Homework 3 - Introduction to Probabilistic Graphical Models

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1 Sampling (Monte-Carlo), MCMC[50 points]

1.1 (Monte-Carlo) [20 points]

Given a random distribution $p(x)$ on $x = [x_1, ..., x_D]^T \in \mathbb{R}^D$. Suppose we want to perform inference $\mathbb{E}_{p(x)}[f(x)]$ using importance sampling, with $q(x)$ as the proposal distribution. According to importance sampling, we draw L i.i.d. samples $x^{(1)}, ..., x^{(L)}$ from $q(x)$, and we have

$$\mathbb{E}_{p(x)}[f(x)] \approx \frac{1}{\sum_{i=1}^{L} u_i} \sum_{i=1}^{L} f(x^{(i)}) u_i$$

where the (unnormalized) importance weights $u_i = \frac{p(x^{(i)})}{q(x^{(i)})}$.

1. (5 points) Find the mean and variance of the unnormalized importance weights $\mathbb{E}_{q(x)}[u_i]$ and $\mathrm{Var}_{q(x)}[u_i]$.

$$\mathbb{E}_{q(x)}[u_i] = \int q(x) \frac{p(x)}{q(x)} dx = \int p(x) dx = 1$$

$$\mathrm{Var}_{q(x)}[u_i] = \int q(x) \left(\frac{p(x)}{q(x)} - 1 \right)^2 dx = \int q(x) \frac{p^2(x)}{q^2(x)} dx - 1$$

2. (5 points) Prove the following lemma: $\mathbb{E}_{p(x)} \left[\frac{p(x)}{q(x)} \right] \geq 1$, and the equality holds only when $p = q$.

$$\mathbb{E}_{p(x)} \left[\frac{p(x)}{q(x)} \right] = \int p(x) \frac{p(x)}{q(x)} dx = \int p^2(x) \frac{1}{q(x)} dx$$

Using Cauchy-Schwarz inequality, we have

$$\int p^2(x) \frac{1}{q(x)} dx \geq \left(\int p(x) dx \right)^2 = 1$$

The equality holds only when $p(x) = q(x)$.

3. (9 points) A measure of the variability of two components in vector $u = [u_1, ..., u_L]^T$ is given by $\mathbb{E}_{q(x)}\left[(u_i - u_j)^2\right]$. Assume that both p and q can be factorized, i.e. $p(x) = \prod_{i=1}^D p_i(x_i)$, and $q(x) = \prod_{i=1}^D q_i(x_i)$. Show that $\mathbb{E}_{q(x)}\left[(u_i - u_j)^2\right]$ has exponential growth with respect to D.

We consider the variability of the unnormalized importance weights $u(x) = \frac{p(x)}{q(x)}$, measured by:

$$\mathbb{E}_{q(x)}[(u_i - u_j)^2]$$

Assume both $p(x)$ and $q(x)$ factorize over dimensions:

$$p(x) = \prod_{i=1}^D p_i(x_i), \qquad q(x) = \prod_{i=1}^D q_i(x_i)$$

Since $u(x) = \frac{p(x)}{q(x)}$, we compute the expected squared difference:

$$\mathbb{E}_{q(x),q(x')}[(u(x) - u(x'))^2] = \mathbb{E}_{q(x)}\left[\left(\frac{p(x)}{q(x)}\right)^2\right] + \mathbb{E}_{q(x')}\left[\left(\frac{p(x')}{q(x')}\right)^2\right] - 2\mathbb{E}_{q(x),q(x')}\left[\frac{p(x)}{q(x)} \cdot \frac{p(x')}{q(x')}\right]$$

Since x and x' are independent and identically distributed under q, this simplifies to:

$$\mathbb{E}_{q(x),q(x')}[(u(x) - u(x'))^2] = 2\,\mathbb{E}_{q(x)}\left[\left(\frac{p(x)}{q(x)}\right)^2\right] - 2\left(\mathbb{E}_{q(x)}\left[\frac{p(x)}{q(x)}\right]\right)^2$$

Let us define:

$$Z_1 = \mathbb{E}_{q(x)}\left[\frac{p(x)}{q(x)}\right] = \int p(x)\,dx = 1$$

$$Z_2 = \mathbb{E}_{q(x)}\left[\left(\frac{p(x)}{q(x)}\right)^2\right] = \int \frac{p(x)^2}{q(x)}\,dx$$

Thus, the variability becomes:

$$\mathbb{E}_{q(x)}[(u_i - u_j)^2] = 2Z_2 - 2$$

Now, using the factorized form of $p(x)$ and $q(x)$, we can write:

$$Z_2 = \int \frac{\prod_{i=1}^D p_i(x_i)^2}{\prod_{i=1}^D q_i(x_i)}\,dx = \prod_{i=1}^D \int \frac{p_i(x_i)^2}{q_i(x_i)}\,dx_i = \prod_{i=1}^D z_i$$

where

$$z_i = \int \frac{p_i(x_i)^2}{q_i(x_i)}\,dx_i$$

If each $z_i > 1$, then:

$$Z_2 = \prod_{i=1}^{D} z_i > 1^D = 1$$

More importantly, if each $z_i \approx c > 1$, then:

$$Z_2 \approx c^D \quad \Rightarrow \quad \mathbb{E}_{q(x)}[(u_i - u_j)^2] \approx 2(c^D - 1)$$

The variance of the difference between importance weights grows exponentially with the dimension D, making standard importance sampling in high-dimensional settings potentially unstable.

$$\boxed{\mathbb{E}_{q(x)}[(u_i - u_j)^2] = 2\left(\prod_{i=1}^{D} \int \frac{p_i(x_i)^2}{q_i(x_i)} dx_i - 1\right) \quad \text{grows exponentially with } D}$$

4. (1 point) Use the conclusion in (c) to explain why the standard importance sampling does not scale well with dimensionality and would blow up in high-dimensional cases.

