More Statistics for IIB Project

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Abstract

1 Understanding of the Big Story

In Michaelmas term (work documented in the previous report), what we did was building a framework for generating and inferring state space models driven by Levy process, NVM process as the most discussed example. In the inference part, we assumed that the exact driving process is known with full details, including the jump sizes and times, making the rest of the system Gaussian (hence called a conditionally Gaussian system), and we implemented a Kalman filter to infer in such case. In this work, we first narrow down the assumption of knowing the exact process driving the system with full details to knowing the exact generator for the driving process, and use it as the proposal for a bootstrap particle filter which can be used alone or combined with a Kalman filter to form the marginalized particle filter to infer in the system. After that, we probably would further narrow down the assumption to knowing the kind of process and infer the parameters? And eventually no prior knowledge?

2 Particle Filter

Inference in stochastic system only has closed form solution for the posterior in some very limited cases, including the simple linear Gaussian model (one continuous case) and the general discrete hidden Markov model. In the vast majority of cases, non-linearity or non-Gaussianity render an analytic solution intractable.

For the Gaussian systems with non-linear dynamics, one classic solution is the extended Kalman filter. The principle is simple, by using Taylor expansion to have a linear approximation of the non-linear dynamics that is compatible with Kalman filter. This method, obviously, fails if the system has substantial non-linearity, or the system is driven by highly non-Gaussian noise. There are some other approaches based on approximation of the non-Gaussian distribution, such as via mixture of Gaussians or second order Taylor series, but all of them have limitations to the form of the posterior distributions.

We hence want a method that can achieve non-linear filtering with no requirements in the form of posterior distribution. And methods based on Monte Carlo satisfy such needs, but with a significant cost in the computational power. However, it is still quite a popular choice because of its generality that allows inference of full posterior distributions in general state-space models.

2.1 General Bayesian Filtering Problem

The main reference for this session is the paper about particle filter tutorail.

Here we study the most important sampling approach for hidden states, particle filtering. Particle filter does similar functions as Kalman filter, but the difference is that the particle filter can be applied to both linear

and non-linear dynamics. The filter enables representing state estimates with arbitrarily shaped probability distributions. The key questions lie in how to set up a particle filter for the inference problem, what would be the outputs and how would the outputs be fed to the system to provide effective inference.

As mentioned before, particle filter solves the problem of similar structure but compatible with non-linear dynamics:

1. Process model for state changes over time given noise and optional inputs:

$$\mathbf{x}_k = f_k(\mathbf{x}_{k-1}, \mathbf{u}_k, \mathbf{v}_{k-1}) \tag{1}$$

2. A measurement model of the form:

$$\mathbf{z}_k = \mathbf{h}_k(\mathbf{x}_k, \mathbf{u}_k, \mathbf{n}_k) \tag{2}$$

   The main difference is that both $\mathbf{f}$ and $\mathbf{h}$ can be arbitrarily shaped distributions.

3.

The particle filter is a Bayesian filter i.e. estimation is performed using Bayesian theory, allowing for estimating a state by combining a statistical model for measurement(likelihood) with a prior probability. The estimation is solved in a similar form to Kalman filter that applies recursive predict-update cycle.

The main steps for such Bayesian filter have the same formulae (both Kalman and Particle filters belong to this class):

1. The **predict step** basically combines the posterior estimate of the previous state with the process model to estimate the current state without observation, via a marginalizing integral. The specific formula can be obtained via marginalizing the posterior estimate of the current state given previous observations:

$$p(\mathbf{x}_k|\mathbf{z}_{1:k-1}) = \int p(\mathbf{x}_k|\mathbf{x}_{k-1})p(\mathbf{x}_{k-1}|\mathbf{z}_{1:k-1})d\mathbf{x}_{k-1} \tag{3}$$

2. The **update step** is basically to estimate the current state after a current observation by combining the prediction posterior and emission mechanism (simply $\mathbf{h}$) and also a marginalisation constant via the Bayes theorem:

$$p(\mathbf{x}_k|\mathbf{z}_{1:k}) = \frac{p(\mathbf{z}_k|\mathbf{x}_k)p(\mathbf{x}_k|\mathbf{z}_{1:k-1})}{p(\mathbf{z}_k|\mathbf{z}_{1:k-1})} \tag{4}$$

   Where $p(\mathbf{z}_k|\mathbf{x}_k) = \mathbf{h}_k(\mathbf{x}_k, \mathbf{u}_k, \mathbf{n}_k)$ and $p(\mathbf{x}_k|\mathbf{z}_{1:k-1})$ is just from the last step.

