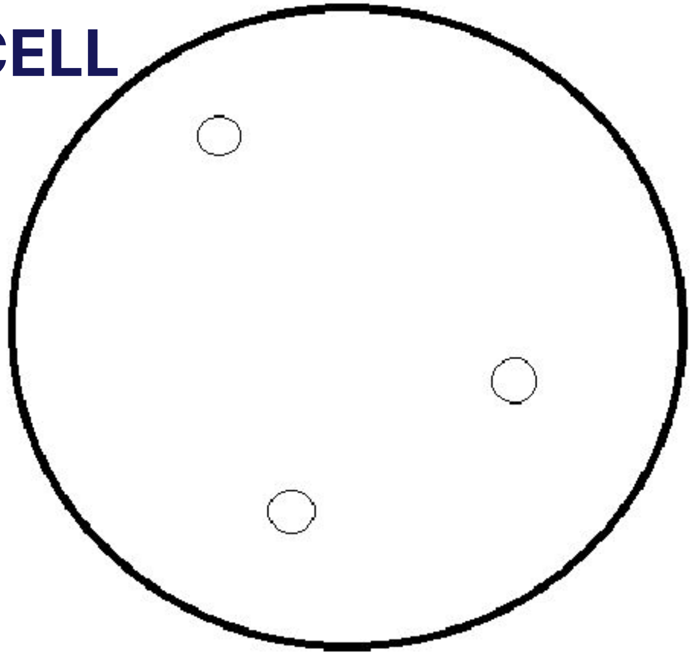
Mentors: Prof Richard Nickl and Fanny Seizilles

# INFERRING DIFFUSION FROM KILLED MOLECULES

Paula Horvat

# **PROBLEM SETUP** - short version

CELL



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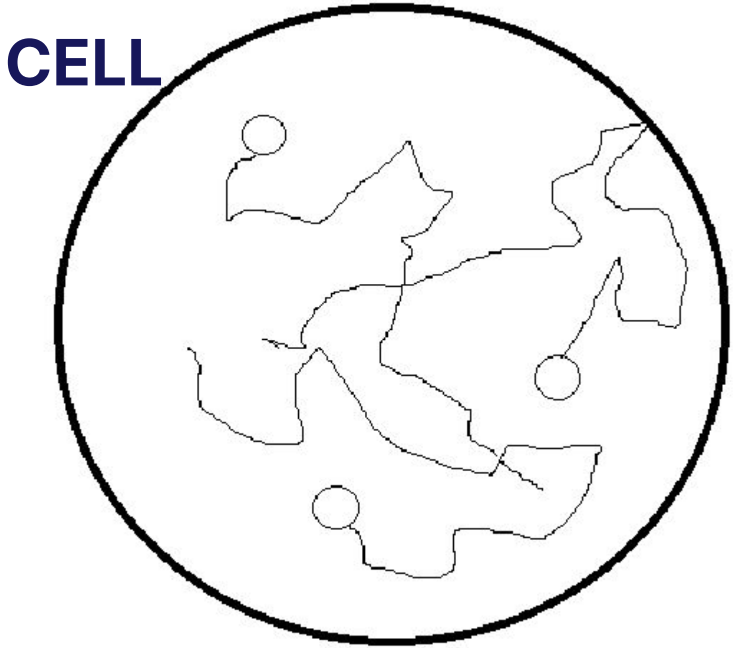

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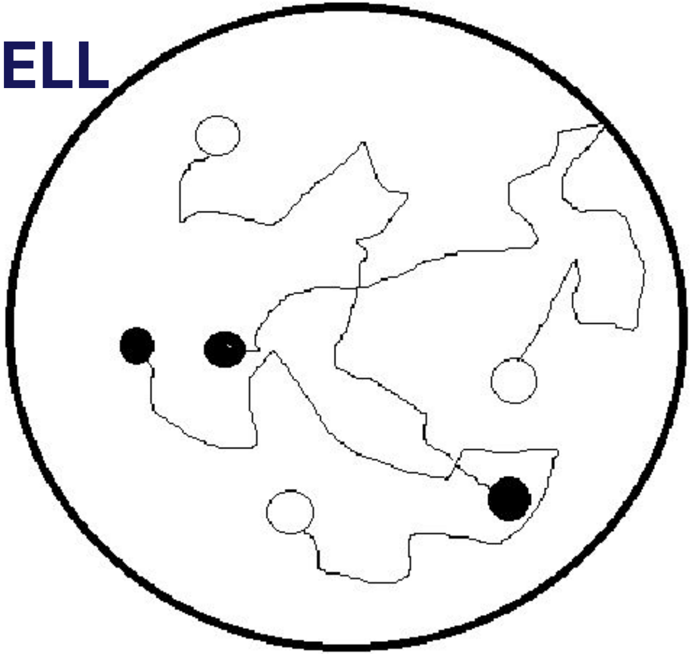

