HW Problems for Summer School on Data Assimilation: Data Assimilation and Inverse Problems

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The objective of this HW assignment is to complement the lecture notes as well as the book material, and give you practice with some important concepts. By the end of this problem set, you will develop intuition for the interplay between prior and the posterior estimate, the properties of the solution of the MAP estimator, the attributes of importance sampling, implementation of MCMC algorithms, and the applicability of 3DVAR & particle filtering algorithms. The first two problems are associated with Chapters 1-6 of the book and will prepare you well for Lecture 1 on Tuesday. The second two problems are associated with Chapters 7-15 of the book and will prepare you well for the Lecture 2 on Tuesday.

Please put your best effort in solving them, as they aid your understanding of the challenges that comes with implementing these algorithms in practice. We encourage you to work on these problems during the summer school, so that you can catch my TA Armeen Taeb for any assistance and clarifications.

1. *Probit Model*: The probit is a natural model for semi-supervised classification. Specifically, for observed labels $j \in 1, 2, \dots J$, the probit model is:

$$y(j) = S(u(j) + \eta(j)),$$

where S is the sigmoid function, e.g. $S(x) = 1$ if $x > 0$, $S(x) = -1$ if $x < 0$. Here, we think of u being "close" to the fiedler vector and y is the noisy observations of the sign of this vector where $\eta(j)$ is noise. In this problem, we will use the probit model to develop Bayesian algorithms. Following the Bayesian perspective, we must construct a natural prior for u. Our intuition suggests that u should be "close" to the fiedler vector. We construct this prior by making connections with the graph Dirichlet energy function.

   (a) Consider the graph Dirichlet energy function $J_0 = \frac{1}{2}\langle u, Lu\rangle$. Show that $J_0 = \frac{1}{4}\sum_{i,j} W_{i,j} u_i u_j$
   Remark: Similar to the classical Dirichlet energy, this quadratic form penalizes nodes from having different function values with penalty being weighted by the weights matrix W. Thus, naturally one is interested in obtaining a small

   (b) Let (q_k, λ_k) denote the eigenpairs of L with $0 = \lambda_0 \le \lambda_1 \le \dots \le \lambda_{N-1}$. In other words, $L = Q\Gamma Q'$ where Q has columns $\{q_k\}_{k=0}^{N-1}$ and Γ is a diagonal matrix with entries $\{\lambda_k\}_{k=0}^{N-1}$. Show that:

$$\frac{1}{2}\langle u, Lu\rangle = \frac{1}{2}\sum_{k=1}^{N-1} \lambda_k(\langle u, v_k\rangle)^2$$

Remark: Clearly $u = v_0$ minimizes the function J. Recall however that the vector v_0 is all ones and does not contain any useful information.

(c) Consider a Gaussian prior $u \sim \mathcal{N}(0, cQ\Sigma Q^\star)$. Here Σ is a diagonal matrix with entries $(0, \lambda_1^{-1}, \ldots, \lambda_{N-1}^{-1})$, and c is a scaling. Use the Karhunen-Loeve theorem to show that the suggested distribution favours the fielder vector and ensures that any draw u from the distribution will be orthogonal to the all ones vector

(d) Select the scaling c that makes the random variable u have unit variance

(e) Show that the log-likelihood function of u is proportional to the Dirichlet energy function $J_0(u)$

(f) Using the constructed prior, obtain a closed form expression (up to CDF of a Gaussian distribution) for the posterior distribution

2. Experiments with the House of Representative Voter Records: In this problem, you will use the knowledge of the previous problems to formulate clustering algorithms for the voter records dataset. Begin by downloading the dataset that is available online. This dataset contains the voting records of 435 U.S. House of Representatives; The first column contains the party affiliation of each representative (-10 democratic, +10 republican) and columns 2-17 contain their votes on each bill (+1 for, -1 against, 0 abstention). For this problem, we will use the probit model with $N = 435$ and $\gamma = 0.1$ in the noise model.

   (a) Compute the weights matrix according to the exponential kernel:

   $$w_{i,j} = \exp(-\|x_i - x_j\|^2/6).$$

   (b) Construct the graph Laplacian and report the classification accuracy using the fielder vector.