   The more difficult one is the denominator, the normalizing term, which is also updated in every update step by combining the predict posterior probability with the emission mechanism:

$$p(\mathbf{z}_k|\mathbf{z}_{1:k-1}) = \int p(\mathbf{z}_k, \mathbf{x}_k)p(\mathbf{x}_k|\mathbf{z}_{1:k-1})d\mathbf{x}_k \tag{5}$$

   Pay attention to the time index in the formulae which provide very important intuition but may be messed up.

The integrals in the predict and update steps for Bayesian filters as shown in equation (3) and (5) are only analytically solvable under strong assumptions : finite dimensional discrete state variables or linear models with Gaussian pdfs. What a particle filter does is basically approximating the posterior pdf by a discrete pdf such that there are minimal restrictions in the models involved. The optimal Bayesian solution is approximated by a sum of weighted samples:

$$p(\mathbf{x}_{0:k}|\mathbf{z}_{1:k}) \sim \sum_{i=1}^{N_s} w_k^i \delta(x_{0:k} - x_{0:k}^i) \tag{6}$$

Like a completely discrete approximation for the integral. The $\mathbf{x}_0$ here is generated from the prior.

Where $\{w_k^i, \mathbf{x}_{0:k}^i\}_{i=1}^{N}{}_s$ is the set containing N_s sample sequences and weights, with each weight representing the relative importance of each of sample sequences, and the sum of weights is 1. Samples associated with high weights are believed to be closer to the true state sequence than samples associated with low weights. The integral of the sum of delta functions i.e. equation (6) is hence the summation of the weights and equal to one, thus a valid probability distribution approximation.

The discrete approximation of a continuous pdf turns intractable integrals into summations over N_s samples, which are often referred to as the particles.

2.2 Algorithms for Particle Filtering

The discrete approximation of a continuous pdf turns intractable integrals into summations over N_s samples. The samples are usually referred to as particles hence the name particle filter. The advantages of representing the posterior by a set of weighted particles include (i) the ability to represent arbitrarily shaped pdfs (assuming enough samples) and (ii) minimal restrictions on the process and measurement models. This combination of advantages is one of the main reasons for the popularity of the particle filter. The most obvious drawbacks are (i) the lack of expressiveness in case the number of particles is too low and (ii) the increased computational costs compared to the usual inference methods.

The sample-based approximation comes with an obvious challenge. The posterior pdf that must be estimated is unknown hence sampling from it is impossible. Samples must therefore be drawn from another distribution instead. This distribution, referred to as importance density (sometimes called proposal density) will be denoted q. The weights compensate for the fact that samples are drawn from the importance density q rather than the posterior pdf. Any function that is positive where the posterior is positive can be used as importance density (sequential importance sampling).

Particles are basically just samples with weights in the filtering scheme.

2.2.1 The Most Basic Particle Filter: Sequential Importance Sampling (SIS)

The simplest particle filter algorithm is hence just sequential importance sampling, and we assume q to be a generator function we have and p to be the desired distribution. In the filtering scheme, both q and p refer to the transition density function in the system.

1. We first define the number of particles we want for the algorithm: N_s, and we draw N_s samples or particles from the prior distribution $q(\mathbf{x}_0)$ and assign the initial weights for each sample as :

$$w_0^i \propto \frac{p(\mathbf{x}_0^i)}{q(\mathbf{x}_0^i)} \tag{7}$$

   The weights are always defined as the ratio of the posterior hidden states probability given observations (none for prior) to the importance probability of observing the data sequence from the generator probability.