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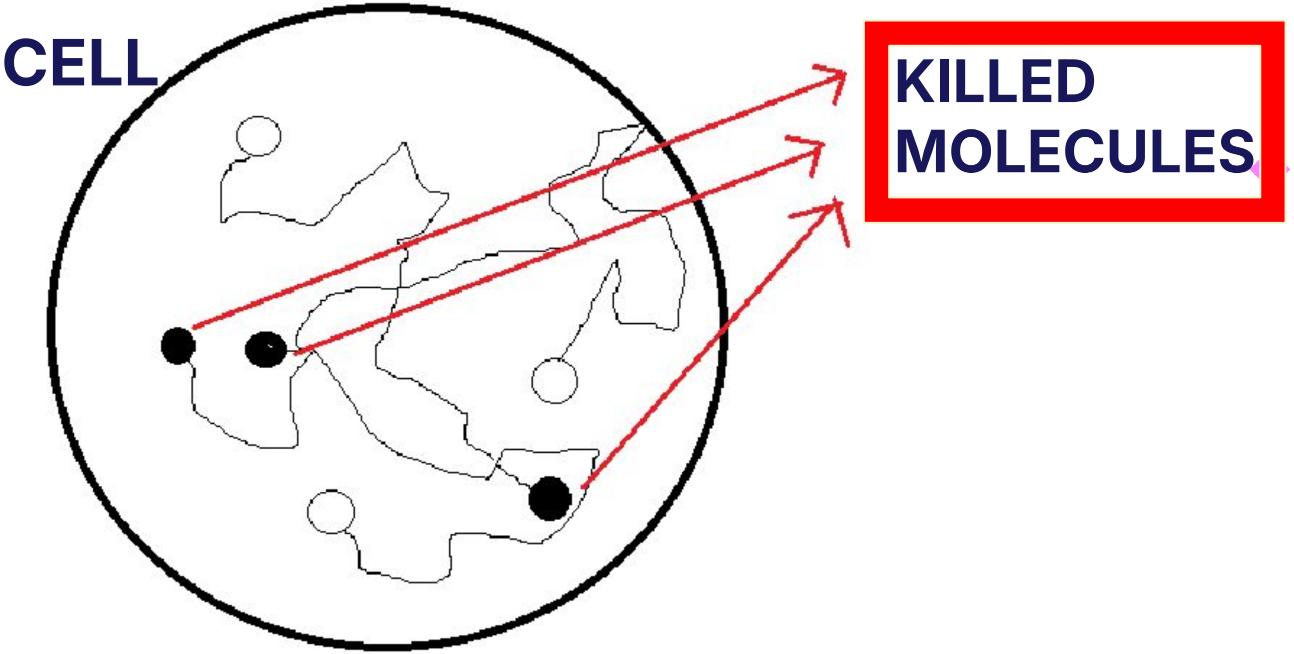

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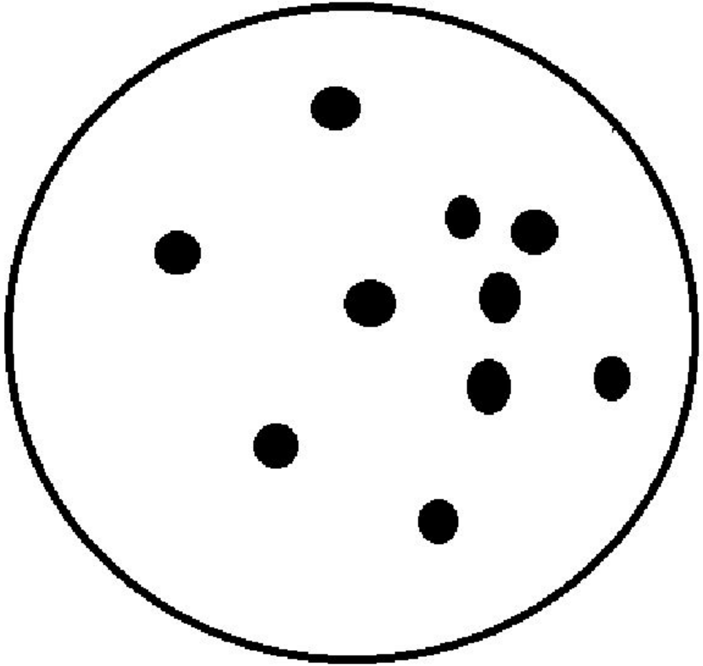
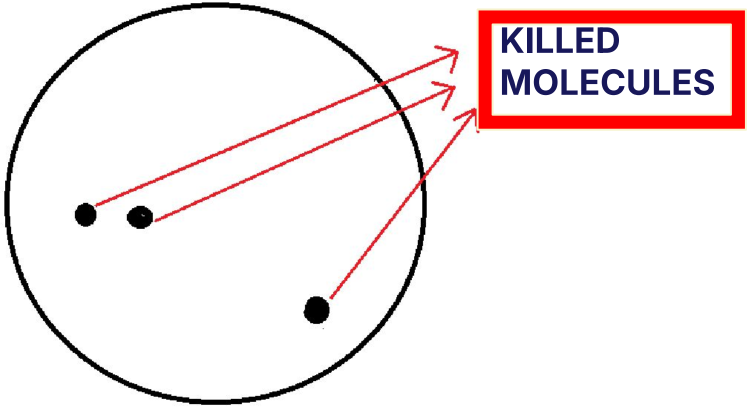


