Ordinary Differential Equations

as an alternative to agent-based modelling

eX Modelo school

OpenMOLE

June 26, 2019

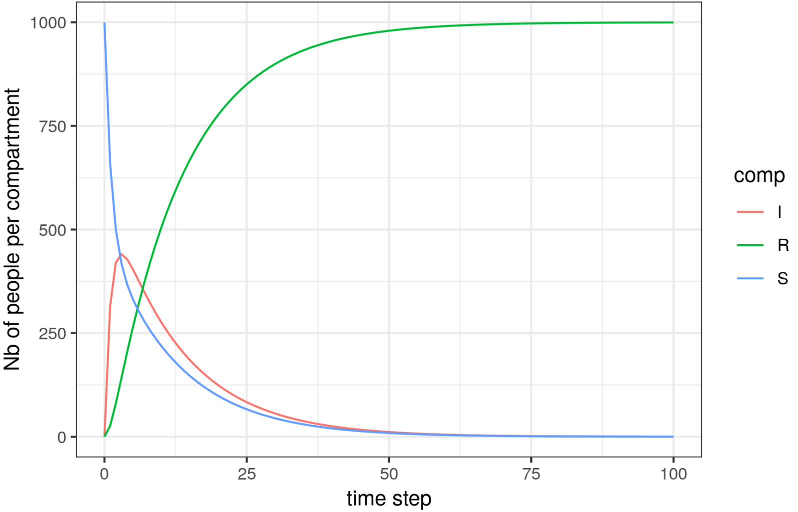
ODE systems

$\rightarrow$ widely used to model transmission phenomena

- population split into compartments
- system of ordinary differential equations

$$\begin{cases} \dfrac{\mathrm{d}S}{\mathrm{d}t} = -\beta S + \lambda I \\[2ex] \dfrac{\mathrm{d}I}{\mathrm{d}t} = \beta S - (\lambda + \gamma) I \\[2ex] \dfrac{\mathrm{d}R}{\mathrm{d}t} = \gamma I \end{cases}$$

SIR model dynamics



ODE	ABM
Equation-based	Individual-based
Generic mechanisms	Precise mechanisms
Population scale	Individual scale
Needs less resources	Computationally expensive

A Zombie situation

How could we model the Zombie invasion?

- Which mechanisms?
- Which parameters?

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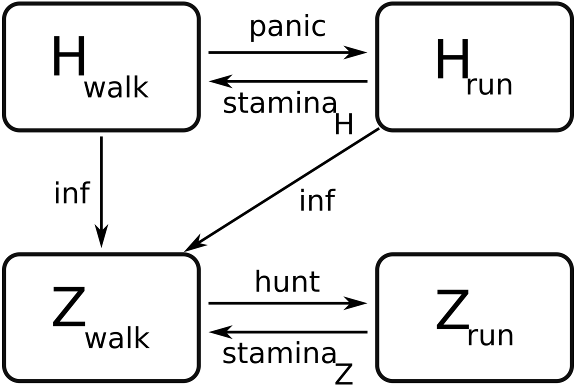
- Which mechanisms?
- Which parameters?

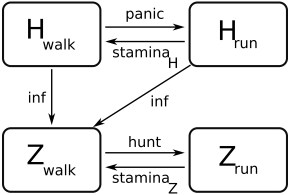
How can we assess our model's ability to reproduce the real data?

- Which metrics?
- Which fitness function?

A very simple ODE model



A very simple ODE model



$$
\begin{cases}
\dfrac{\mathrm{d}H_{walk}}{\mathrm{d}t} = -(panic + inf) * H_{walk} + exhaustH * H_{run} \\[2ex]
\dfrac{\mathrm{d}H_{run}}{\mathrm{d}t} = panic * H_{walk} - (exhaustH + inf) * H_{run} \\[2ex]
\dfrac{\mathrm{d}Z_{walk}}{\mathrm{d}t} = inf * (H_{walk} + H_{run}) - hunt * Z_{walk} + exhaustZ * Z_{run} \\[2ex]
\dfrac{\mathrm{d}Z_{run}}{\mathrm{d}t} = hunt * Z_{walk} - exhaustZ * Z_{run}
\end{cases}
$$

