Friedrich-Alexander-Universität
Technische Fakultät

Machine Learning
Data Analytics

Machine Learning for Time Series (MLTS)

Lecture 5: Sequential Monte Carlo and Particle Filtering

Dr. Dario Zanca

Machine Learning and Data Analytics (MaD) Lab
Friedrich-Alexander-Universität Erlangen-Nürnberg
14.11.2024

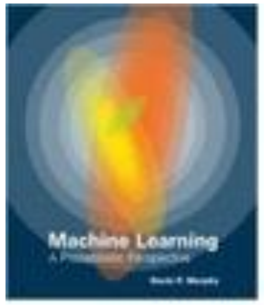
Topics overview

Topics overview

References

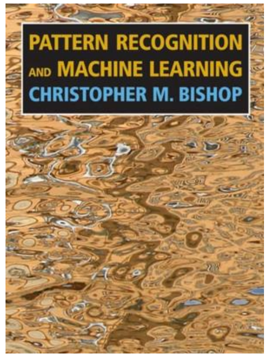
Machine learning: A Probabilistic Perspective,

by Kevin Murphy (2012)



Pattern Recognition and Machine Learning

by C. M. Bishop (2008)



In this lecture…

Sequential Monte Carlo and Particle Filtering

Concepts recap

Review concept: State Space Models (SSMs)

LG-SSMs are characterized by:

- Transition density: $p(z_n | z_{n-1})$
- Measurement/Observation density: $p(y_n | z_n)$

Joint density can be expressed using the *chain rule*:

$$p(z_{1:n} | y_{1:n}) = p(z_1) \prod_{i=2}^{n} p(z_i | z_{i-1}) \prod_{i=1}^{n} p(y_i | z_i)$$

where $z_{1:n} = (z_1, \dots, z_n)$ and $y_{1:n} = (y_1, \dots, y_n)$.

Filtering is the task of estimating $p(z_n | y_{1:n})$.

Review concept: Bayesian filtering

Let $p(z_{n-1}|y_{1:n-1})$ be the filtering density at time step $n-1$ and we wish to determine $p(z_n|y_{1:n})$.

We can use the following iterative steps:

- Prediction step:

$$p(z_n|y_{1:n-1}) = \int \underbrace{p(z_n|z_{n-1})}_{\text{transition density}} \; \underbrace{p(z_{n-1}|y_{1:n-1})}_{\text{filtering density}} dz_n$$

- Correction step:

$$p(z_n|y_{1:n}) = \frac{\overbrace{p(y_n|z_n)}^{\text{likelihood}}\, p(z_n|y_{1:n-1})}{p(y_n|y_{1:n-1})}$$

Review concept: Bayesian filtering

Let $p(z_{n-1}|y_{1:n-1})$ be the filtering density at time step $n-1$ and we wish to determine $p(z_n|y_{1:n})$.

We can use the following iterative steps:

- Prediction step:

$$p(z_n|y_{1:n-1}) = \int \underbrace{p(z_n|z_{n-1})}_{\text{transition density}} \underbrace{p(z_{n-1}|y_{1:n-1})}_{\text{filtering density}} dz_n$$

- Correction step:

$$p(z_n|y_{1:n}) = \frac{\overbrace{p(y_n|z_n)}^{\text{likelihood}} p(z_n|y_{1:n-1})}{p(y_n|y_{1:n-1})}$$

If the variables are normally distributed and the transitions are linear, the Bayes filter becomes equal to the Kalman filter.

Review concepts: Kalman Filters

Prediction step (time update):

$$\bar{z}_n = F_n z_{n-1} + B_n u_n$$

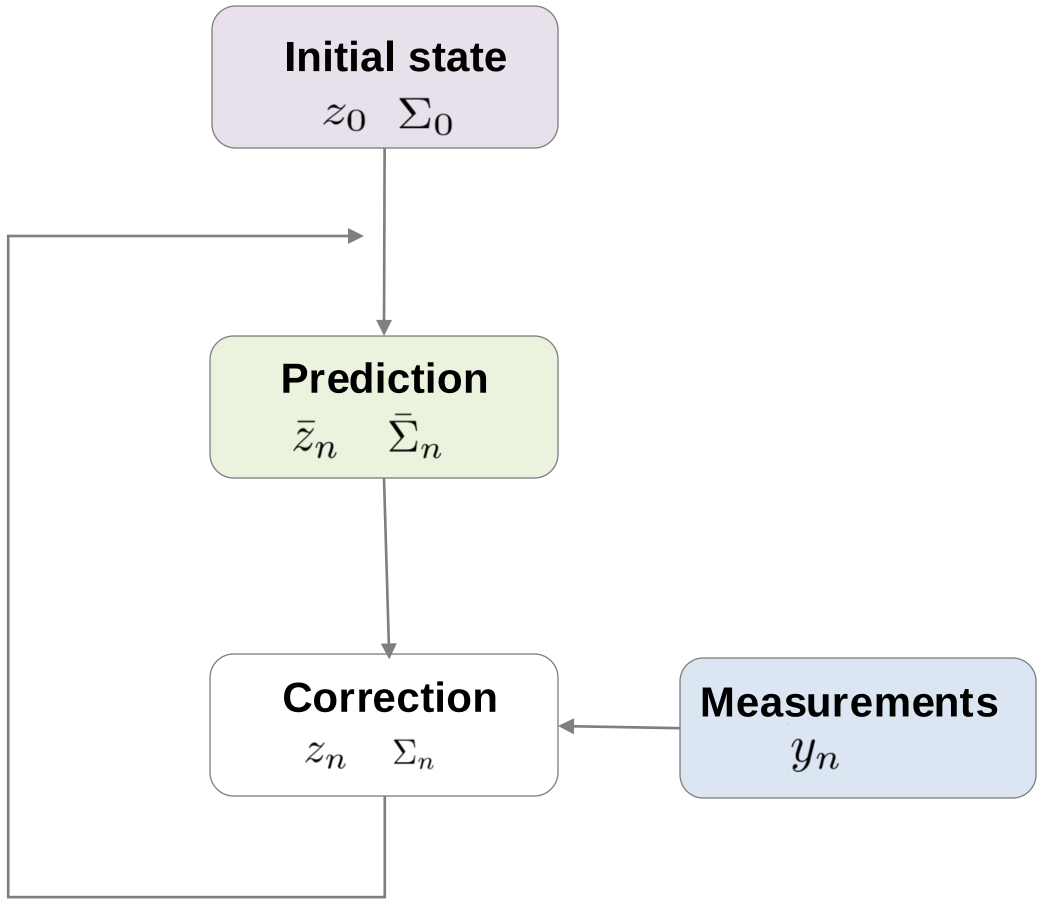
$$\bar{\Sigma}_n = F_n \Sigma_{n-1} F_n^T + R_n$$