**KILLED MOLECULES**

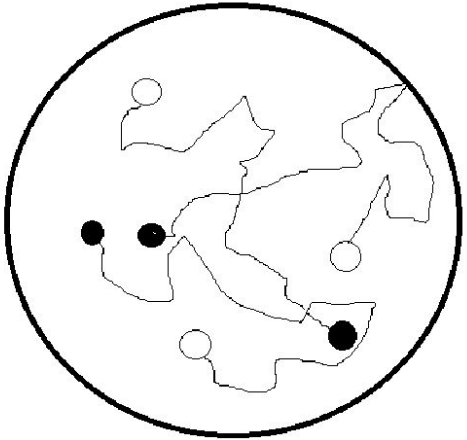
# **PROBLEM SETUP** - short version

**INPUT:**




**QUESTION:**
Given the positions of killed molecules, can we reconstruct their trajectories?

**OUTPUT:**



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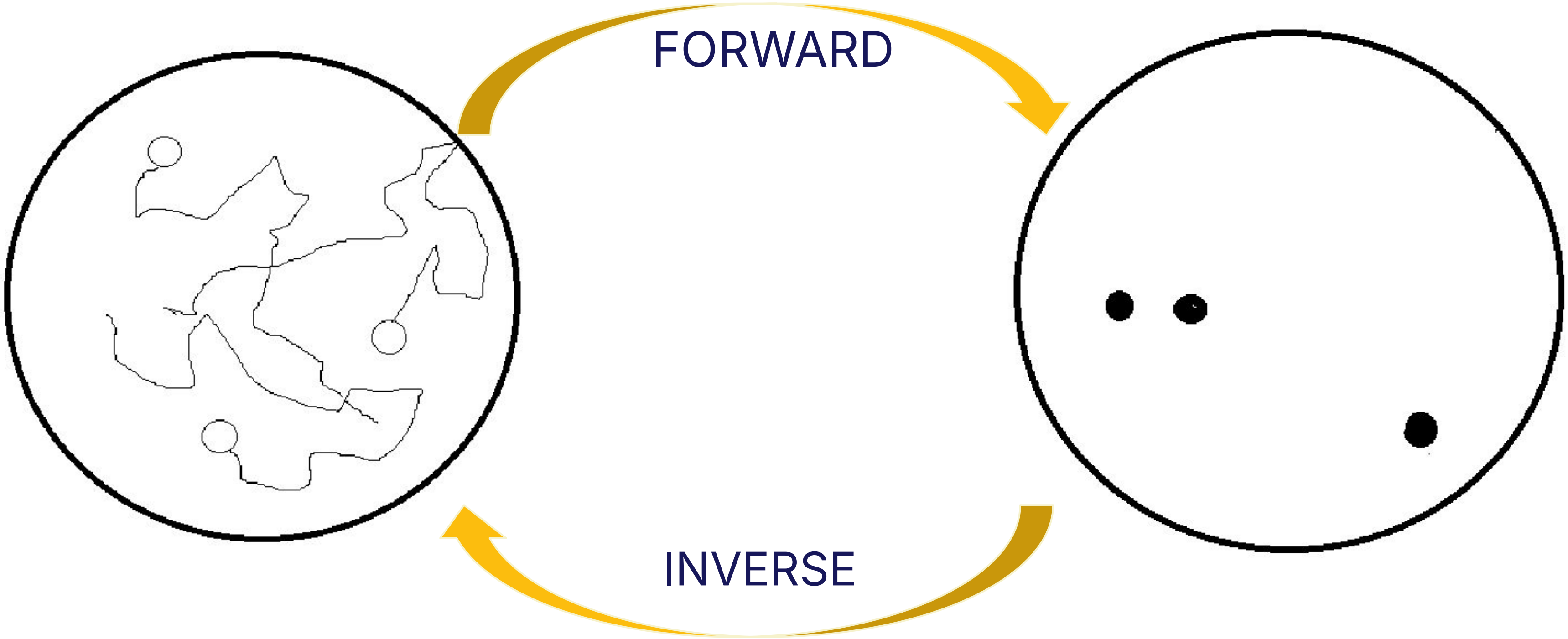

# PROBLEM SETUP

- $\Omega \subset \mathbb{R}^2$ - bounded domain
- $(X_t,\ t \geq 0)$ - Markov process, $X_0 \sim \phi$

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$$dX_t = \nabla D(X_t)\, dt + \sqrt{2\, D(X_t)}\, dW_t + \nu(X_t)\, dL_t,\ \ t > 0$$

Deterministic movement

Random shaking

Reflection at the boundary

# PROBLEM SETUP

- $\Omega \subset \mathbb{R}^2$ - bounded domain
- $(X_t,\ t \geq 0)$ - Markov process, $X_0 \sim \phi$

$$dX_t = \nabla D(X_t)\,dt + \sqrt{2\,D(X_t)}\,dW_t + \nu(X_t)\,dL_t,\ \ t > 0$$

$$D : \Omega \to [D_{min}, \infty)$$

→ diffusivity
→ everything we need to know about the movement of molecules

# PROBLEM SETUP

- $dX_t = \nabla D(X_t)\, dt + \sqrt{2\, D(X_t)}\, dW_t + \nu(X_t)\, dL_t, \;\; t > 0$
- $q : \Omega \to [0, \infty)$ - killing potential

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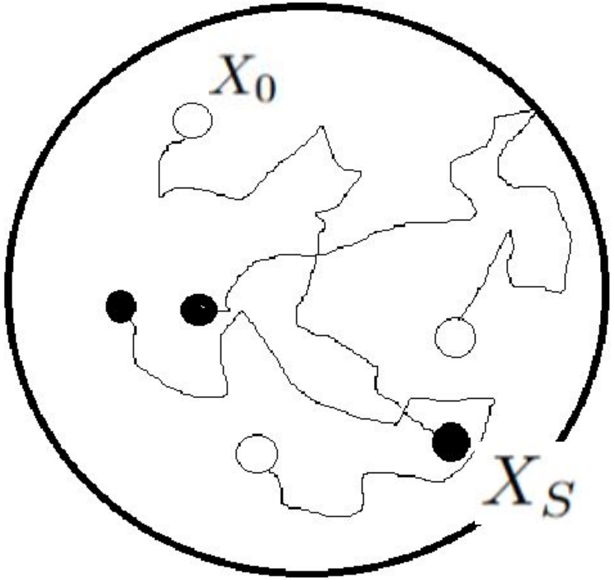
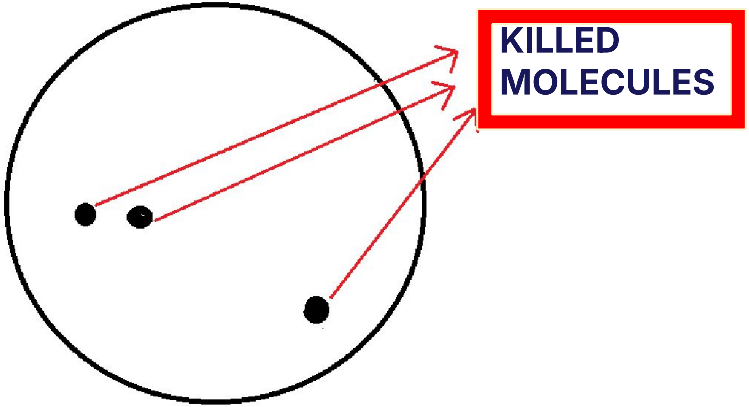