   (c) Select 3 democrats (with indices 12, 31, 38) and 3 republicans (with indices 370, 322, 274) as known labels so that $J = 6$. Using gradient descent, solve the MAP estimator for u. Report the classification accuracy based on the sign of this vector.

   (d) Use importance sampling with the number of samples equalling $n = \{10, 50, 100, 200, 1000\}$. For each n, report the posterior mean and variance for each node in the graph and the corresponding classification accuracy based on the sign of the posterior mean.

   (e) Let $\{w_j\}_{j=1}^n$ be the weights (normalized so that they sum to 1 and thus define a probability distribution)) that you obtained from the likelihood function in (d). Then the effective sample size is given by the ratio:

   $$\text{ESS} = \frac{(\sum_j w_j)^2}{\sum_j w_j^2}$$

   Prove that $\text{ESS} \geq 1$ and the equality is achieved when $w_i = 1$ for some i and $w_j = 0$ for $j \neq i$. Justify that this phenomena occurs when the prior is a very bad approximation of the posterior. Furthermore, prove that ESS $\leq n$and the equality is achieved when $w_i = w_j$ or all (i, j). Justify that this phenomena occurs when the prior distribution is exactly the posterior distribution, and the importance sampling reduces to Monte Carlo sampling. Report the ESS for the voter record data with $n = 1000$. What can you conclude?

3. The Ising Model: (The content of this question does not require you to seek background information from outside sources. Interested readers should look at the book "Monte Carlo Methods in Statistical Physics" by Newman and Barkema). Graphical models are a family of multivariate distributions which are Markov in accordance to a particular undirected graph. Each node in the graph $i \in V$ is associated to a random variable. The set of edges $E \subset \binom{V}{2}$ encode the conditional dependency relationships: a variable conditioned on its neighbours is independent of the remaining variables.
In this problem we focus on the setting where the collection of random variables $\{x_i\}_{i=1}^p$ take on discrete values ± 1. This is known as the Ising model and is described with the following joint distribution over the variables x:

$$\mathbb{P}(x) = \frac{1}{Z} \exp\Big\{ \sum_{\{s,t\} \in E} \theta_{s,t} x_s x_t \Big\}$$

Here $\theta \in \mathbb{R}^{p \times p}$ encodes the graph structure. (We consider the diagonal elements of θ equalling zeros). In particular, $\theta_{s,t}$ is non-zero if variables s and j are connected via an edge.

   (a) Suppose that you were tasked with sampling from this joint distribution. One approach that we learned earlier was importance sampling, a technique that is based on sampling from another distribution, and reweighting the samples based on the likelihood of the original joint distribution. While this is a natural approach, it becomes tractable in the setting where the number of variables p is large (say $p = 20$). Why?

   (b) Show that the conditional distribution of a variable x_r given the rest $(x_{V \setminus r})$ is given by:

$$\mathbb{P}(x_r | x_{V \setminus r}) = \frac{\exp(2x_r \sum_{t \in V \setminus r} \theta_{rt} x_t)}{\exp(2x_r \sum_{t \in V \setminus r} \theta_{rt} x_t) + 1}$$

   Remark: Notice that sampling from the conditional distribution is tractable. Why? This suggests that Gibbs sampling could be used to draw samples from the joint distribution.

   (c) We consider a specific example to showcase the use of Gibbs sampling for this problem. Consider a collection of $x \in \mathbb{R}^5$ discrete variables specified by the following $\theta^\star \in \mathbb{R}^{5\times 5}$:

$$\theta^\star = \begin{pmatrix} 0 & 0.5 & 0 & 0.5 & 0 \\ 0.5 & 0 & 0.5 & 0 & 0.5 \\ 0 & 0.5 & 0 & 0.5 & 0 \\ 0.5 & 0 & 0.5 & 0 & 0 \\ 0 & 0.5 & 0 & 0 & 0 \end{pmatrix}$$

Use Gibbs sampler with initialization $x^0 = \begin{pmatrix} 1 & -1 & -1 & 1 & 1 \end{pmatrix}^T$, burn-in period of 5000 samples, draw $N = 1000$ samples from the joint distribution. Report the sample mean and sample variance for each of the variables. From your samples, compute a correlation matrix of all the 5 variables and plot an image of the correlation values. Do you see a pattern? Does this confirm the validity of the sampling technique?