A very simple ODE model

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$$\begin{cases} N & = & H_{walk} + H_{run} + Z_{walk} + Z_{run} \\ panic & = & panic_0 * (Z_{walk} + Z_{run})/N \\ hunt & = & hunt0 * (H_{walk} + H_{run})/N \end{cases}$$

Exploration

First step: Calibrate

We have some real time series of zombie invasion
$\rightarrow$ find the parameter values to best fit them

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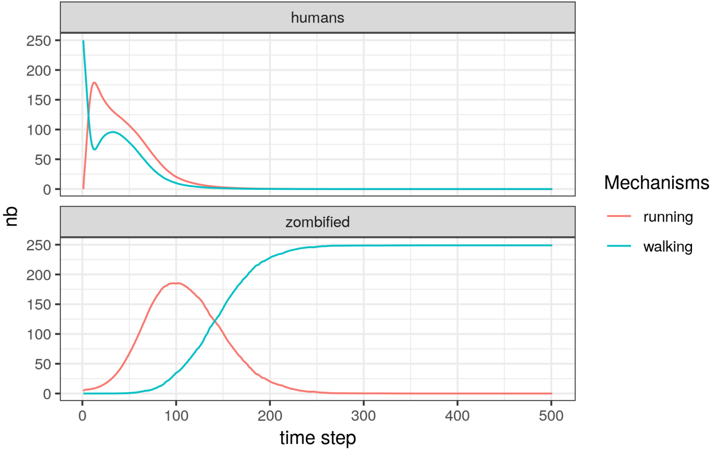

Process

Process

- Embed the model in OpenMOLE

First step: Calibrate

Process

- Embed the model in OpenMOLE
- Define a fitness function

Process

- Embed the model in OpenMOLE
- Define a fitness function
- Write a calibration task

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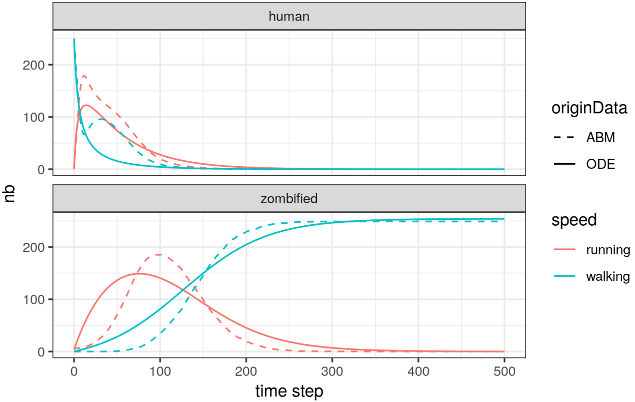
Parameter set

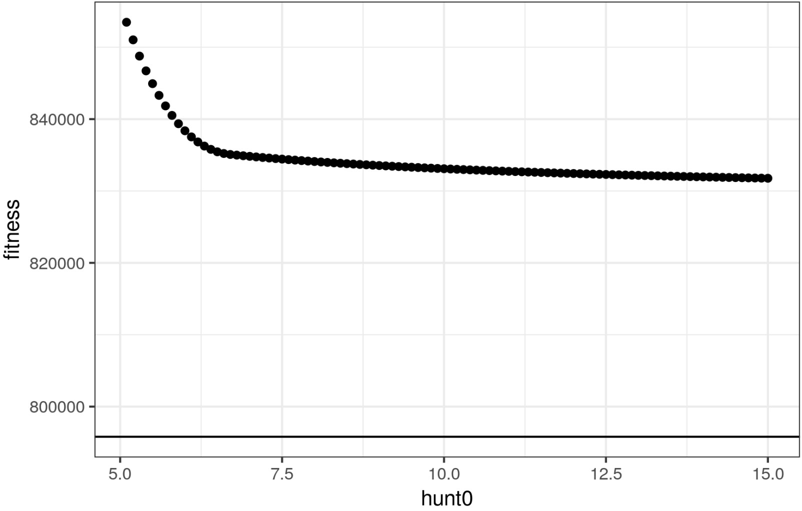
$panic_0$	7.25
$stamina_H$	0.99
$hunt_0$	10.15
$stamina_Z$	1.28
inf	0.02
fitness	780 394



