$

$$⑥,⑦ \left\{ \begin{array}{l} - \Big(\sum_{q=1}^{K} t_{N,rq}(\cdot,s) + d_{N,r}(\cdot,s)\Big) f(\cdot,s) \rangle \\ + \sum_{q=1}^{K} \langle S_{N,q}(s), (t_{N,qr}(\cdot,s) + b_{N,qr}(\cdot,s))\, f(\cdot,s) \rangle \Big) ds \\ + M^2_{N,r}(f,t) \end{array} \right.$$

$$⑤ \quad + M^1_{N,r}(f,t)$$

For definitions of the martingales $M^2_{N,r}$ and $M^1_{N,r}$, see Oelschläger (1989) pg. 570.

3 Heuristic argument for RD system as $N \to \infty$

1. Note that $\lim_{N\to\infty} V_N = \lim_{N\to\infty} \hat{V}_N = \delta_0$
(in the sense of distributions because of our scalings)

2. Assume (in some yet unspecified sense) that

$$\lim_{N\to\infty} S_{N,r}(t) = S_r(t) \quad \text{for} \quad \begin{matrix} r=1,\dots,k \\ t\geq 0 \end{matrix}$$

where the measures $S_r(t)$ have smooth densities $s_r(\cdot,t)$

such that

$$\lim_{N\to\infty} s_{N,r}(\cdot,t) = \lim_{N\to\infty} \hat{s}_{N,r}(\cdot,t) = s_r(\cdot,t)$$

and

$$\lim_{N\to\infty} \nabla s_{N,r}(\cdot,t) = \nabla s_r(\cdot,t)$$

3. It can be shown that the quadratic variations of the martingales $M^1_{N,r}(f,\cdot)$ and $M^2_{N,r}(f,\cdot)$ go to 0 as $N\to\infty$, so we can neglect these terms.

Formally, this means that as $N\to\infty$, we go from $\langle S_{N,r}(t), f(\cdot,t)\rangle$ to $\langle s_r(\cdot,t), f(\cdot,t)\rangle$ by replacing

$S_{N,r}(0)$ with $s^*_r(\cdot)$ = the density of $S_r(0)$ 1

$s_r(\cdot,s)$ with $s_{N,r}(s)$ 2, 7

$G_{N,r}$, $D_{N,rq}$, $t_{N,rq}$, $b_{N,rq}$, $d_{N,r}$ with
$G_{\infty,r}$, $D_{\infty,rq}$, $t_{\infty,rq}$, $b_{\infty,rq}$, $d_{\infty,r}$ 3, 6, 7

After integrating by parts, the result is the weak formulation of this system of RD equations:

$$\frac{\partial}{\partial t} s_r(x,t) = \nabla \cdot \left(s_r(x,t) \left(-G_{\infty,r}(x,t) + \sum_{q=1}^{K} D_{\infty,qr}(x,t) \nabla s_q(x,t) \right) \right)$$

$$+ \frac{1}{2} \sum_{m,n=1}^{d} A_{r,mn} \nabla_m \nabla_n s_r(x,t)$$

$$- \left(\sum_{q=1}^{K} t_{\infty,rq}(x,t) + d_{\infty,r}(x,t) \right) s_r(x,t)$$

$$+ \sum_{q=1}^{K} \left(t_{\infty,qr}(x,t) + b_{\infty,qr}(x,t) \right) s_q(x,t) \qquad t \geq 0$$

$$s_r(x,0) = s_r^*(x) \qquad \text{for} \quad r = 1, \ldots, K.$$