2. Then in each step, we propagate the particles in last step: $\{x_{k-1}^i, w_{k-1}^i\}_{i=1}^{N_s}$as the current observations $\mathbf{z}_k$ arrive, to obtain the new particles $\{x_k^i, w_k^i\}_{i=1}^{N_s}$.

   We first draw samples from the proposal distribution q, conditional on the last trajectory of the particle and the current observation (need Bayesian expansion to evaluate, note that this is not the transition density):

$$x_k^i \sim q(x_k^i | x_{k-1}^i, \mathbf{z}_k) \tag{8}$$

   Next we assign weights to the samples to make them particles, which equal to the ratio of the exact posterior distribution to the proposed one, but note that these are evaluated over the whole trajectory for each particle, not just the instantaneous values:

$$w_k^i \propto \frac{p(\mathbf{x}_{0:k}^i | \mathbf{z}_{1:k})}{q(\mathbf{x}_{0:k}^i | \mathbf{z}_{1:k})} \tag{9}$$

But note that this equation is not trivial to evaluate directly, and instead, we solve it by using a similar recursive update form by rewriting the equation as:

$$w_k^i \propto w_{k-1}^i \frac{p(z_k|x_k^i)p(x_k^i|x_{k-1}^i)}{q(x_k^i|x_{k-1}^i, z_k)} \tag{10}$$

with the numerator terms being the emission and transition density functions, and the denominator term being the proposal density function that needs Bayesian expansion to evaluate (samples generated not just based on the last states but also the current observation, two inference paths). Use simple sum-to-one constraint to have the exact expression from the variation part.

Then we have the particles for the current time step: $\{x_k^i, w_k^i\}_{i=1}^{N_s}$

3. The particles give us a probability distribution of the hidden states at the time step accoridng to formula (6) i.e.

$$p(\mathbf{x}_{0:k}|\mathbf{z}_{1:k}) \sim \sum_{i=1}^{N_s} w_k^i \delta(x_{0:k} - x_{0:k}^i) \tag{11}$$

with the sum of weight history of a particle equal to the probability of the hidden states being the trajectory of a specific particle (discrete distribution approximation over some particular sequences). Then we could do something like ML estimate to infer the hidden states of the noisy signal using non-linear dynamics.

An additional thing to note is that we often use the normalized weights for the particles instead. So the weight of the ith particle now becomes:

$$\hat{w}^{(i)} = \frac{w^{(i)}}{\sum_j w^{(j)}} \tag{12}$$

This has a simple derivation:

1. Say the target of estimate is some random function h(x), such that we want to know the expectation:

$$E(h(x)) = \int h(x)p(x)dx \tag{13}$$

2. Again by importance sampling, we have the estimation formula:

$$E(h(x)) = \int h(x)p(x)\frac{q(x)}{q(x)}dx \sim \frac{1}{N}\sum_i \frac{p(x^{(i)})}{q(x^{(i)})}h(x^{(i)}) = \frac{1}{N}\sum w^{(i)}h(x^{(i)}) \tag{14}$$

3. To use the normalized weights, we need an additional relation:

$$1 = \int p(x)dx = \int p(x)\frac{q(x)}{q(x)}dx \sim \frac{1}{N}\sum_i \frac{p(x^{(i)})}{q(x^{(i)})} = \frac{1}{N}\sum_i w^{(i)} \tag{15}$$

The key to note is that we have the similarity:

$$N \sim \sum_i w^{(i)} \tag{16}$$

4. Finally, we put the expression for N in (16) into (14) to obtain the estimation formula in the normalized weights:

$$E(h(x)) \sim \sum_i \frac{w^{(i)}}{N}h(x^{(i)}) = \sum_i \frac{w^{(i)}}{\sum_j w^{(j)}}h(x^{(i)}) = \sum_i \hat{w}^{(i)}h(x^{(i)}) \tag{17}$$

Note that the important thing is that h can be anything we want to estimate. The most straight forward example is the mean E(x), which would be just the weighted sum of the particles, way more reasonable than the simple average.

