11. Sampling Methods
Sampling Methods

Sampling Methods are widely used in Computer Science

- as an **approximation** of a deterministic algorithm
- to represent **uncertainty** without a parametric model
- to obtain higher computational **efficiency** with a small approximation error

Sampling Methods are also often called **Monte Carlo Methods**

Example: Monte-Carlo Integration

- Sample in the bounding box
- Compute fraction of inliers
- Multiply fraction with box size
Non-Parametric Representation

Probability distributions (e.g. a robot’s belief) can be represented:

- **Parametrically**: e.g. using mean and covariance of a Gaussian
- **Non-parametrically**: using a set of hypotheses (samples) drawn from the distribution

Advantage of non-parametric representation:
- No restriction on the type of distribution (e.g. can be multi-modal, non-Gaussian, etc.)
Non-Parametric Representation

The more samples are in an interval, the higher the probability of that interval

But:

How to draw samples from a function/distribution?
Sampling from a Distribution

There are several approaches:

- Probability transformation
  - Uses inverse of the c.d.f $h$
- Rejection Sampling
- Importance Sampling
- MCMC

Probability transformation:

- Sample uniformly in $[0,1]$
- Transform using $h^{-1}$

But:

- Requires calculation of $h$ and its inverse

\[ h(y) = \int_{-\infty}^{y} p(\hat{y}) d\hat{y} \]
Rejection Sampling

1. Simplification:
   • Assume $p(z) < 1$ for all $z$
   • Sample $z$ uniformly
   • Sample $c$ from $[0, 1]$

   • If $f(z) > c$ : keep the sample
     otherwise: reject the sample
Rejection Sampling

2. General case:
Assume we can evaluate \( p(z) = \frac{1}{Z_p} \tilde{p}(z) \) (unnormalized)

- Find proposal distribution \( q \)
  - Easy to sample from \( q \)
- Find \( k \) with \( kq(z) \geq \tilde{p}(z) \)
- Sample from \( q \)
- Sample uniformly from \([0,kq(z_0)]\)
- Reject if \( u_0 > \tilde{p}(z_0) \)

But: Rejection sampling is inefficient.
 Importance Sampling

• **Idea:** assign an importance weight $w$ to each sample

• With the importance weights, we can account for the “differences between $p$ and $q$”

\[ w(x) = \frac{p(x)}{q(x)} \]

• $p$ is called **target**

• $q$ is called **proposal** (as before)
Importance Sampling

**Explanation:** The prob. of falling in an interval $A$ is the area under $p$

- This is equal to the expectation of the indicator function $I(x \in A)$

$$E_p[I(z \in A)] = \int p(z)I(z \in A)dz$$
Importance Sampling

• **Explanation:** The prob. of falling in an interval $A$ is the area under $p$

• This is equal to the expectation of the indicator function $I(x \in A)$

$$E_p[I(z \in A)] = \int p(z)I(z \in A)\,dz$$

$$= \int \frac{p(z)}{q(z)}q(z)I(z \in A)\,dz = E_q[w(z)I(z \in A)]$$

**Requirement:**

$$p(x) > 0 \Rightarrow q(x) > 0$$

Approximation with samples drawn from $q$:

$$E_q[w(z)I(z \in A)] \approx \frac{1}{L} \sum_{l=1}^{L} w(z_l)I(z_l \in A)$$
The Particle Filter

- **Non-parametric** implementation of Bayes filter
- Represents the belief (posterior) \( \text{Bel}(x_t) \) by a set of random state samples.
- This representation is **approximate**.
- Can represent distributions that are **not Gaussian**.
- Can model **non-linear** transformations.

**Basic principle:**
- Set of state hypotheses ("particles")
- Survival-of-the-fittest
The Bayes Filter Algorithm (Rep.)

\[
Bel(x_t) = \eta \ p(z_t | x_t) \int p(x_t | u_t, x_{t-1})Bel(x_{t-1})dx_{t-1}
\]

Algorithm Bayes\_filter \( (Bel(x), d) \)

1. if \( d \) is a sensor measurement \( z \) then
2. \( \eta = 0 \)
3. for all \( x \) do
4. \( Bel'(x) \leftarrow p(z | x)Bel(x) \)
5. \( \eta \leftarrow \eta + Bel'(x) \)
6. for all \( x \) do \( Bel'(x) \leftarrow \eta^{-1}Bel'(x) \)
7. else if \( d \) is an action \( u \) then
8. for all \( x \) do \( Bel'(x) \leftarrow \int p(x | u, x')Bel(x')dx' \)
9. return \( Bel'(x) \)
Mathematical Description