# PROBLEM SETUP

- $n_{mol} = \#$ of molecules in the domain
- $X_t^m, m = 1, .., n_{mol} - i.i.d.$

# **PROBLEM SETUP** - short version

**INPUT:**




**QUESTION:**
Given the positions of killed molecules, can we reconstruct their trajectories?

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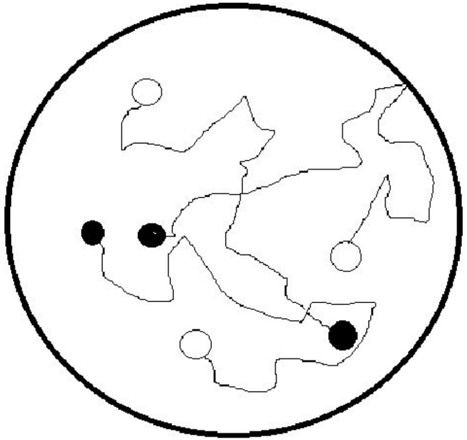


# **PROBLEM SETUP** - short version

**INPUT:**

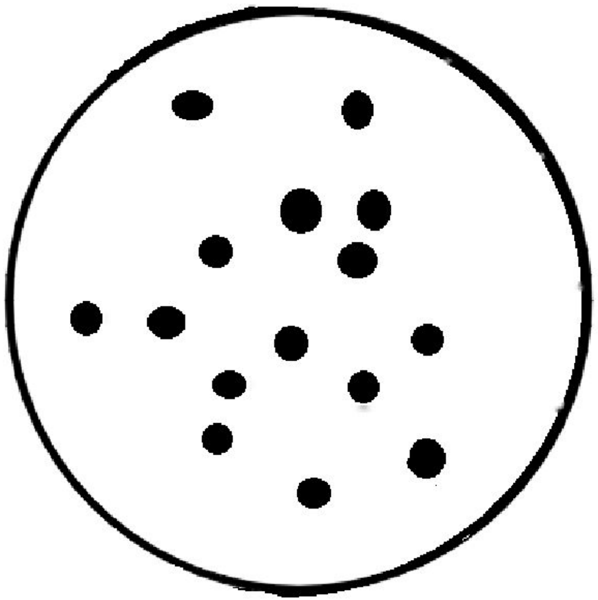
$$X_S^m, m = 1, .., n_{mol}$$

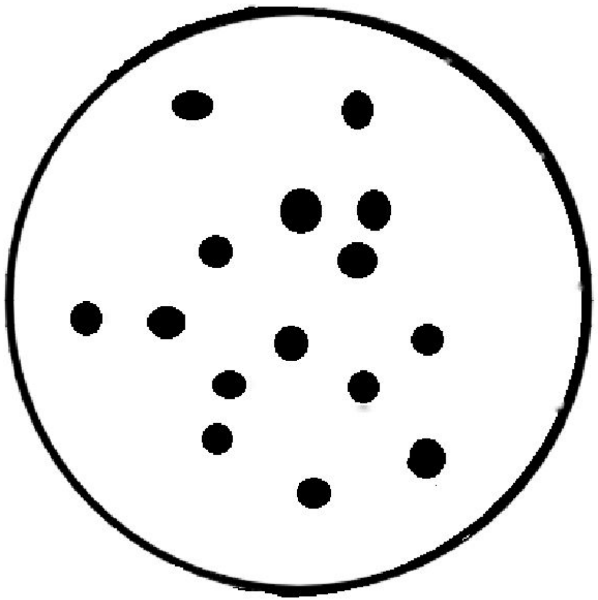
**QUESTION:**
Given the positions of killed molecules, can we reconstruct their trajectories?