2.2.2 Bootstrap Particle Filter: SIS with Resampling

However, the simplest SIS algorithm has several problems and modifications are needed to make it an effective particle filter algorithm. The most famous problem is the weight degeneracy problem.Weight degeneracy often occurs in scenarios where the likelihood function sharply contrasts the prior or proposal distribution. In such cases, particles that are not close to the high probability regions of the likelihood function end up with negligible weights. Another common cause is the accumulation of errors over time in the estimated state, which leads to a situation where most particles fail to predict the observed data accurately, resulting in their weights becoming insignificant. Note that this doesn't have much relation to the MH problem of acceptance probability tending to 0.

The solution to that is by implementing a sequential importance sampling algorithm with resampling for the particles.

The problem is defined as below:

After a few iterations one particle weight will be very close to one and all other particle weights will be almost zero. The consequences of the degeneracy problem are (i) almost all computational effort will be put into computations related to particles that have negligible or no contribution to the overall estimate and (ii) the number of effective particles is only one. The latter greatly limits the performance and expressiveness of the filter. The expressiveness is limited since a single particle can only represent one point in the state space rather than pdfs of arbitrary shapes. Performance is poor since the particle filter will diverge. Divergence occurs in case state estimation errors increase over time and are unacceptably large. Once diverged, the filter fails to "follow" the true state or reduce estimation errors to acceptable values.

The solution to this problem is resampling. In the most basic resampling, say we have decided to have N trajectories, using the normalized weights as the probabilities of selection of the particles, we draw N particles with replacement. Therefore, trajectories with small importance weights are eliminated, whereas those with large importance weights are replicated.The normalized importance weights are set to 1/N after the resampling step.

Therefore we have an algorithm for the basic particle filter with resampling:

1. To start the algorithm, we need several inputs, including the number of trajectories we want N, initial particles $\{X_0\}$, observation data, emission function from samples to observation g, and the transition function for particles q (we denote f as the actual transition function). In bootstrap particle filter, f=q directly.

   Note also that we need to compute the initial weights for the initial set of particles as in (18) which shows the weight for the ith particle without normalization yet. Note that we are only interested in the contribution form the ith particle, so the condition is on the ith hidden state but not the whole hidden states in the beginning, where π_0 is the initial state distribution. We need the initial probabilities for the weights. Note that we need to normalize the weights after the computation.

   $$w_0^{(i)} = \frac{g(y_0|x_0^{(i)})\pi_0(x_0^{(i)})}{q_0(x_0^{(i)}|y_0)} \tag{18}$$

   The transition function should take the particles and return the propagated particles to the next time step through the system. The emission function should take the observation and particles at the same time step to return the corresponding emission probability.

   The initial particles should be sampled form some initial prior.

2. Then we run the algorithm through each time step in the observation data to infer the hidden states. Note that SIS method applies to time series data.

3. In each iteration after initialization, we perform **resampling** first for the particles from the last step, based on the normalized weights $\{\hat{w}_{t-1}\}$ which are taken directly as the selection probabilities. We draw N particles with replacement according to the normalized weights. After resampling, we set the normalized weights of the resampled particles evenly to $\frac{1}{N}$.

Then we perform the **propagation** step for the resampled particles based on the transition kernel function provided (return new proposed samples directly). For the ith trajectory (often no dependence on observation y, just the previous particles):

$$x_t^{(i)} \sim q(x_{t-1}^{(i)}, y_t) \tag{19}$$

Finally we **update and normalize the weights**. The unnormalized weights are computed according to equation (20). Note that we need the kernel to compute the transition probability in the general case. Remember to normalize the weights. w_{t-1} is basically the uniform weights passed form the last step.