Set of weighted samples:

$$\mathcal{X}_t := \{ \langle x_t^{[1]}, w_t^{[1]} \rangle, \langle x_t^{[2]}, w_t^{[2]} \rangle, \ldots, \langle x_t^{[M]}, w_t^{[M]} \rangle \}$$

The samples represent the probability distribution:

$$p(x) = \sum_{i=1}^{M} w_t^{[i]} \cdot \delta_{x_t^{[i]}}(x)$$

Point mass distribution ("Dirac")
The Particle Filter Algorithm

Algorithm $\text{Particle\_filter}(\mathbf{x}_{t-1}, u_t, z_t)$:

1. $\tilde{\mathbf{x}}_t = \mathbf{x}_t = \emptyset$
2. for $m = 1$ to $M$ do
3. sample $x_t^{[m]} \sim p(x_t | u_t, x_{t-1}^{[m]})$
4. $w_t^{[m]} \leftarrow p(z_t | x_t^{[m]})$
5. $\tilde{\mathbf{x}}_t \leftarrow \tilde{\mathbf{x}}_t \cup \langle x_t^{[m]}, w_t^{[m]} \rangle$
6. for $m = 1$ to $M$ do
   - draw $i$ with prob. $\propto w_t^{[i]}$
   - $\mathbf{x}_t \leftarrow \mathbf{x}_t \cup \langle x_t^{[i]}, 1/M \rangle$
7. return $\mathbf{x}_t$
Localization with Particle Filters

• Each particle is a potential pose of the robot
• Proposal distribution is the motion model of the robot (prediction step)
• The observation model is used to compute the importance weight (correction step)

Randomized algorithms are usually called Monte Carlo algorithms, therefore we call this:

Monte-Carlo Localization
A Simple Example

• The initial belief is a uniform distribution (global localization).
• This is represented by an (approximately) uniform sampling of initial particles.
Sensor Information

The sensor model \( p(z_t | x_t^{[m]}) \) is used to compute the new importance weights:

\[
    w_t^{[m]} \leftarrow p(z_t | x_t^{[m]})
\]
After resampling and applying the motion model

$$p(x_t \mid u_t, x^{[m]}_{t-1})$$

the particles are distributed more densely at three locations.
Again, we set the new importance weights equal to the sensor model.

\[ w_t^{[m]} \leftarrow p(z_t \mid x_t^{[m]}) \]
Resampling and application of the motion model:
One location of dense particles is left.

*The robot is localized.*
Algorithm **Particle_filter** $(\mathcal{X}_t, u_t, z_t)$:

1. $\tilde{\mathcal{X}}_t = \mathcal{X}_t = \emptyset$
2. for $m = 1$ to $M$ do
3. sample $x_t^{[m]} \sim p(x_t | u_t, x_{t-1}^{[m]})$
4. $w_t^{[m]} \leftarrow p(z_t | x_t^{[m]})$
5. $\tilde{\mathcal{X}}_t \leftarrow \tilde{\mathcal{X}}_t + \langle x_t^{[m]}, w_t^{[m]} \rangle$
6. for $\tilde{\mathcal{X}}_t$ do
   - for $m = 1$ to $M$ do
     - draw $i$ with prob. $\propto w_t^{[i]}$
     - $\mathcal{X}_t \leftarrow \mathcal{X}_t \cup x_t^{[i]}$
7. return $\mathcal{X}_t$
Sampling from Proposal

This can be done in the following ways:

- Adding the motion vector to each particle directly (this assumes perfect motion)
- Sampling from the motion model, e.g. for a 2D motion with translation velocity \( v \) and rotation velocity \( w \) we have:

\[
\begin{align*}
\text{sample } x_t^m & \sim p(x_t | u_t, x_{t-1}^m) \\
\end{align*}
\]
Motion Model Sampling (Example)
Computation of Importance Weights

Computation of the sample weights:

- Proposal distribution: 
  \[ g(x_t^{[m]}) = p(x_t^{[m]} | u_t, x_{t-1}^{[m]}) \text{Bel}(x_{t-1}^{[m]}) \]  
  (we sample from that using the motion model)

- Target distribution (new belief):
  \[ f(x_t^{[m]}) = \text{Bel}(x_t^{[m]}) \]  
  (we can not directly sample from that → importance sampling)