Filtering step (Measurement update):

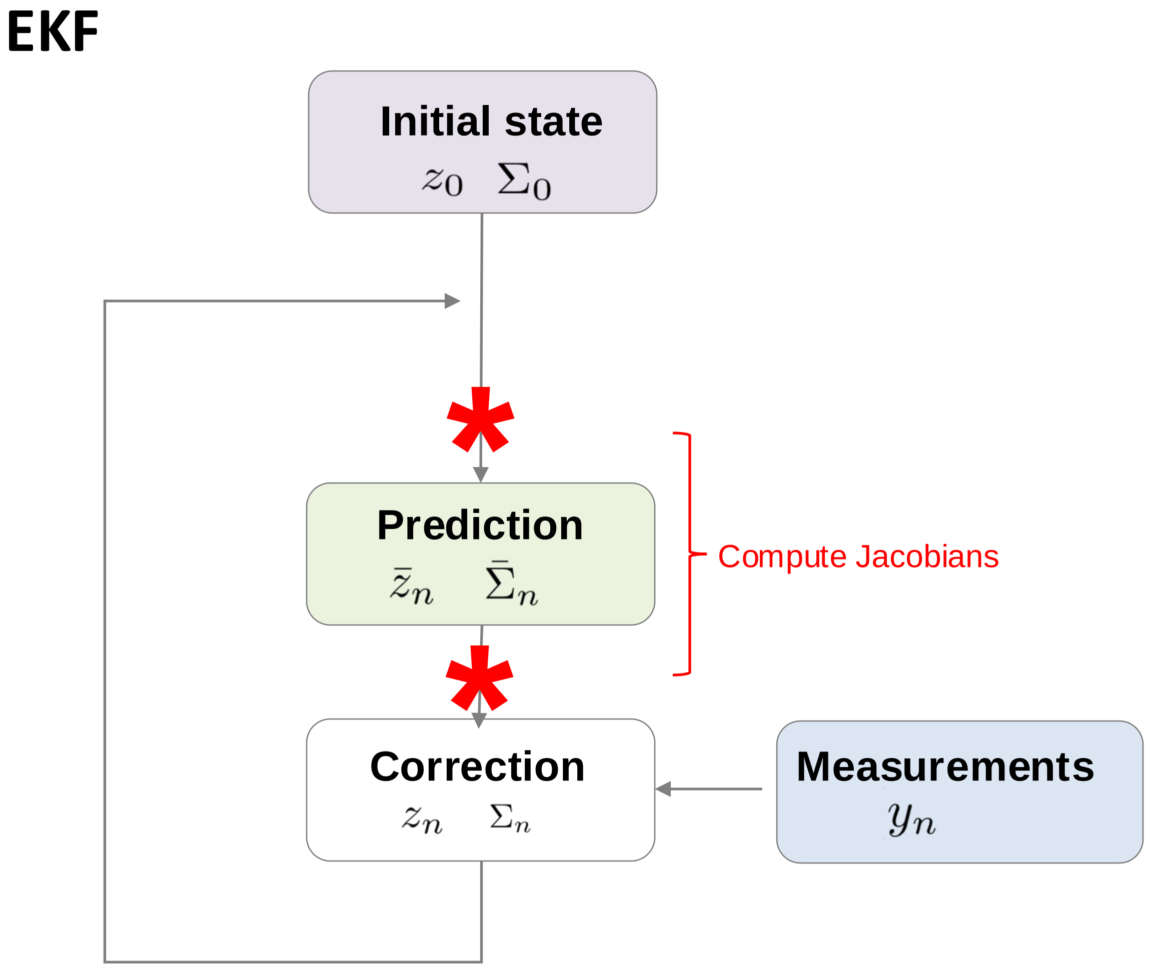
$$K_n = \bar{\Sigma}_n H_n^T \left(H_n \bar{\Sigma}_n H_n^T + Q_n\right)^{-1}$$