$$w_t^{(i)} = w_{t-1}^{(i)} \frac{g(y_t|x_t^{(i)}) f(x_t^{(i)}|x_{t-1}^{(i)})}{q_t(x_t^{(i)}|x_{t-1}^{(i)}, y_t)} \tag{20}$$

But for the **weight update in the bootstrap particle filter**, f=g and we need only the emission probability as shown in (21). Remember also to normalize the weights.

$$w_t^{(i)} = w_{t-1}^{(i)} g(y_t|x_t^{(i)}) \tag{21}$$

2.3 Particle Filter for Levy State Space Model

We first implement a basic bootstrap particle filter to the Levy state space model. Hence, what we need are the transition function for propagating the particles, and the emission function for computing the probability of a particle given an observation.

First, revise the formula for the Levy state space model driven by an NVM process, the Normal Gamma process to be more specific, as shown in equation (22).

$$\mathbf{X(t)} = \mathbf{e}^{\mathbf{A}(t-s)}\mathbf{X}(s) + \sum_{\frac{s}{T} \le V_i \le \frac{t}{T}} [\mu_W Z_i + \sigma_W \sqrt{Z_i} U_i] \mathbf{e}^{\mathbf{A}(t-V_i)}\mathbf{h} \tag{22}$$

We further evaluate it into the form that is convenient for simulation, with Δt being the simulation time step size, $\{Z_i,V_i\}$ being the jump sizes and times for the subordinator process, and σ_w μ_w being the NVM parameters. Note that such system has a fixed transition function given uniform simulation time step, but the system exponent in the noise has to be calculated for each jump and evaluation point. We compute the new sample by simulate the driving process first and then finidng the corresponding jumps in the interval using formula (22). **Note that in our simulation scheme, we divide the time axis into many dt intervals. So the jump times we obtained are essentially $\tau_i = V_i - t$, thus whats inside the bracket is just minus of the offseted jump time in the dt interval $-\tau_i$. Hence, we dont need to bother with the exact time point of the system t**.

$$X_{n+1} = e^{\mathbf{A}\Delta t} X_n + \sum_{\frac{t-\Delta t}{T} \le V_i \le \frac{t}{T}} [\mu_W Z_i + \sigma_W \sqrt{Z_i} U_i] \mathbf{e}^{\mathbf{A}(t-V_i)}\mathbf{h} \tag{23}$$

The observations are again the true hidden states covered by Gaussian noise of some variance.

$$\mathbf{Y}_n = \mathbf{X}_n + \sigma \mathbf{U}_n \tag{24}$$

Then, what we need to do is to draw samples from the transition function f($\mathbf{X}_{n+1}|\mathbf{X}_n$) and define the observation function g($\mathbf{Y}_n|\mathbf{X}_n$) to run a bootstrap particle filter. Note that the transition function here probably does not have a closed form, and there is no need to define it, because we just need to simulate forwards to have new samples proposed. That is for the transition function, all we need is the exact driving process generator to simulate forwards by dt to obtain the jump sizes and times. We can therefore understand particle filtering scheme as simulating multiple paths to try to reconstruct the real one. It is just having multiple simulations from zero, and using weights as the measure for matching of a simulation to the real one (constrained by weight which is higher for more likely simulations given the observations). It is something

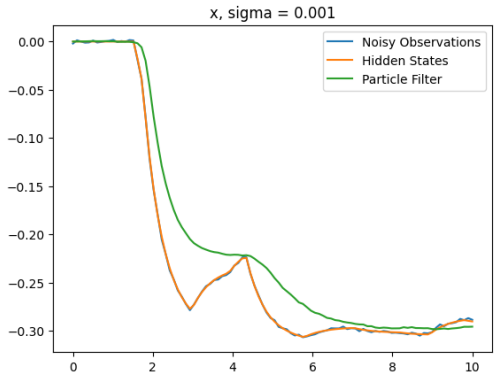
like the weighted sum of all simulated paths. The observation probability is shown in equation (25). Note that since additional normalisation step would be carried out, and the normalisation constant is the same for all samples, there is no need to include it in the function. We just need a score for matching.