(d) You will now reverse engineer θ from the samples you generated! You will use the Metropolis Hastings algorithm to get the posterior distribution $\mathbb{P}(\theta|\{x^{(i)}\}_{i=1}^N)$. Notice that θ is symmetric and has has zeros on the diagonal, meaning that there are $p(p-1)/2$ free parameters. Hence we work with a vector $\tilde{\theta} \in \mathbb{R}^{p(p-1)/2}$ containing all the degrees of freedom of θ. Recall that for Metropolis Hastings, we need to construct a prior on $\tilde{\theta}$ and a proposal distribution. Since we expect the graph structure to be sparse (i.e. $\tilde{\theta}$ sparse), a natural prior on each element of $\tilde{\theta}_i$ is the Laplace distribution $\tilde{\theta}_i \overset{iid}{\sim} \text{Laplace}(0, \lambda)$. Further, we use a random-walk proposal distribution:

$$v^\star \sim \tilde{\theta}^{(i)} + \mathcal{N}(0, \sigma^2 \mathcal{I}),$$

with $\sigma^2 = 0.1$. With $\lambda = 0.2$, a burn-in time of 10000 samples, use Metropolis Hasting to generate $n = 1000$ samples from the posterior $\mathbb{P}(\theta|\{x^{(i)}\}_{i=1}^N)$. Compute and report the sample mean and variance of these samples. Does your findings match the underlying $\theta^\star$?

Remark: We know that the accept function in the Metropolis Hasting algorithm often removes the normalization constant in the target probability distribution. In this scenario, this does not happen. Why? What does this say about this method for large p?

4. The Pendulum Problem The dynamics of a pendulum is characterized by the following linear system:

$$\ddot{u} + \delta \dot{u} + \sin(u) = 0$$

where $u(t)$ denotes the location of the pendulum, and $\dot{u}(t)$ denotes the velocity.

(a) Show that the dynamical system can be written by:

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big[\frac{1}{2}\dot{u}^2 - \cos(u)\Big] = -\delta \dot{u}^2$$

Justify that for $\delta \geq 0$, the solution will not blow up in finite time. What happens when $\delta = 0$?

(b) Notice that the dynamical system can be equivalently expressed by the system of equations:

$$\begin{cases} \dot{u} = w \\ \dot{w} = -\delta w - \sin(u) \end{cases} \tag{1}$$

with $v = \begin{pmatrix} u \\ w \end{pmatrix}$ denoting the state-space. We consider the solution of (1) at discrete intervals of T so that $v^{j+1} = \psi(v^j)$ where $\Psi(\cdot)$ denotes the solution of (1) with initial conditions $(u^0, w^0) = (\pi/4, 0)$. Suppose we have noisy observations of the state of the dynamical systems at discrete times:

$$\begin{cases} v^{j+1} = \Psi(v^j) \\ y^j = u^j + \eta \end{cases} \tag{2}$$

Set $T = 0.2$, consider $\eta \sim \mathcal{N}(0, \gamma)$ with $\gamma = 0.1^2$ as the noise term, and set $\delta = 0.1$. Using MATLAB, solve the different equation (2) and obtain 20 measurement of y. Plot these values.

(c) Letting $H = \begin{pmatrix} 1 & 0 \end{pmatrix}$, recall that 3DVAR obtains estimates $m_{(j+1)}$ of the state space from the following sequential computations:

$$m_{j+1} = (\mathcal{I} - KH)\psi(m_j) + Ky_{j+1},$$

a tradeoff between fitting to data and getting accurate dynamics. Here the matrix K satisfies the relations:

$$S = HCH' + \gamma \quad K = CH'S^{-1},$$

with $C \in \mathbb{R}^{2\times 2}$ diagonal is to be specified. In this problem, show that there is only one degree of freedom. Play around with this parameter to find one that gives you a small $\sum_{j=1}^{20} \|v^j - m^j\|_{\ell_2}$. (This is a bit of an open ended problem. We want you to play around a bit!).

(d) Starting with $n = \{5, 20, 50, 100\}$ random particles of the state-space v, apply Particle Filtering and count the effective samples after each iteration of the dynamics. What do you observe? Plot the mean particle filter against the true observations. What do you see?

(e) With $n = 100$ random particles of the state-space v, apply Ensemble Kalman Inversion and compare the mean particle filter against true observations