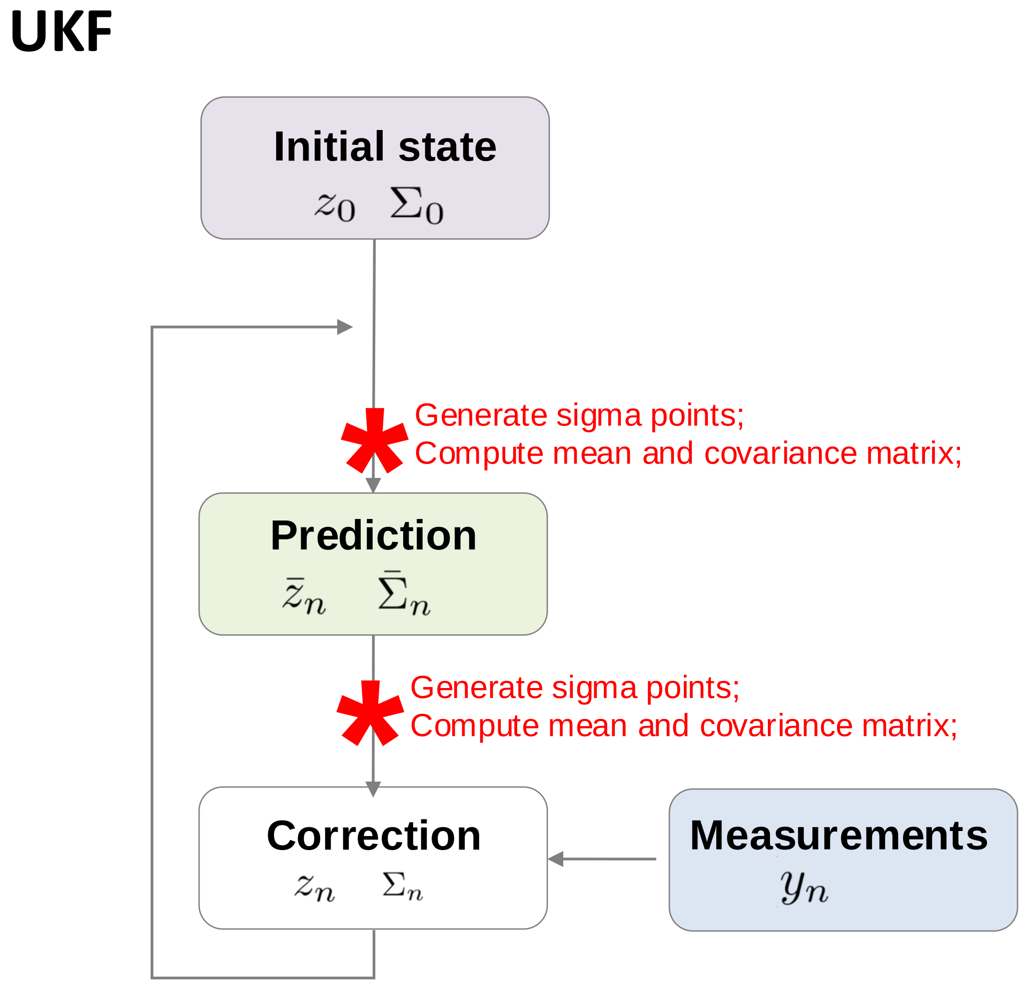
$$z_n = \bar{z}_n + K_n \left(y_n - H_n \bar{z}_n\right)$$

$$\Sigma_n = \left(1 - K_n H_n\right) \bar{\Sigma}_n$$



Review concepts: EKF and UKF





Review concepts: KFs comparison

Estimator	State-transition / Measurement models assumptions	Assumed noise distribution	Computational cost
Kalman Filter	Linear	Gaussian	Low
Extended Kalman Filter	Non-linear (but locally linear)	Gaussian	Low / Medium (depending on the difficulty of computing the Jacobian)
Unscented Kalman Filter	Non-linear	Gaussian	Medium

Sequential Monte Carlo and Particle Filtering

Monte Carlo methods

Motivation

The fundamental goal of this section is **"how to find the expectation of a function $\boldsymbol{f(z)}$ with respect to a probability distribution $\boldsymbol{p(z)}$".**

$$\mathbb{E}[f] = \int f(z)p(z)dz$$

Motivation

The fundamental goal of this section is **"how to find the expectation of a function $\boldsymbol{f(z)}$ with respect to a probability distribution $\boldsymbol{p(z)}$".**

$$\mathbb{E}[f] = \int f(z)p(z)dz$$

Sampling methods can be used to approximate this expectation using a set of samples $z^s \sim p(z)$, by the finite sum:

$$\frac{1}{S}\sum_{s=1}^{S} f(z^s)$$

where $S \in \mathbb{Z}^+$.

Motivation

However, possible problems are:

- Samples z^s might not be independent
- Depending on f, expectation might be dominated by examples with small probability

→ We need relatively large sample size S.

Monte Carlo methods (MC)

Monte Carlo methods include a wide class of **algorithms that rely on random sampling** to obtain numerical results.

- Use randomness to solve problem that might be deterministic in principle.
- Used, e.g., in optimization, numerical integration and for generating draws from a probability distribution.

Monte Carlo methods (MC)

Monte Carlo methods include a wide class of **algorithms that rely on random sampling** to obtain numerical results.

- Use randomness to solve problem that might be deterministic in principle.
- Used, e.g., in optimization, numerical integration and for generating draws from a probability distribution.

E.g., if we are interested in applying a filtering method, and the filtering density is complicated → Computations of prediction and correction steps cannot be done analytically.

In such cases, we use Monte Carlo methods for numerical computations.

General idea behind MC methods

The general ideal behind Monte Carlo methods can be summarised in 4 essential steps:

Define a domain of possible inputs

Generate input randomly from a probability distribution

Perform deterministic computations on the input

Aggregate results

Rejection sampling

Rejection sampling is a Monte Carlo algorithm to sample data from a sophisticated (“difficult to sample from”) distribution with the help of a proxy distribution.