$$g(\mathbf{Y}_n|\mathbf{X}_n) = N(\mathbf{X}_n, \sigma^2\mathbf{I}) \sim exp((\mathbf{Y}_n - \mathbf{X}_n)^T(\mathbf{Y}_n - \mathbf{X}_n)/2\sigma^2) \tag{25}$$

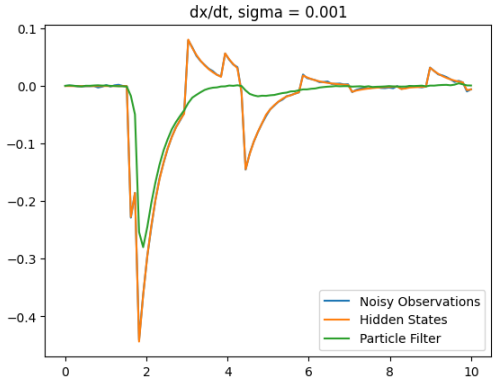
The main problem in building the particle filter transition function is that since it is just some random process generator, but we do not necessarily know the type of process or the exact parameters for such generator. For this case, we would just assume that we know exactly the type of process and parameters, by using the exact generator that generates the data, and leave such problem for latter discussion.

Note that in coding, always remember that sample generation always has the chance of returning empty array which could cause dimension mismatch.

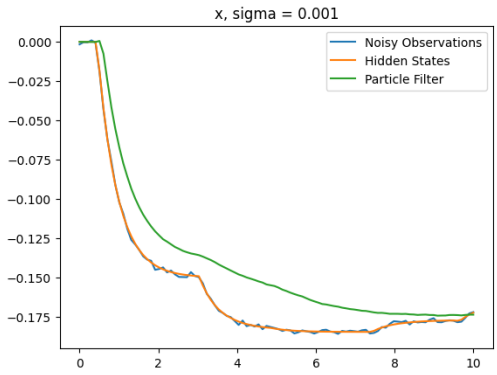
Hence, we have a simple implementation of particle filtering in the Levy state space model. Some example results are shown in figure 1 below.



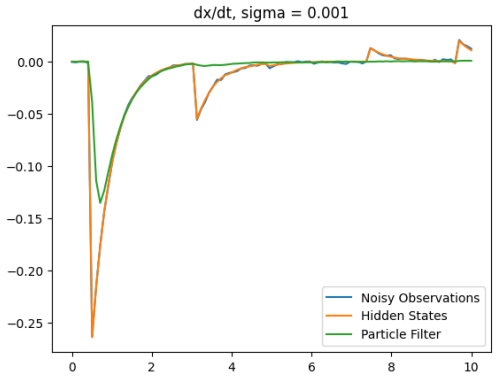
(a) Particle Filtering with 1000 Particles (x)



(b) Particle Filtering with 1000 Particles ($\frac{dx}{dt}$)



(c) Particle Filtering with 10000 Particles (x)



(d) Particle Filtering with 1000 Particles ($\frac{dx}{dt}$)

Figure 1: Particle Filtering Implementation Example Results

3 Marginal Particle Filter

As discussed in the particle filtering session, this implementation is also narrowing down the assumption of knowing exact driving process, to knowing the exact process generator. The assumption here is the same, and the only difference is that instead of using particle filter to do all the inference, we include an additional Kalman filter to do the inference for the linear part, and particle filter will do the non-linear part of the problem.

3.1 Marginal Particle Filter in the Levy State Space Model

Since in the previous particle filtering scheme, all we did was

As proven in the conditional Gaussian system part before, the second term on the right hand side when conditional to the jump sizes and times follow a Gaussian distribution with mean and variance shown in equation (27) and (28) respectively. Note that instead of the Normal Gamma jumps, we are now interested in the jumps of the Gamma process, since the former cannot convert directly into the mean and variance terms now. Using these two formulae, we can convert the jump sizes and times proposal into Gaussian mean and variance.