- Computation of importance weights:

\[
w_t^{[m]} = \frac{f(x_t^{[m]})}{g(x_t^{[m]})} \propto \frac{p(z_t | x_t^{[m]})p(x_t^{[m]} | u_t, x_{t-1}^{[m]}) \text{Bel}(x_{t-1}^{[m]})}{p(x_t^{[m]} | u_t, x_{t-1}^{[m]}) \text{Bel}(x_{t-1}^{[m]})} = p(z_t | x_t^{[m]})
\]
Proximity Sensor Models

- How can we obtain the sensor model $p(z_t \mid x_t^{[m]})$?
- Sensor Calibration:

![Graph for Laser sensor](image1.png)

![Graph for Sonar sensor](image2.png)

Laser sensor

Sonar sensor
Resampling

• Given: Set $\tilde{X}_t$ of weighted samples.
• Wanted: Random sample, where the probability of drawing $x_i$ is equal to $w_i$.
• Typically done $M$ times with replacement to generate new sample set.

for $m = 1$ to $M$

draw $i$ with prob. $\propto w_t^{[i]}$

$X_t \leftarrow X_t \cup x_t^{[i]}$ for $t$ to do
Resampling

- Standard n-times sampling results in high variance
- This requires more particles
- $O(n \log n)$ complexity

- Instead: low variance sampling only samples once
- Linear time complexity
- Easy to implement
Sample-based Localization (sonar)
Initial Distribution
After Ten Ultrasound Scans
After 65 Ultrasound Scans
Estimated Path
Kidnapped Robot Problem

The approach described so far is able to
- track the pose of a mobile robot and to
- globally localize the robot.

- How can we deal with localization errors (i.e., the kidnapped robot problem)?

**Idea:** Introduce uniform samples at every resampling step
- This adds new hypotheses
Summary

- There are mainly 4 different types of sampling methods: Transformation method, rejections sampling, importance sampling and MCMC

- Transformation only rarely applicable

- Rejection sampling is often very inefficient

- Importance sampling is used in the particle filter which can be used for robot localization

- An efficient implementation of the resampling step is the low variance sampling
Markov Chain Monte Carlo
Markov Chain Monte Carlo

- In high-dimensional spaces, rejection sampling and importance sampling are very inefficient.
- An alternative is Markov Chain Monte Carlo (MCMC).
- It keeps a record of the current state and the proposal depends on that state.
- Most common algorithms are the Metropolis-Hastings algorithm and Gibbs Sampling.
Markov Chains Revisited

A Markov Chain is a distribution over discrete-state random variables $x_1, \ldots, x_M$ so that

$$p(x_1, \ldots, x_T) = p(x_1)p(x_2 \mid x_1) \cdots = p(x_1) \prod_{t=2}^{T} p(x_t \mid x_{t-1})$$

The graphical model of a Markov chain is this:

We will denote $p(x_t \mid x_{t-1})$ as a row vector $\pi_t$

A Markov chain can also be visualized as a state transition diagram.
The State Transition Diagram

The diagram illustrates the state transitions across different time steps, denoted as $t-2$, $t-1$, and $t$, with corresponding states $k=1$, $k=2$, and $k=3$. The transitions are represented by matrices $A_{11}$ and $A_{33}$, indicating the probability of state changes over time.
Some Notions

• The Markov chain is said to be **homogeneous** if the transitions probabilities are all the same at every time step \( t \) (here we only consider homogeneous Markov chains)

• The transition matrix is **row-stochastic**, i.e. all entries are between 0 and 1 and all rows sum up to 1

• Observation: the probabilities of reaching the states can be computed using a vector-matrix multiplication
The Stationary Distribution

The probability to reach state $k$ is $\pi_{k,t} = \sum_{i=1}^{K} \pi_{i,t-1} A_{ik}$

Or, in matrix notation: $\pi_t = \pi_{t-1} A$

We say that $\pi_t$ is **stationary** if $\pi_t = \pi_{t-1}$

**Questions:**

- How can we know that a stationary distribution exists?
- And if it exists, how do we know that it is unique?
The Stationary Distribution (Existence)

To find a stationary distribution we need to solve the eigenvector problem $A^T \mathbf{v} = \mathbf{v}$

The stationary distribution is then $\pi = \mathbf{v}^T$ where $\mathbf{v}$ is the eigenvector for which the eigenvalue is 1.