Let us suppose that:

- We wish to sample from a “non-standard” distribution $p(z)$
- Sampling directly from $p(z)$ is difficult
- We are able to evaluate $\mathrm{p}(z)$ for any z, up to a certain (unknown) normalizing constant Z_p:

$$\mathrm{p}(z) = \tilde{p}(z)/Z_p$$

To apply rejection sampling, we make use of a simpler distribution $q(z)$, also called **proposal distribution** →We are able to readily draw samples from $q(z)$

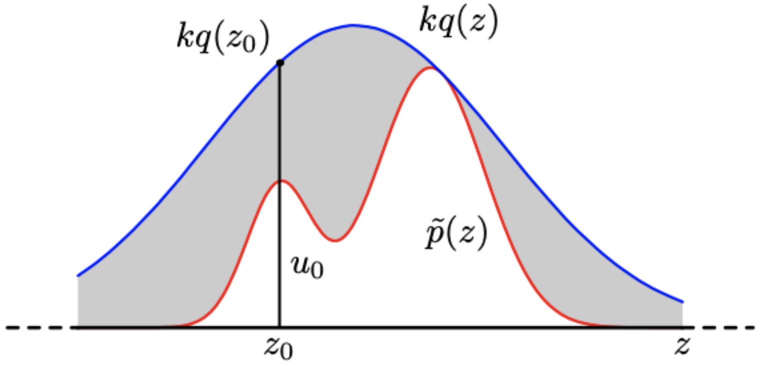
Rejection sampling

Samples are generated from the proposal distribution $q(z)$ and **rejected** if they fall between the unnormalized $\tilde{p}(z)$ and the scaled distribution $kq(z)$.

→ In the side figure, samples are rejected if they fall in the grey area.

→ Samples are accepted with probability $\frac{\tilde{p}(z)}{kq(z)}$

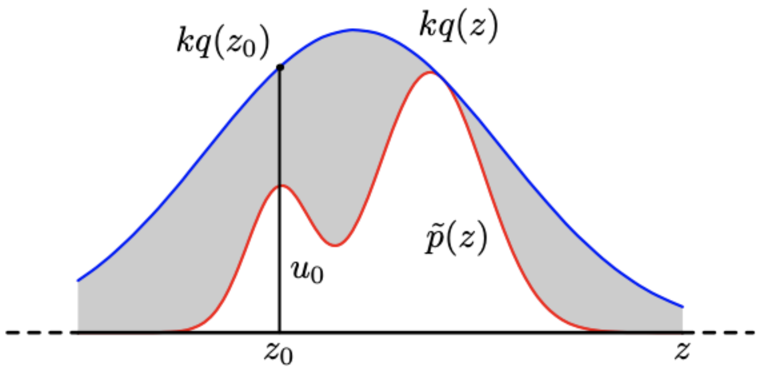
Note: k is a constant value which is chosen such that $kq(z) \geq \tilde{p}(z)$ for all values of z.



Rejection method

The success of the rejection method depend on the success in determining a suitable value for the constant k.

→ This is impractical in many cases, which leads to very small acceptance rates.



Importance sampling

Importance sampling is a method which allows approximating expectations directly.

Suppose, similarly to the previous case, that:

- It is impractical to draw samples from $p(z)$
- But we can evaluate $p(z)$ easily for any z

Uniform sampling from the space of z is inefficient (high-dimensionality) and only few samples will have significant contribution.

$\rightarrow$ We would like to chose samples from regions where $p(z)$ is large.

Importance sampling

We draw samples from a proposal distribution $q(z)$. Then,

$$\mathbb{E}[f] = \int f(z)p(z)dz = \int f(z)\frac{p(z)}{q(z)}q(z)dz \approx \boldsymbol{\frac{1}{S}\sum_{s=1}^{S}\frac{p(z^s)}{q(z^s)}f(z^s)}$$

The quantity $\frac{p(z^s)}{q(z^s)}$ measures the importance of each sample and are called **importance weights**.

- Compared to rejection sampling, no samples are rejected.
- Importance sampling do not provide itself a mechanism for drawing samples from a distribution $q(z)$.

Sampling-importance-resampling approach

The **sampling-importance-resampling** approach also makes use of a proposal distribution $q(z)$ and **avoids determining a constant $\boldsymbol{k}$**.

It consists of there *general* steps:

1. Sampling of $\{z_1, \dots, z_s\}$ from the proposal distribution $q(z)$
2. Construction of importance weights $\{w_1, \dots, w_s\}$
3. Resampling from a discrete distribution with probabilities given by the weights

Property. The resulting samples are approximately distributed according to $p(z)$ and the distribution becomes correct for $S \to \infty$.

Sequential Monte Carlo and Particle Filtering

Particle Filtering (PF): Theory

Motivations

Estimator	State-transition / Measurement models assumptions	Assumed noise distribution	Computational cost
Kalman Filter	Linear	Gaussian	Low
Extended Kalman Filter	Non-linear (but locally linear)	Gaussian	Low / Medium (depending on the difficulty of computing the Jacobian)
Unscented Kalman Filter	Non-linear	Gaussian	Medium

Particle Filtering (PF)

We can use sampling-importance-resampling formalism to obtain a **sequential Monte Carlo**, also said **particle filtering**.

PF is a Monte Carlo (or simulation-based) approach for recursive Bayesian inference.

- It **approximates the prediction-correction cycle**
- It can be used for systems that are **not linear-Gaussian,** to make tractable inference algorithms
- It is widely applied in many areas (e.g., tracking, forecasting, online parameter learning, …)

🔍 The term “particle filters” originated in in reference to mean-field interacting particle methods used in fluid mechanics since early 1960s (Del Moral, 1966).

Particle Filtering (PF)

First, we update the belief state using importance sampling.