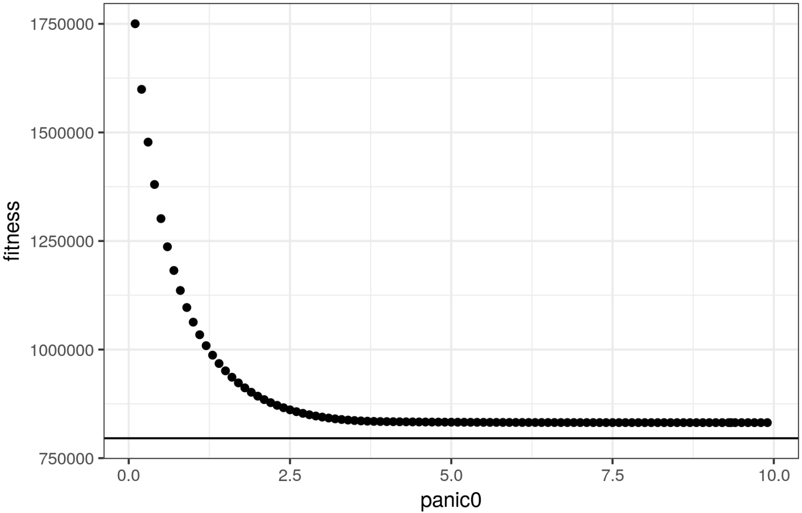
Second step: Profiles

Profiles for each of the 5 parameters:
$rightarrow\ panic_0, stamina_H, hunt_0, stamina_Z, inf_0$