This eigenvector needs to be normalized so that it is a valid distribution.

Theorem (Perron-Frobenius): Every row-stochastic matrix has such an eigenvector, but this vector may not be unique.
Stationary Distribution (Uniqueness)

- A Markov chain can have many stationary distributions
- Sufficient for a unique stationary distribution: we can reach every state from any other state in finite steps at non-zero probability (i.e. the chain is **ergodic**)
- This is equivalent to the property that the transition matrix is **irreducible**:

\[ \forall i, j \exists m \quad (A^m)_{ij} > 0 \]
Main Idea of MCMC

• So far, we specified the transition probabilities and analysed the resulting distribution
• This was used, e.g. in HMMs

Now:

• We want to sample from an arbitrary distribution
• To do that, we design the transition probabilities so that the resulting stationary distribution is our desired (target) distribution!
Detailed Balance

**Definition:** A transition distribution $\pi_t$ satisfies the property of **detailed balance** if $\pi_i A_{ij} = \pi_j A_{ji}$.

The chain is then said to be **reversible**.

![Graph with detailed balance](attachment:image.png)
Making a Distribution Stationary

**Theorem:** If a Markov chain with transition matrix $A$ is irreducible and satisfies detailed balance wrt. the distribution $\pi$, then $\pi$ is a stationary distribution of the chain.

**Proof:**

$$\sum_{i=1}^{K} \pi_i A_{ij} = \sum_{i=1}^{K} \pi_j A_{ji} = \pi_j \sum_{i=1}^{K} A_{ji} = \pi_j \quad \forall j$$

it follows $\pi = \pi A$.

This is a sufficient, but not necessary condition.
Sampling with a Markov Chain

The idea of MCMC is to sample state transitions based on a proposal distribution $q$.

The most widely used algorithm is the Metropolis-Hastings (MH) algorithm.

In MH, the decision whether to stay in a given state is based on a given probability.

If the proposal distribution is $q(x' \mid x)$, then we stay in state $x'$ with probability

$$
\min \left( 1, \frac{\tilde{p}(x')q(x \mid x')}{\tilde{p}(x)q(x' \mid x)} \right)
$$

Unnormalized target distribution
The Metropolis-Hastings Algorithm

- Initialize $x^0$
- for $s = 0, 1, 2, \ldots$
  - define $x = x^s$
  - sample $x' \sim q(x' \mid x)$
  - compute acceptance probability
    $$\alpha = \frac{\tilde{p}(x')q(x \mid x')}{\tilde{p}(x)q(x' \mid x)}$$
  - compute $r = \min(1, \alpha)$
  - sample $u \sim U(0, 1)$
  - set new sample to
    $$x^{s+1} = \begin{cases} 
      x' & \text{if } u < r \\
      x^s & \text{if } u \geq r
    \end{cases}$$
Why Does This Work?

We have to prove that the transition probability of the MH algorithm satisfies detailed balance wrt the target distribution.

**Theorem:** If \( p_{MH}(x' \mid x) \) is the transition probability of the MH algorithm, then

\[
p(x)p_{MH}(x' \mid x) = p(x')p_{MH}(x \mid x')
\]

**Proof:**
Why Does This Work?

We have to prove that the transition probability of the MH algorithm satisfies detailed balance wrt the target distribution.

**Theorem:** If $p_{MH}(x' \mid x)$ is the transition probability of the MH algorithm, then

$$p(x)p_{MH}(x' \mid x) = p(x')p_{MH}(x \mid x')$$

**Note:** All formulations are valid for discrete and for continuous variables!
Choosing the Proposal

- A proposal distribution is valid if it gives a non-zero probability of moving to the states that have a non-zero probability in the target.
- A good proposal is the Gaussian, because it has a non-zero probability for all states.
- **However:** the variance of the Gaussian is important!
  - with low variance, the sampler does not explore sufficiently, e.g. it is fixed to a particular mode
  - with too high variance, the proposal is rejected too often, the samples are a bad approximation
Example

Target is a mixture of 2 1D Gaussians.
Proposal is a Gaussian with different variances.
Summary

• Markov Chain Monte Carlo is a family of sampling algorithms that can sample from arbitrary distributions by moving in state space

• Most used methods are the Metropolis-Hastings (MH) and the Gibbs sampling method

• MH uses a proposal distribution and accepts a proposed state randomly

• Finding a good proposal distribution is important for the quality of the approximation to the target distribution