If the proposal distribution has the form $q(z^s_{1:n}|y_{1:n})$, then the importance weights are given by

$$w^s_n \propto \frac{p(z^s_{1:n}|y_{1:n})}{q(z^s_{1:n}|y_{1:n})}$$

which can be normalized as follow:

$$\hat{w}^s_n \propto \frac{w^s_n}{\sum_{s'} w^{s'}_n}$$

Particle Filtering (PF)

We observe that we can rewrite the numerator recursively as follows:

$$p(z_{1:n}|y_{1:n}) = \frac{p(y_n|z_{1:n}, y_{1:n-1})p(z_{1:n}|y_{1:n-1})}{p(y_n|y_{1:t-1})}$$

$$= \frac{p(y_n|z_n)p(z_n|z_{1:n-1}, y_{1:n-1})p(z_{1:n-1}|y_{1:n-1})}{p(y_n|y_{1:t-1})}$$

$$\propto p(y_n|z_n)p(z_n|z_{n-1})p(z_{1:n-1}|y_{1:n-1})$$

Markov property

And, similarly, the denominator:

$$q(z_{1:n}|y_{1:n}) = q(z_n|z_{1:n-1}, y_{1:n})\, q(z_{1:n-1}|\, y_{1:n-1})$$

Particle Filtering (PF)

Therefore, we use this formulation to derive an iterative update for the weights:

$$w_n^s \propto \frac{p(z_{1:n}^s|y_{1:n})}{q(z_{1:n}^s|y_{1:n})}$$

$$\propto \frac{p(y_n|z_n^s)p\left(z_n^s\middle|z_{n-1}^s\right)p(z_{1:n-1}^s|y_{1:n-1})}{q(z_n^s|z_{1:n-1}^s, y_{1:n})\ q(z_{1:n-1}^s|\ y_{1:n-1})}$$

$$= w_{n-1}^s \frac{p(y_n|z_n^s)p\left(z_n^s\middle|z_{n-1}^s\right)}{q(z_n^s|z_{1:n-1}^s, y_{1:n})}$$

And we can approximate the posterior filtered density using

$$p(\mathrm{z_n}|\mathrm{y_{1:n}}) \approx \sum_{s=1}^{S} \widehat{w}_n^s \delta_{z_n^s}(z_n)$$

Particle Filtering (PF)

Therefore, we use this formulation to derive an iterative update for the weights:

$$w_n^s \propto \frac{p(z_{1:n}^s|y_{1:n})}{q(z_{1:n}^s|y_{1:n})}$$

$$\propto \frac{p(y_n|z_n^s)p\left(z_n^s\middle|z_{n-1}^s\right)p(z_{1:n-1}^s|y_{1:n-1})}{q(z_n^s|z_{1:n-1}^s, y_{1:n})\ q(z_{1:n-1}^s|\ y_{1:n-1})}$$

$$= w_{n-1}^s \frac{p(y_n|z_n^s)p\left(z_n^s\middle|z_{n-1}^s\right)}{q(z_n^s|z_{1:n-1}^s, y_{1:n})}$$

And we can approximate the posterior filtered density using

$$p(\mathrm{z_n}|\mathrm{y_{1:n}}) \approx \sum_{s=1}^{S} \hat{w}_n^s \delta_{z_n^s}(z_n)$$

The Dirac delta represents a spike at each particle location allowing approximation of theposterior as weighted sum of discrete particles.

Particle Filtering: the degeneracy problem

The basic sequential importance fails after a few steps because most of the particles will have negligible weights.

→ This problem is know as **degeneracy problem** and it occurs when sampling in high dimensional spaces

We can quantify the degree of degeneracy by using the effective sampling size, defined by:

$$S_{eff} = \frac{1}{\sum_{s=1}^{S} (w_n^s)^2}$$

When the variance of the weights is too large, we are wasting resources updating particles with negligible weights.

Particle filtering: the resampling step

The degeneracy problem can be solved by **adding a resampling step.**

Wheneven the effective sampling size S_{eff} drops a certain threshold:

- we eliminate particles with low weights and
- we create replicates of the survival particles.

In particular, we generate a new set $\{z_n^{s*}\}_{s=1}^{S}$ by sampling replacement S times according to the weighted distribution obtained previously $\sum_{s=1}^{S} \widehat{w}_n^s \delta_{z_n^s}(z_n)$.

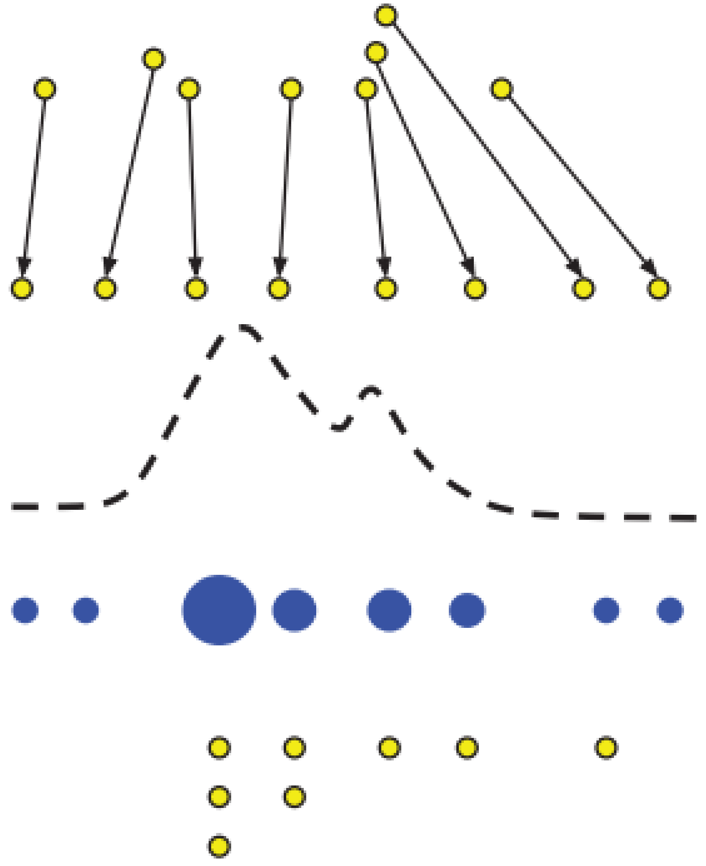
The result is an *i.i.d. unweighted sample* from the discrete density, so we set the new weights to $w_n^s = 1/S$.