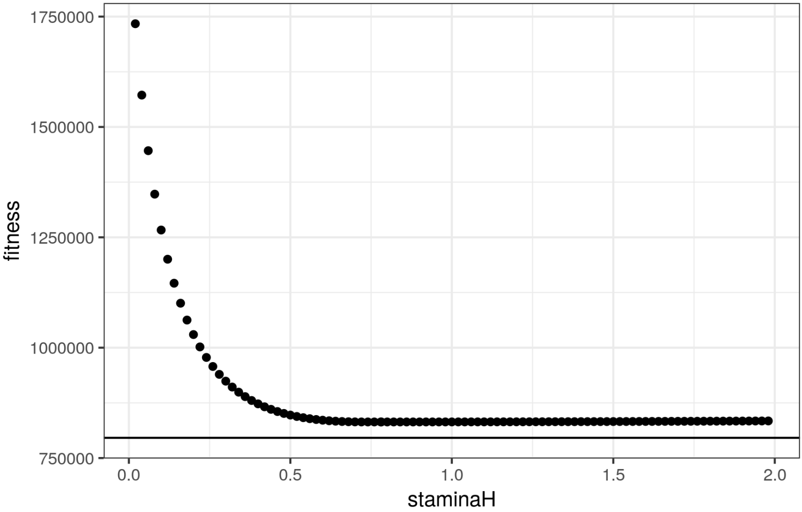
Profiles



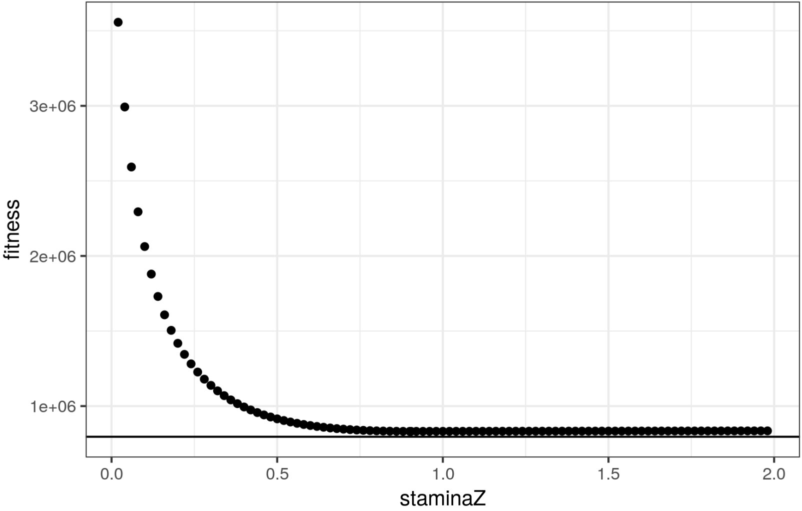
Profiles

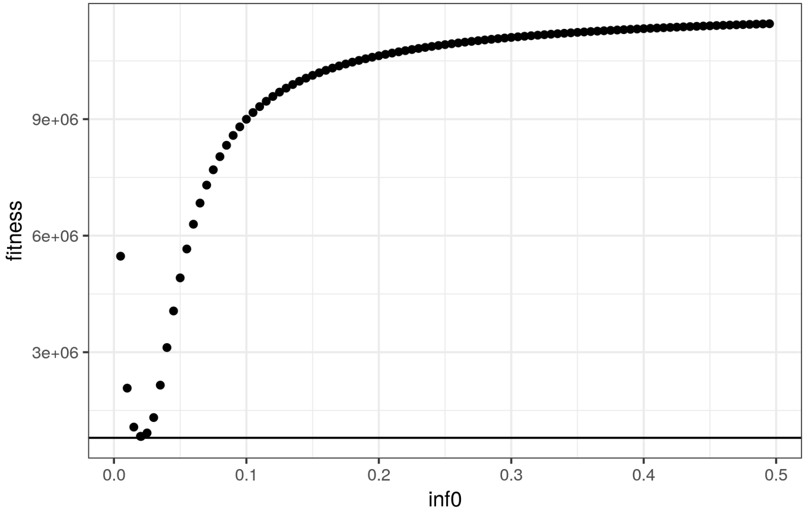


1750000
1500000
1250000
1000000
750000
fitness
0.0
2.5
5.0
7.5
10.0
panic0


1750000
1500000
1250000
1000000
750000
fitness
0.0
0.5
1.0
1.5
2.0
staminaH

Profiles




fitness
9e+06
6e+06
3e+06
0.0
0.1
0.2
0.3
0.4
0.5
inf0

Adding complexity

New mechanisms

What mechanisms could we add to better represent the complexity of our Zombie situation?

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The parcimony issue

- Do the new mechanisms really improve the fitness?
- Do we need them all?
- What are the best combinations?