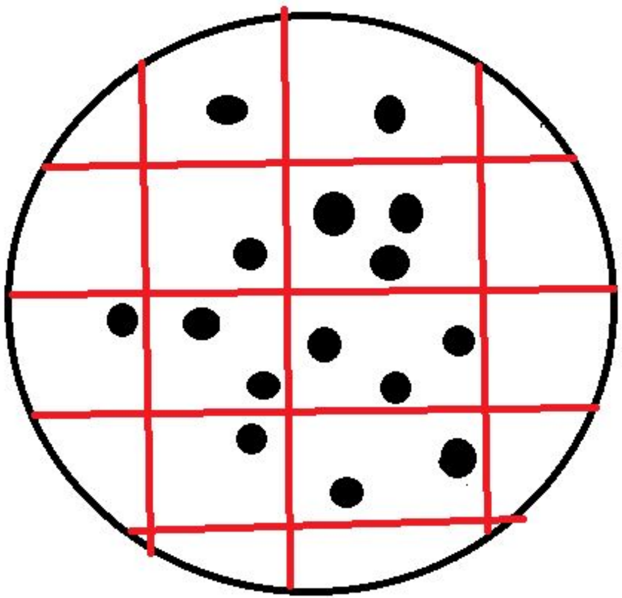
**OUTPUT:**

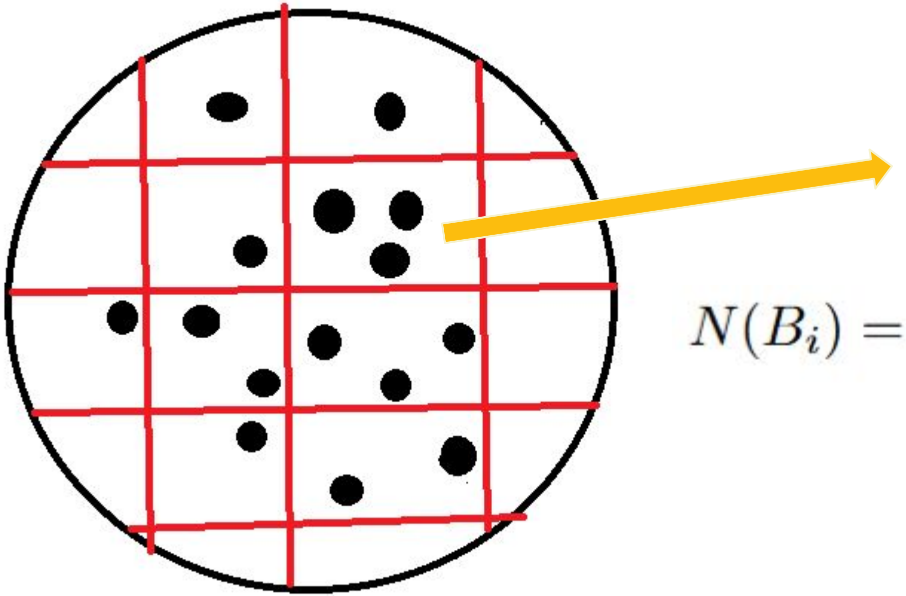
$D$ - diffusivity

# SOLUTION



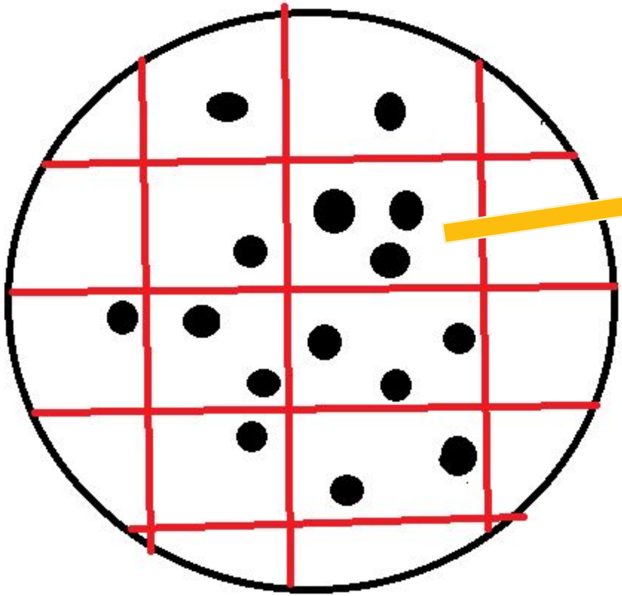






$B_i$ - bin $i$

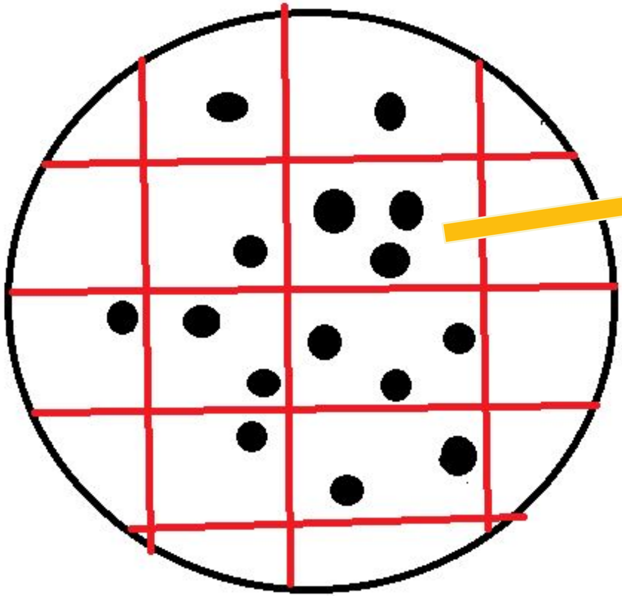
$N(B_i) = \#$ of killed molecules in $B_i$



$B_i$ - bin $i$

$N(B_i) = \#$ of killed molecules in $B_i$

$$N(B_i) \sim Poisson(n_{mol}\Lambda_D(B_i))$$



$B_i$ - bin $i$

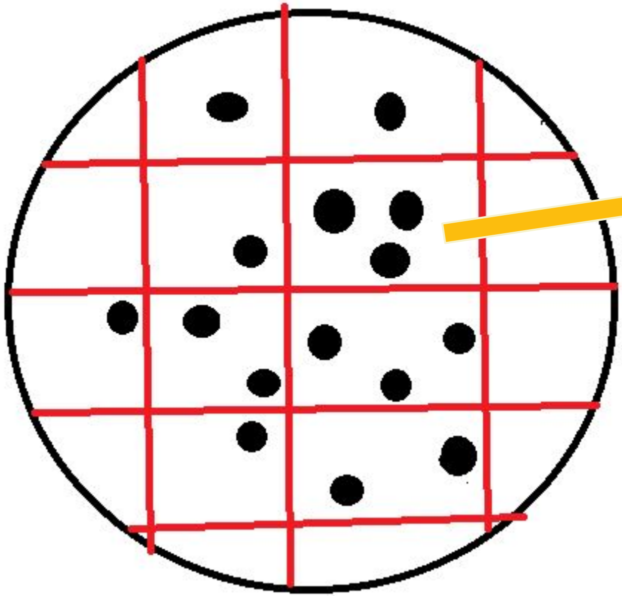
$N(B_i) = \#$ of killed molecules in $B_i$