PF: the overall scheme

Proposal

Weighting

Resampling



$p(z_{1:n-1}|y_{1:n-1})$

$p(z_{1:n}|y_{1:n-1})$

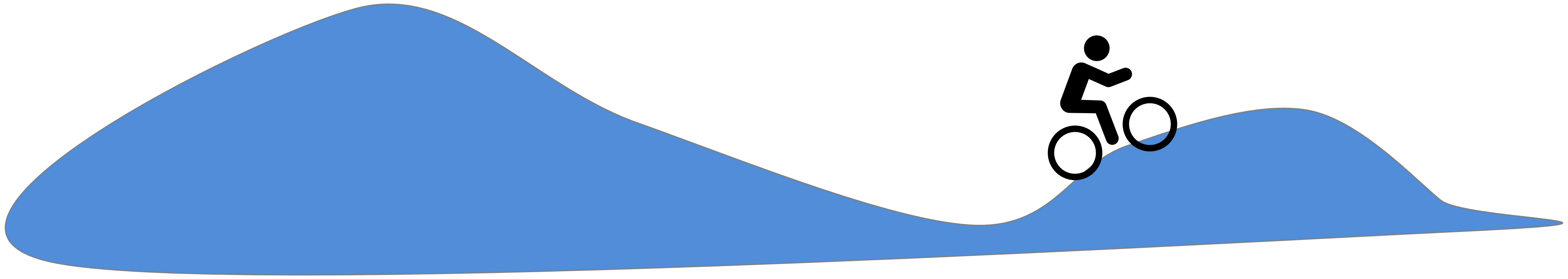
$p(y_n\ |z_n)$

$p(z_n\ |y_{1:n})$

Sequential Monte Carlo and Particle Filtering

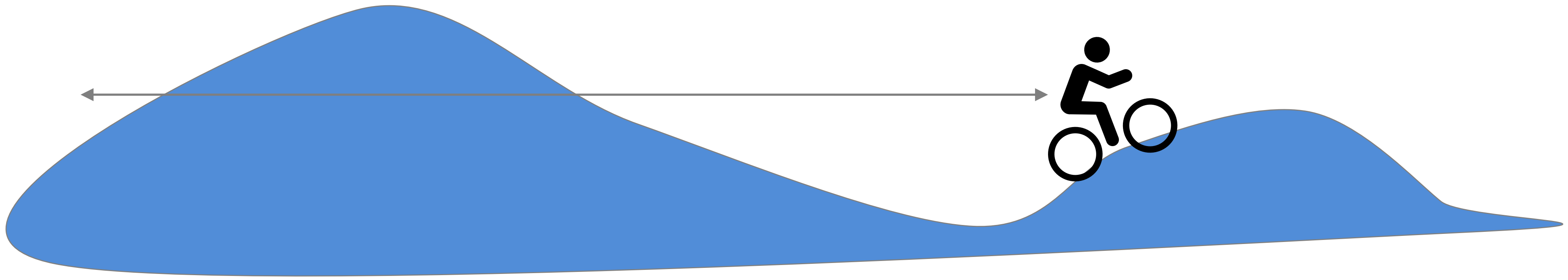
Particle Filtering (PF): Example and Algorithmic View