Process

- Embed the model in OpenMOLE **DONE**

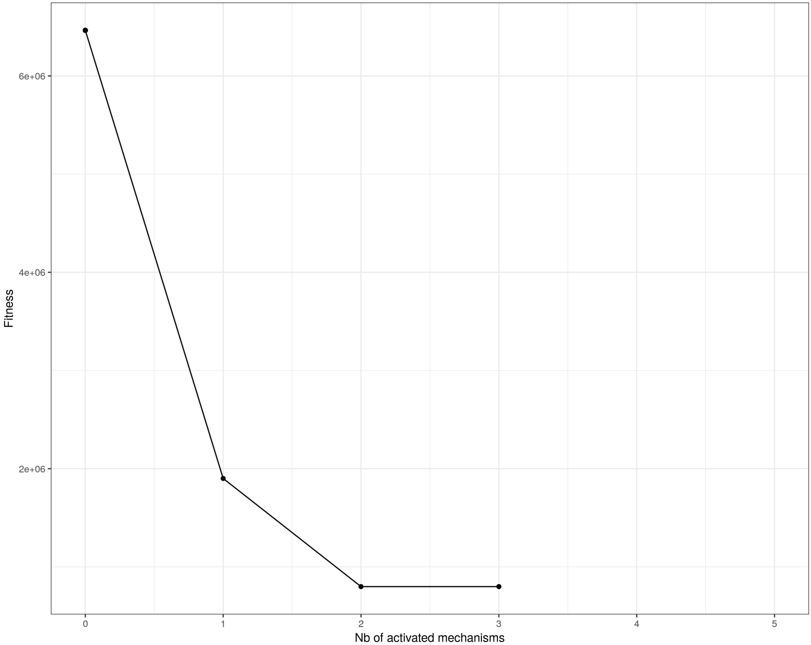
Process

- Embed the model in OpenMOLE **DONE**
- Define a **second** fitness function

Process

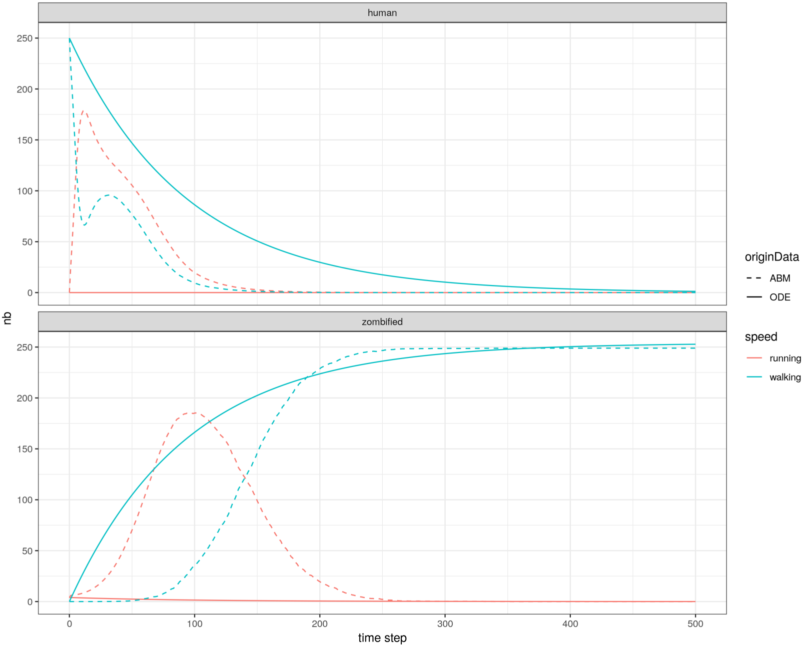
- Embed the model in OpenMOLE **DONE**
- Define a **second** fitness function
- **Modify** the calibration task