$$N(B_i) \sim Poisson(n_{mol}\Lambda_D(B_i))$$

$N$ - Poisson point process with intensity measure $\Lambda_D$

# Questions for my project:

What if we don’t know **when** all the molecules were killed?
What if we don’t know **if** the molecules stopped moving?
Is it possible to reach the same **conclusions**?



$B_i$ - bin $i$

~~$N(B_i) = \#$ of killed molecules in $B_i$~~

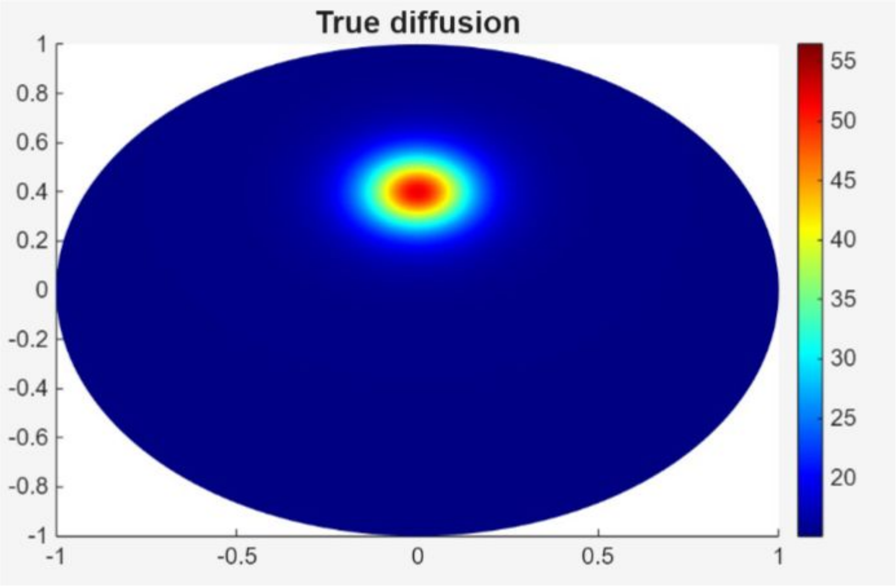
$N(B_i) := \#$ of molecules in $B_i$ at time $t$