PF: Example



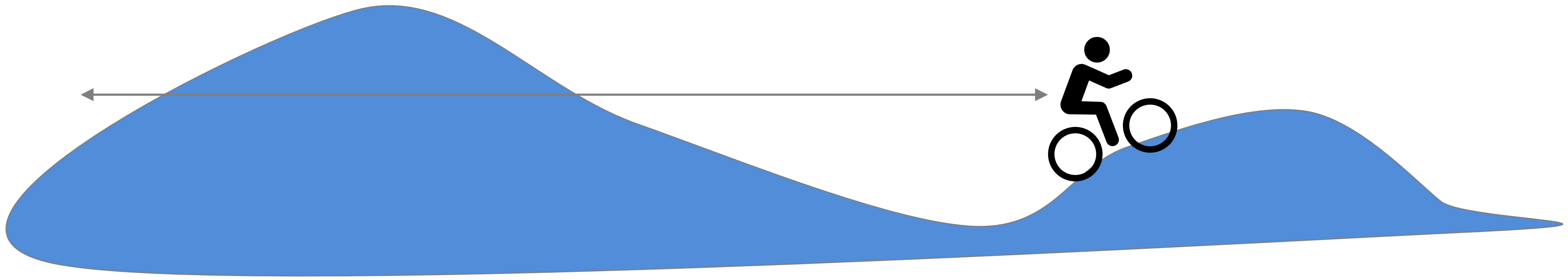
PF: Example

1. We want to estimate the **horizontal position** of the cyclist.



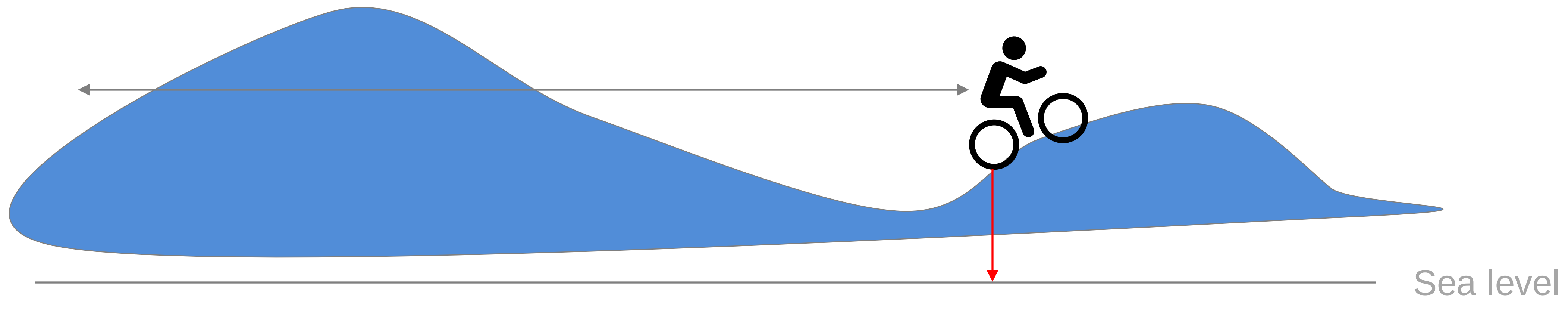
PF: Example

1. We want to estimate the **horizontal position** of the cyclist.
2. We have **knowledge** about the hills' morphology

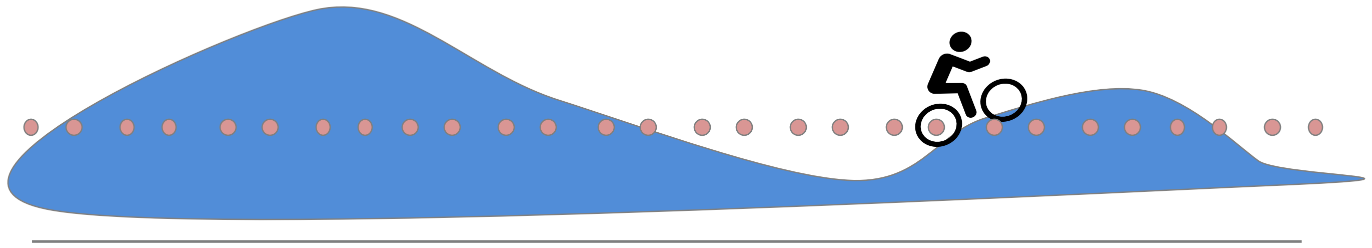


PF: Example

1. We want to estimate the **horizontal position** of the cyclist.
2. We have **knowledge** about the hills’ morphology
3. We receive noisy **measures of the altitude** (e.g., in relation to sea level).



PF: Example



▬ Particles (time n)

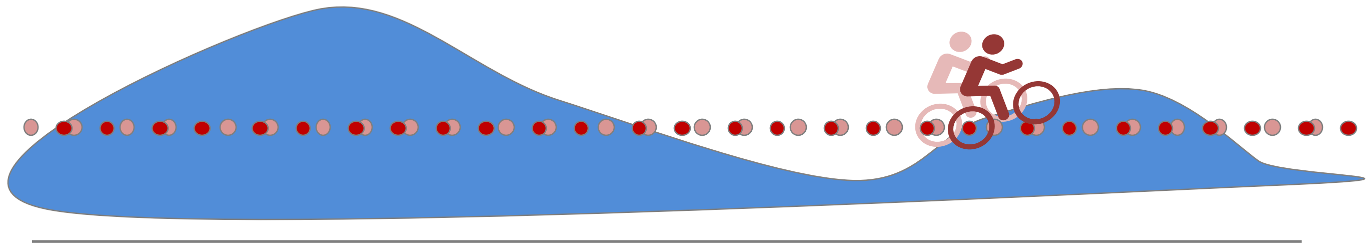
We draw a **set of particles** $\langle z_n^s, w_n^s \rangle_{s\in\{1,\dots,S\}}$

- n is the time index,
- z_n^s is a state hypothesis,
- w_n^s corresponding weights.

These samples represent the prior probability:

$$p(z_n|y_1,\dots,y_n) \simeq \sum_{s=1}^{S} w_n^s * \delta(z_n^s)$$

PF: Example



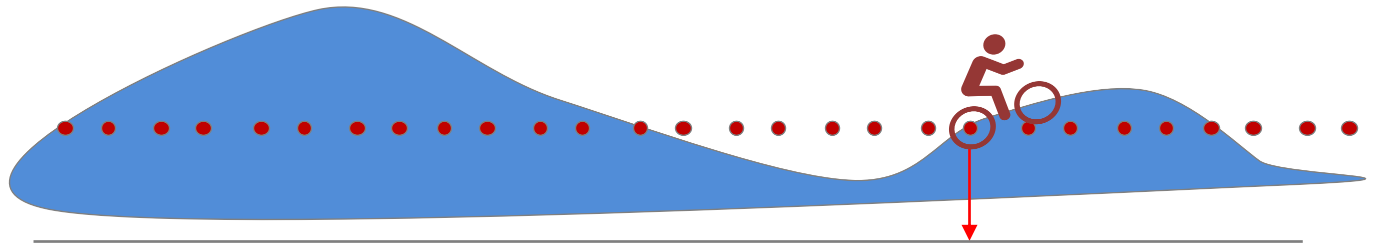
🟥 Particles (time n)

🟥 Propagated Particles (time $n+1$)

In the **prediction step,** we use our transition model f to **propagate** particles forward in time:

$$z_{n+1}^{s} = f(z_n^s) + \epsilon$$

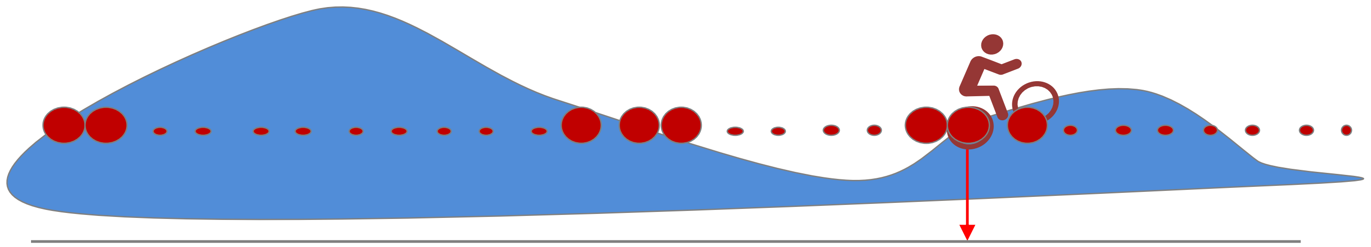
PF: Example



In the **correction step,** we **compute particle weights** based on the new sensory information y_{n+1}:

$$w_{n+1}^{s} = w_{n}^{s} * p(y_{n+1} | z_{n+1}^{s})$$

PF: Example



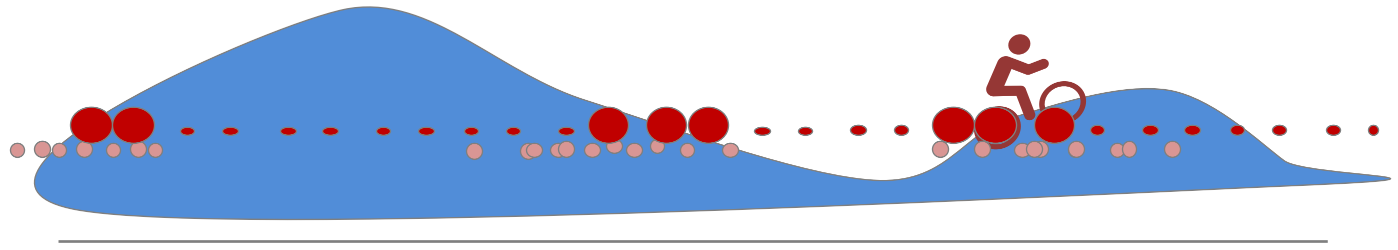
In the **correction step,** we **compute particle weights** based on the new sensory information y_{n+1}:

$$w_{n+1}^s = w_n^s * p(y_{n+1} | z_{n+1}^s)$$

Now the distribution $p(z_{n+1} | y_{1:t+1})$ is represented by the particle set:

$$\langle z_{n+1}^s, w_{n+1}^s \rangle_{s \in \{1, \ldots, S\}}$$

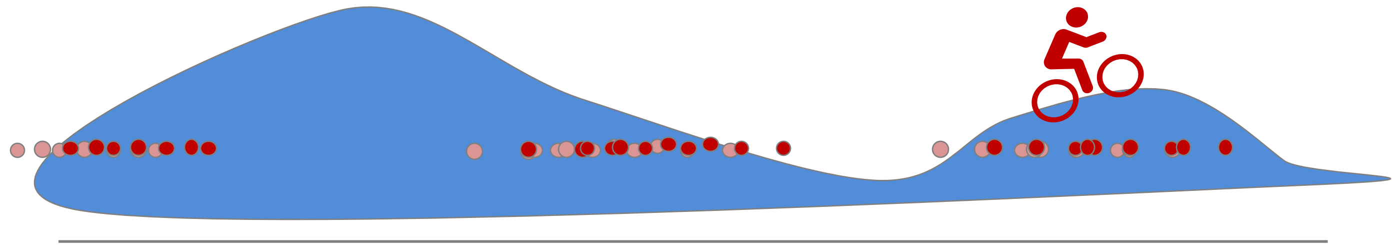
PF: Example



We **repeat** the previous steps:

- Sampling again from the new distribution (we have more particles close to the more likely state’s hypothesis).

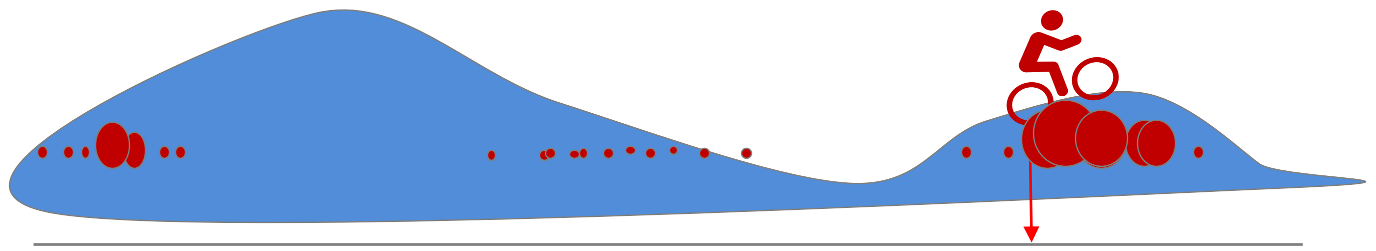
PF: Example



We **repeat** the previous steps:

- Sampling again from the new distribution (we have more particles close to the more likely state's hypothesis).
- We propagate again through time.

PF: Example



We **repeat** the previous steps:

- Sampling again from the new distribution (we have more particles close to the more likely state's hypothesis).
- We propagate again through time.
- We perform again a correction, based on the new measurement, and update the particles' weights.
- …

PF: An algorithmic view

```
Initially sample $S$ particles $z_1^S$
For $n = 1, \dots, N$
    For $s = 1, \dots, S$
        Draw $z_n^s \sim q(z_n^s | z_{n-1}^s, y_n)$
        update and normalize $w_{n+1}^s$
        if $S_{eff} < \mathrm{S}_{\min}$:
                Resample particles
                Re-initialize weights
        End
    End
End
```

Sequential Monte Carlo and Particle Filtering

Recap

Recap

- Monte Carlo methods
  - Rejection method
  - Importance sampling
  - Sampling-importance-resampling approach
- Particle filtering

Particle Filtering: pros and cons

Advantages:

- Ability to represent arbitrary densities
- Adaptive focusing on probable regions of state-space
- Dealing with non-Gaussian noise

Disadvantages:

- High computational complexity
- It is difficult to determine optimal number of particles
- Number of particles increase with increasing model dimension
- Potential problems: degeneracy