Pareto front

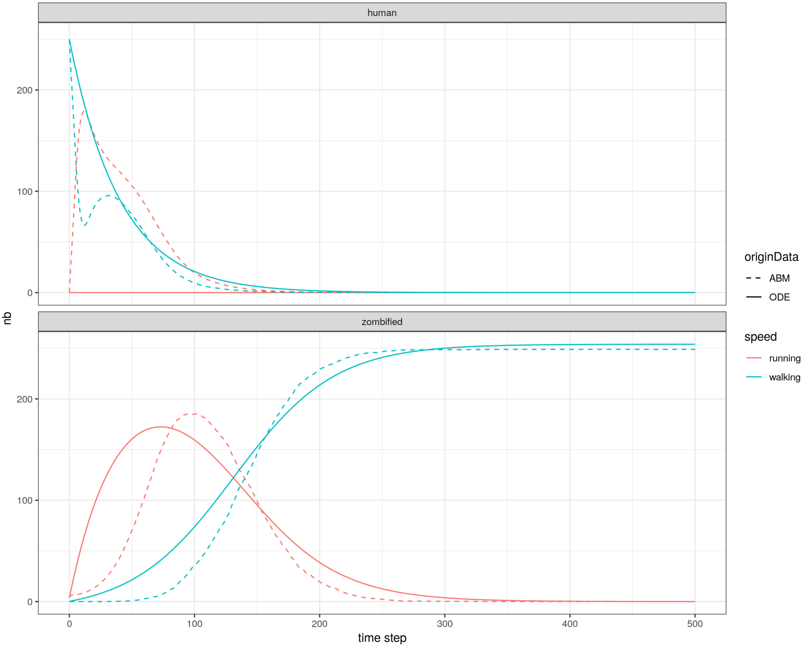


Dynamics for 0 mechanism activated

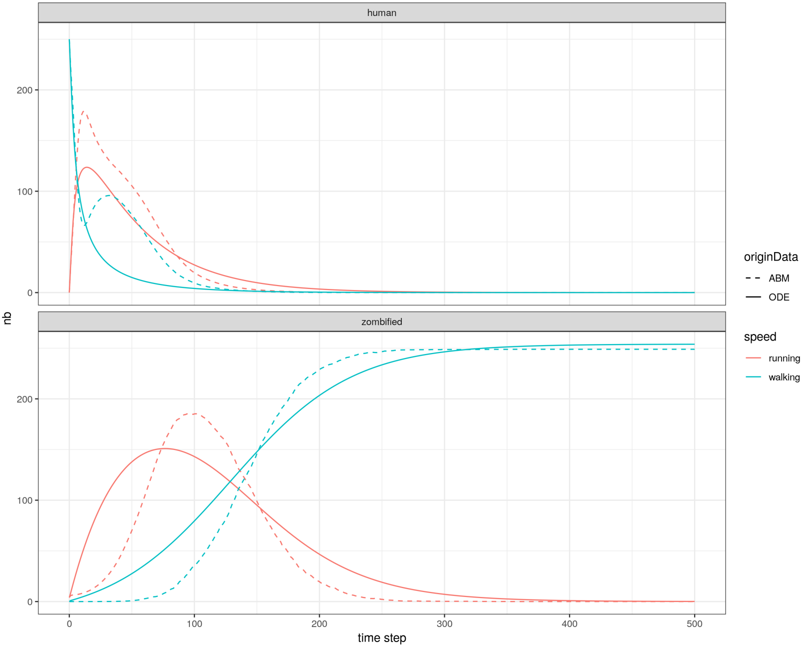
OpenMOLE



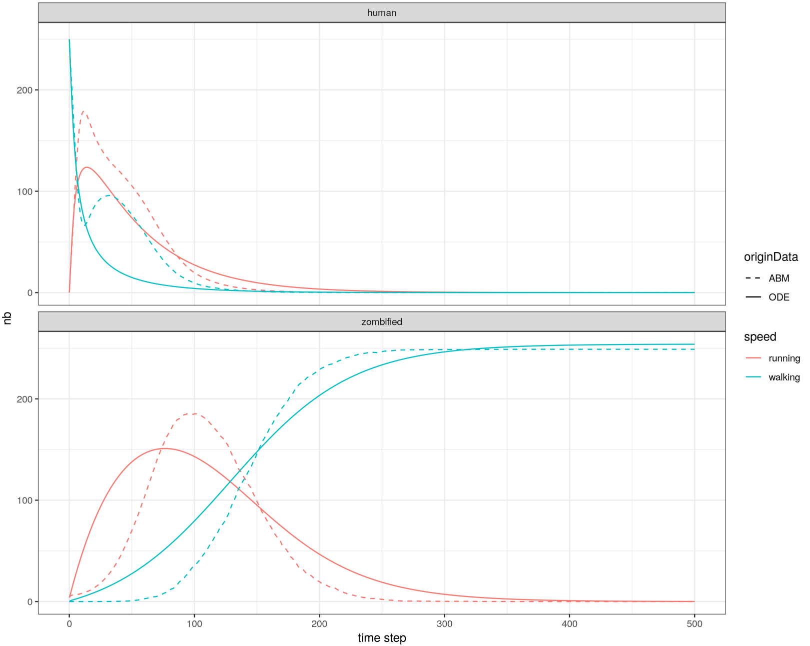
Dynamics for 1 mechanism activated



Dynamics for 2 mechanisms activated



Dynamics for 3 mechanisms activated



Some mathematics

Recall the ODE system:

$$\begin{cases} \dfrac{\mathrm{d}H_{walk}}{\mathrm{d}t} & = & -(panic0 * \dfrac{Z_{walk} + Z_{run}}{N} + inf) * H_{walk} + exhaustH * H_{run} \\ \dfrac{\mathrm{d}H_{run}}{\mathrm{d}t} & = & panic0 * \dfrac{Z_{walk} + Z_{run}}{N} * H_{walk} - (exhaustH + inf) * H_{run} \\ \dfrac{\mathrm{d}Z_{walk}}{\mathrm{d}t} & = & inf * (H_{walk} + H_{run}) - hunt0 * \dfrac{H_{walk} + H_{run}}{N} * Z_{walk} + exhaustZ * Z_{run} \\ \dfrac{\mathrm{d}Z_{run}}{\mathrm{d}t} & = & hunt0 * \dfrac{H_{walk} + H_{run}}{N} * Z_{walk} - exhaustZ * Z_{run} \end{cases}$$

Where $N := H_{walk} + H_{run} + Z_{walk} + Z_{run}$

First-order **nonlinear** (autonomous) ordinary differential equation... a priori no explicit solution, hence numerical solutions.

Total population size

Summing the 4 equations, we have:

$$\frac{\mathrm{d}N}{\mathrm{d}t} = \frac{\mathrm{d}H_{walk}}{\mathrm{d}t} + \frac{\mathrm{d}H_{run}}{\mathrm{d}t} + \frac{\mathrm{d}Z_{walk}}{\mathrm{d}t} + \frac{\mathrm{d}Z_{run}}{\mathrm{d}t} = 0$$

So $N(t)$ is constant:

$$N(t) = N(0), \text{ for all } t.$$

We find back that the population size (human + zombies) is constant: natural !

Human / zombies population size

Let's note $H := H_{walk} + H_{run}$
Summing the first equations, we have:

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\mathrm{d}H_{walk}}{\mathrm{d}t} + \frac{\mathrm{d}H_{run}}{\mathrm{d}t} = -inf * (H_{walk}(t) + H_{run}(t)) = -inf * H(t)$$

First-order linear ordinary differential equation with constant coefficient: explicit solution !

$$H(t) = H(0) * e^{-inf * t}$$

Likewise,

$$Z(t) := Z_{walk} + Z_{run} = N - H(t)$$

Equilibrium points

Definition: The point $x \in \mathbb{R}^4$ is an *equilibrium point* for the differential equation $X' = F(X)$ if $F(X) = 0$.

For example, points of the form $(0, 0, N, 0)$ are equilibrium points. They correspond to a population composed of walking zombies.

New mechanism

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$$
\begin{cases}
\dfrac{\mathrm{d}H_{walk}}{\mathrm{d}t} & = & -(panic + inf + out) * H_{walk} + exhaustH * H_{run} \\
\dfrac{\mathrm{d}H_{run}}{\mathrm{d}t} & = & panic * H_{walk} - (exhaustH + inf + out) * H_{run} \\
\dfrac{\mathrm{d}Z_{walk}}{\mathrm{d}t} & = & inf * (H_{walk} + H_{run}) - (hunt + die) * Z_{walk} + exhaustZ * Z_{run} \\
\dfrac{\mathrm{d}Z_{run}}{\mathrm{d}t} & = & hunt * Z_{walk} - (exhaustZ + die) * Z_{run}
\end{cases}
$$

New mechanism

$$
\begin{cases}
N & = & H_{walk} + H_{run} + Z_{walk} + Z_{run} \\
panic & = & panic0 * (Z_{walk} + Z_{run})/N \\
hunt & = & hunt0 * (H_{walk} + H_{run})/N \\
inf & = & inf0 * (1 - fightback) \\
out & = & out0 * (H_{walk} + H_{run})/N \\
die & = & die0 * (H_{walk} + H_{run})/N
\end{cases}
$$

However, the population size is no more constant, due to $out0$ and $die0$.

Then, $H := H_{walk} + H_{run}$ satisfies :

$$\frac{\mathrm{d}H}{\mathrm{d}t} = -(inf + out0.\frac{H}{N}).H$$

for which a solution is not as simple as for the previous model.