$$X_{n+1} = e^{\mathbf{A}\Delta t}X_n + \sum_{\frac{t-\Delta t}{T} \leq V_i \leq \frac{t}{T}} [\mu_W Z_i + \sigma_W \sqrt{Z_i} U_i] \mathbf{e}^{\mathbf{A}(-\tau_i)}\mathbf{h} \tag{26}$$

$$\mathbf{m} = \mu_W \sum_{\frac{s}{T} \leq V_i \leq \frac{t}{T}} Z_i \mathbf{e}^{\mathbf{A}(-\tau_i)}\mathbf{h} \tag{27}$$

$$\mathbf{S} = \sigma_W^2 \sum_{\frac{s}{T} \leq V_i \leq \frac{t}{T}} (\sqrt{Z_i}\mathbf{e}^{\mathbf{A}(-\tau_i)}\mathbf{h})(\sqrt{Z_i}\mathbf{e}^{\mathbf{A}(-\tau_i)}\mathbf{h})^T \tag{28}$$

After proposing the means and variances in every single time point, what we can do is to run a Kalman filter exactly as the conditional Gaussian case to the system, using the means and variances proposed by the particle filter. This implementation would be exactly the same as the previous ideal marginalised particle filtering problem, and all we need to do is to pass the mean and covariance matrices. Therefore, since we can use a similar proposal scheme from particle filtering case just with all jumps and jump times packed into something else, all we need is to formulate the likelihood function for the weight computation. For the simplicity of derivation, we would just use $\mathbf{U}_n$ for the biased noise term. Hence the transition function is $\mathrm{p}(\mathbf{U}_{n+1}|\mathbf{U}_n)$ (again no need to know), and the observation function is $\mathrm{p}(\mathbf{Y}_{n+1}|\mathbf{m}_{n+1}, \mathbf{S}_{n+1})$.

1. To derive the likelihood function, first we have our hidden Markov system looks like:

$$X_{n+1} = e^{\mathbf{A}\Delta t}X_n + \mathbf{U}_{n+1} \tag{29}$$

   The emission function is again:

$$\mathbf{Y}_{n+1} = \mathbf{X}_{n+1} + \sigma_n \mathbf{V}_{n+1} \tag{30}$$

   with $\mathbf{U}_{n+1} \sim N(\mathbf{m}, \mathbf{S})$ and $\mathbf{V}_{n+1} \sim N(\mathbf{0}, \mathbf{I})$

2. The contribution of the conditional is that we now know all the noise characteristics, and the likelihood function is hence the marginal of $\mathbf{Y}$ in the Gaussian system. We obviously have $\mathbf{X}_{n+1}$ to follow a Gaussian distribution since it is just a modified Gaussian noise and distributed as $N(e^{\mathbf{A}\Delta t}X_n + \mathbf{m}_{n+1}, \mathbf{S}_{n+1})$, denoted the mean here as $\mathbf{m}'$. $\mathbf{Y}_{n+1}$ is obtained by the summation of two Gaussian samples then, so it also follows a Gaussian distribution as a result. Since the Gaussian terms should be independent, the resultant distribution is just a Gaussian with mean being the sum of means and covariance matrix being the sum of covariance matrices. Also note that this only works for summation of multivariate Gaussians of the same dimensions, and do not confuse it with joining Gaussian distributions where the total covariance would be the inverse of the inverse sum. So, the likelihood function would just be:

$$p(\mathbf{Y}_n|\mathbf{m}_n, \mathbf{S}_n) = N(\mathbf{m}'_n, \mathbf{S}_n + \sigma_n^2\mathbf{I}) \sim \frac{1}{|\mathbf{S}_n + \sigma_n^2\mathbf{I}|^{\frac{1}{2}}} exp(-\frac{1}{2}(\mathbf{Y}_n - \mathbf{m}'_n)^T(\mathbf{S}_n + \sigma_n^2\mathbf{I}))^{-1}(\mathbf{Y}_n - \mathbf{m}'_n)) \tag{31}$$

   We still dont need the normalisation constant, as additional normalisation would be carried out.