$$N(B_i) \sim Poisson(n_{mol} \Lambda_{D,t}(B_i))$$

$N$ - Poisson point process with intensity measure $\Lambda_{D,t}$

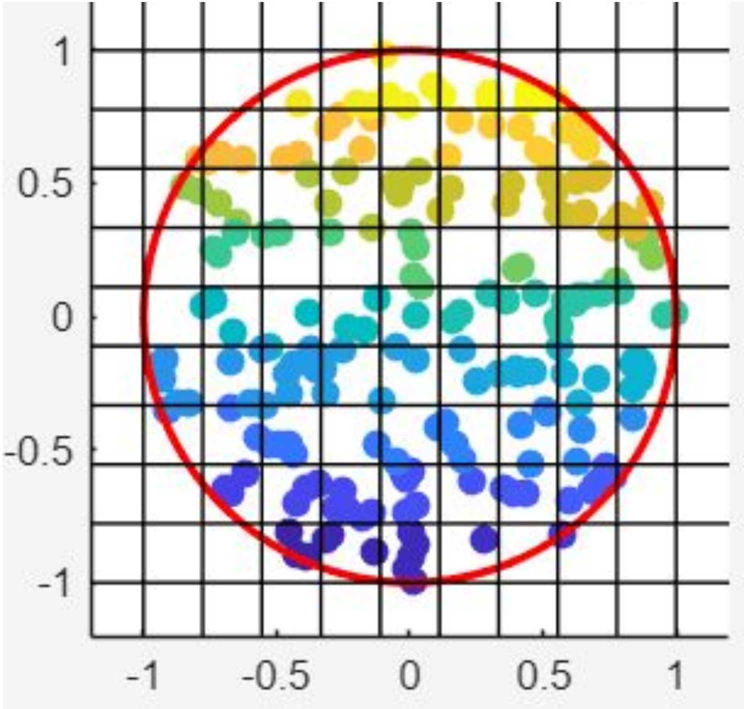
# Results

1. Simulation of observations with known diffusivity



# Results

1. Simulation of observations with known diffusivity
2. $Y_1, .., Y_K$ - counts of molecules



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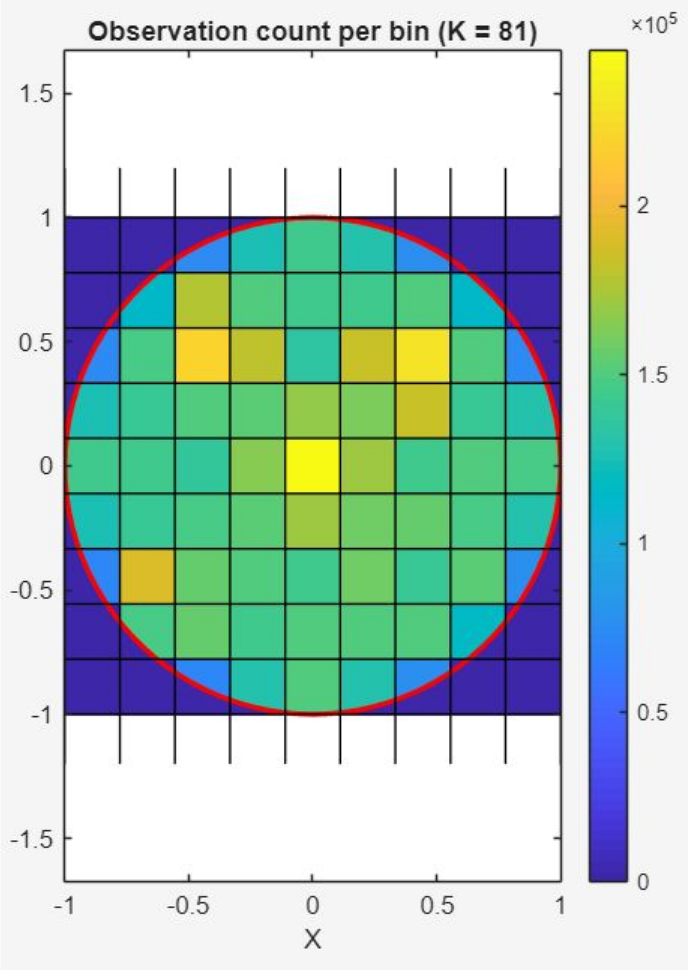
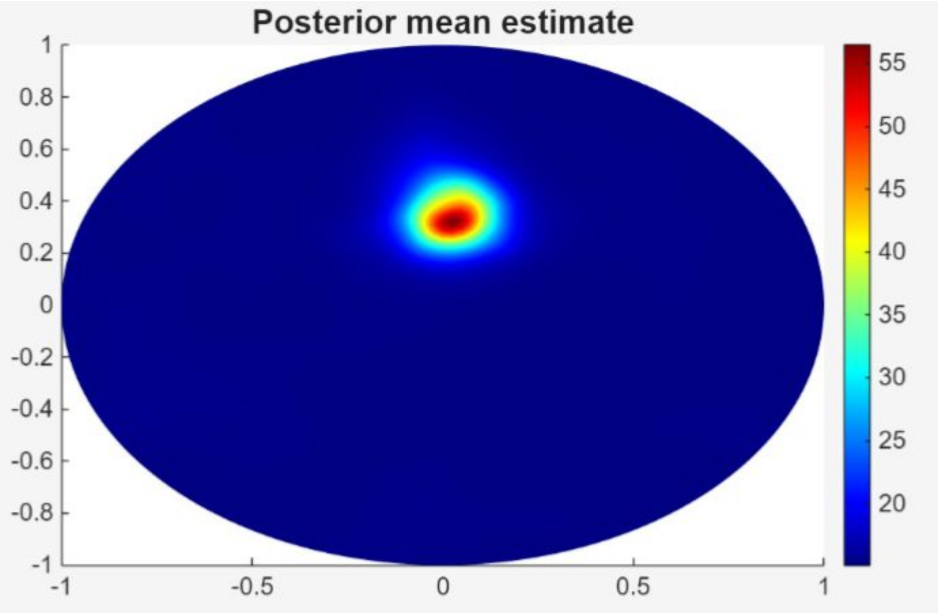
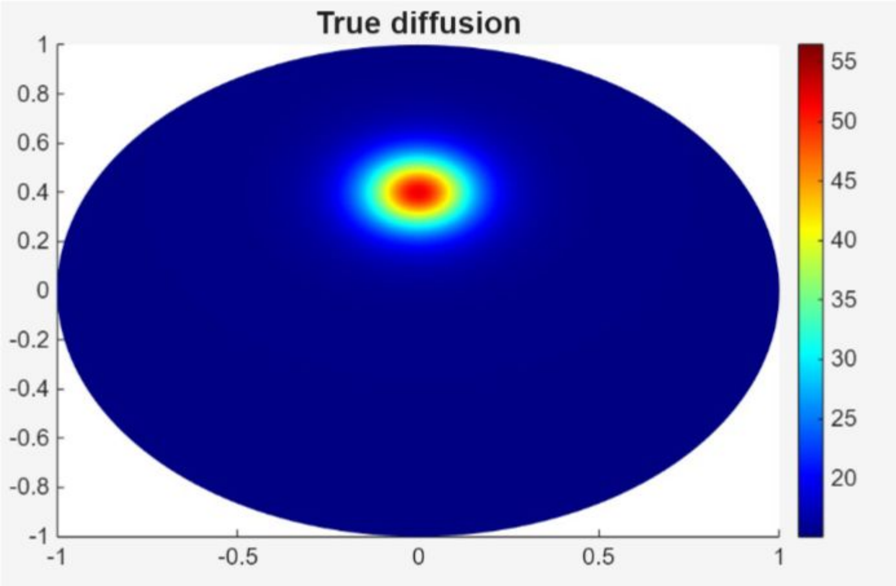
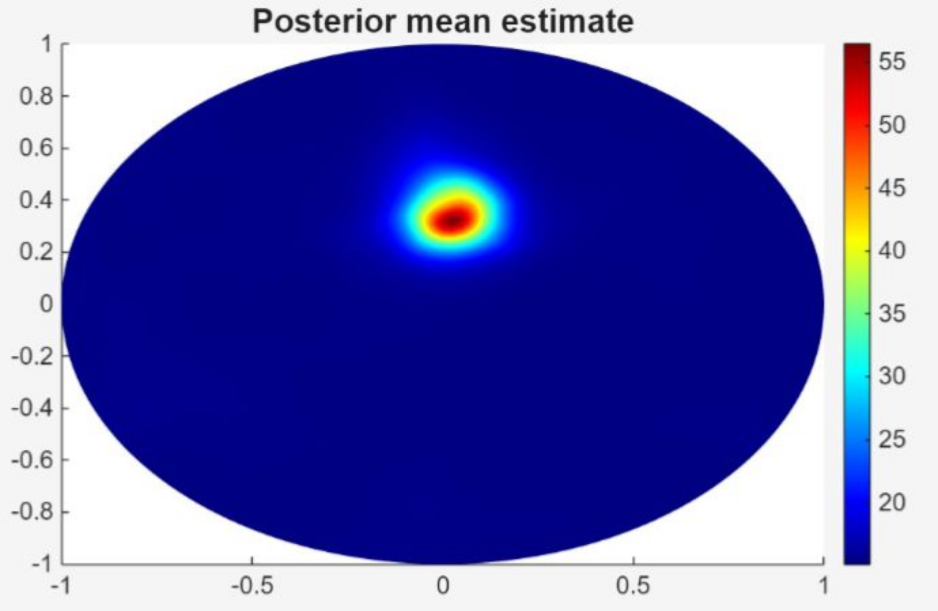