4 Particle MCMC

4.1 Comparison between Sequential Monte Carlo and Markov Chain Monte Carlo

Particle filtering is a **sequential Monte Carlo algorithm**, that samples from a state space system **with time evolution** like a Markov chain. **MCMC**, on the other hand, samples from a **static** distribution by using proposal to explore the sample space constrained by the acceptance probability (basically a measure of likelihood of the proposal compared to the current position). SMC samples based on the Markov structure of the state space system, whereas MCMC samples from a known distribution that is more similar to the distribution of variables at a particular time step in a Markov chain.

These are both Monte Carlo based algorithms, which implies that they can do general distributions, including those with non-linear dynamics, but they are both quite computationally expensive.

4.2 The Foundation for MCMC Algorithm: Metropolis Hasting (Reference from 4M24 Lectures)

Metropolis Hasting is an algorithm derived for sampling from the invariant distribution of a Markov chain, with the invariant distribution being the target distribution. More advanced algorithms such as Gibbs sampler and Langevin MCMC are just Metropolis Hasting using the exact proposal (acceptance probability equal to 1) and using Langevin dynamics for the proposal from a given state.

We always tend to sample from the stationary distribution of the Markov chain $\pi(dy)$. By detailed balance assuming the reversibility of the Markov Chain that:

$$\pi(x)p(x,dy) = \pi(dy)p(dy,x) \tag{32}$$

In practice, we don't always have the exact transition function p(,), and instead, we use a proposal function q(,), but the proposal transition kernel may not satisfy the equality if not perfectly match, leading to biased transition to one side. Metropolis Hasting is a solution to this problem by introducing an acceptance probability of transition $\alpha(,)$:

$$\pi(x)q(x,y)\alpha(x,y) = \pi(y)q(y,x) \tag{33}$$

However, this is subject to the condition that the transition from x to y is more frequent than that from y to x for the proposal kernel q(,), since α is a probability and takes value from the range [0,1]:

$$\pi(x)q(x,y) > \pi(y)q(y,x) \tag{34}$$

In such case, we have the expression for the acceptance probability that enforces balance in the bidirectional transitions:

$$\alpha(x,y) = \frac{\pi(y)q(y,x)}{\pi(x)q(x,y)} \tag{35}$$

In practice, we don't swap x and y if the tilt is the other way round, and instead we introduce a unity cap to the acceptance probability as follows:

$$\alpha(x,y) = min(\frac{\pi(y)q(y,x)}{\pi(x)q(x,y)}, 1) \tag{36}$$

Note that although the variables in $\pi()$ are different in the numerator and denominator, the functions are the same and hence the normalisation constants are the same. Therefore, in computing the acceptance probability, we don't need to know the normalisation constant for π, since the one at the top and bottom cancel. (But we need for q, since these would be completely different posterior functions)

Using the acceptance probability shown in equation (36), the full proposal in MH is:

$$q_{MH}(x,y) = q(x,y)\alpha(x,y) \tag{37}$$

Note that the definition of MH still needs only the proposal, as the proposal is also the only information needed to calculate the acceptance probability. In MH, the moves to the higher probability regions are always accepted with 100% probability, but those to the lower probability regions could be rejected.

The overall algorithm for Metropolis Hasting is hence simply:

1. Simulate a sample y from $q(x^j, .)$
2. Compute $\alpha(x^j, y)$. And with the probability α(this could be obtained by generating a sample from a uniform distribution [0,1] and see if the sample is greater than α), set the next sample x^{j+1}as y, otherwise set it as the same as x^j.
3. Repeat the process and end until enough samples have been obtained.

Eventually we are sampling from the invariant distribution of the Markov chain.

Gibbs sampling is just a special case of Metropolis Hasting with acceptance probability always being 1. Metropolis Hasting is the most general way to sample from a joint distribution. It also decomposes the joint distribution into a series of product of univariate conditionals which are calculated by the kernels. The only difference is that the transition could be rejected and samples may stay in the same place.