# Results

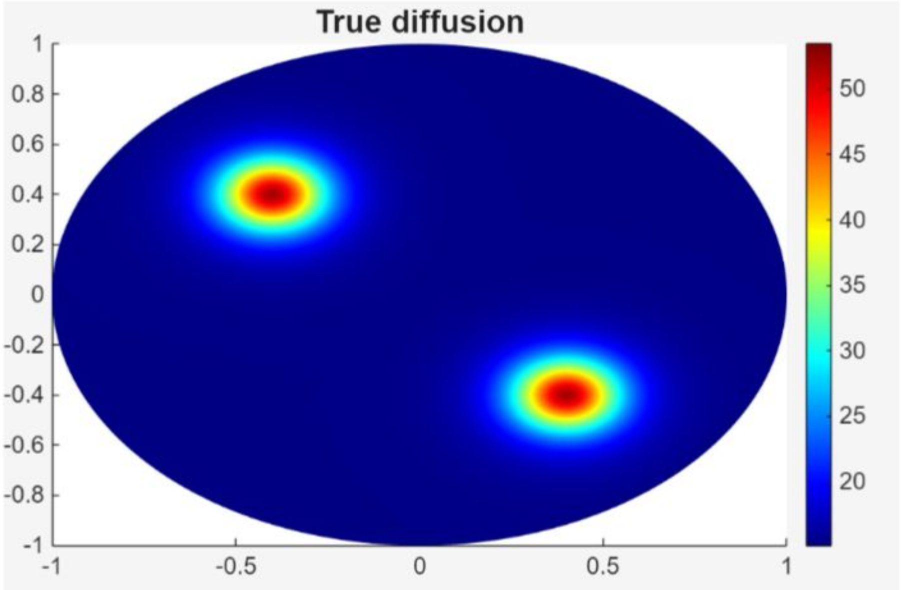
1. Simulation of observations with known diffusivity
2. $Y_1, .., Y_K$ - counts of molecules
3. Estimation of diffusivity




True diffusion
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-1
-0.5
0
0.5
1
55
50
45
40
35
30
25
20


Posterior mean estimate
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-1
-0.5
0
0.5
1
55
50
45
40
35
30
25
20

# Results


True diffusion
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0.6
0.4
0.2
0
-0.2
-0.4
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-1
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0
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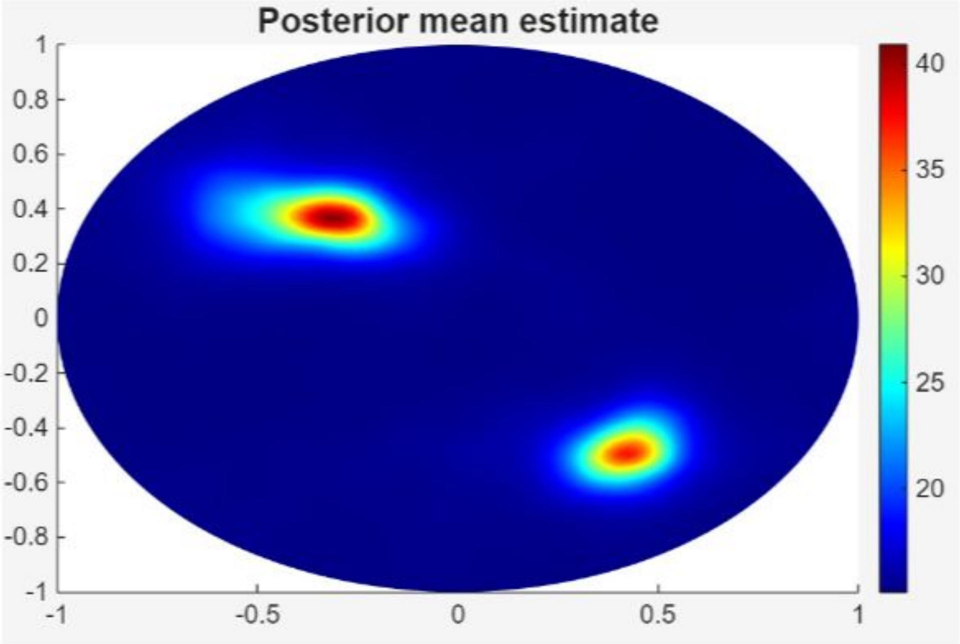
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-0.8
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-1
-0.5
0
0.5
1
40
35
30
25
20

# Thank you!