   Standard importance sampling does not scale well with dimensionality because the variance of the importance weights grows exponentially with dimension, making the estimator unstable in high-dimensional spaces.

1.2 (MCMC)[40 points]

1.2.1 Multiple Choice [10 points]

1. (5 points) Which of the following statements is true for the acceptance probability $A(x'|x) = \min(1, \frac{P(x')Q(x|x')}{P(x)Q(x'|x)})$ of Metropolis-Hastings algorithm?

   (a) It satisfies detailed balance.

   (b) We can just evaluate $P(x')$ and $P(x)$ up to a normalization constant.

   (c) It ensures that the MH algorithm eventually converges to the true distribution.

   (d) All of the above.

   The correct answer is **(d)**. The acceptance probability satisfies detailed balance, we can evaluate $P(x')$ and $P(x)$ up to a normalization constant, and it ensures that the MH algorithm eventually converges to the true distribution.

2. (5 points) Which of the following statements is true for Hamiltonian Monte Carlo in comparison with vanilla MCMC?

(a) It can improve acceptance rate and give better mixing.

(b) Stochastic variants can be used to improve performance in large dataset scenarios.

(c) It may not be used for discrete variable.

(d) All of the above.

The correct answer is **(d)**. Hamiltonian Monte Carlo can improve acceptance rate and give better mixing, stochastic variants can be used to improve performance in large dataset scenarios, and it may not be used for discrete variable.

1.2.2 Modeling with Markov Chain Monte Carlo [30 points]

We are going to use the data from the 2013-2014 Premier League PL1 to build a predictive model on the number of goals scored in a single game by the two opponents. Bayesian hierarchical model is a good candidate for this kind of modeling task. We model each team's strength (both attacking and defending) as latent variables. Then in each game, the goals scored by the home team is a random variable conditioned on the attacking strength of the home team and the defending strength of the away team. Similarly, the goals scored by the away team is a random variable conditioned on the attack strength of the away team and the defense strength of the home team. Therefore, the distribution of the scoreline of a specific game is dependent on the relative strength between the home team A and the away team B, which also depends on the relative strength between those teams with their other opponents.

Table 1: 2013-2014 Premier League teams

Index	0	1	2	3
Team	Arsenal	Aston Villa	Cardiff City	Chelsea
Index	4	5	6	7
Team	Crystal Palace	Everton	Fulham	Hull City
Index	8	9	10	11
Team	Liverpool	Manchester City	Manchester United	Newcastle United
Index	12	13	14	15
Team	Norwich City	Southampton	Stoke City	Sunderland
Index	16	17	18	19
Team	Swansea City	Tottenham Hotspur	West Bromwich Albion	West Ham United

Here we consider using the same model as described by Baio and Blangiardo. The Premier League has 20 teams, and we index them as in Table 1. Each team would play 38 matches every season (playing each of the other 19 teams home and away), which totals 380 games in the entire season. For the g-th game, assume that the index of home team is $h(g)$ and the index of the away team is $a(g)$. the observed number of goals is:

$$y_{gj}|\theta_{gj} = \text{Poisson}(\theta_{gj})$$

where the $\theta = (\theta_{g1}, \theta_{g2})$ represent the scoring intensity in the g-th game for the team playing at home ($j = 1$) and away ($j = 2$), respectively. We put a log-linear model for the θs:

$$\log \theta_{g1} = \text{home} + \text{att}_{h(g)} - \text{def}_{a(g)}$$
$$\log \theta_{g2} = \text{att}_{a(g)} - \text{def}_{h(g)}$$

Note that team strength is broken into attacking and defending strength. And home represents home- team advantage, and in this model is assumed to be constant across teams. The prior on the home is a normal distribution

$$\text{home} \sim \mathcal{N}(0, \tau_0^{-1})$$

where the precision $\tau_0 = 0.0001$.

The team-specific attacking and defending effects are modeled as exchangeable:

$$\text{att}_t \sim \mathcal{N}(\mu_{\text{att}}, \tau_{\text{att}}^{-1})$$
$$\text{def}_t \sim \mathcal{N}(\mu_{\text{def}}, \tau_{\text{def}}^{-1})$$

We use conjugate priors as the hyper-priors on the attack and defense means and precisions:

$$\mu_{\text{att}} \sim \mathcal{N}(0, \tau_1^{-1})$$
$$\mu_{\text{def}} \sim \mathcal{N}(0, \tau_1^{-1})$$
$$\tau_{\text{att}} \sim \text{Gamma}(\alpha, \beta)$$
$$\tau_{\text{def}} \sim \text{Gamma}(\alpha, \beta)$$

where the precision $\tau_1 = 0.0001$, and we set parameters $\alpha = \beta = 0.1$.

This hierarchical Bayesian model can be represented using a directed acyclic graph as shown in Figure 1. Where the goals of each game $y = \{y_{gj}|g = 0, ..., 379, j = 1, 2\}$ are 760 observed variables, and parameters $\theta = (\text{home}, \text{att}_0, ..., \text{att}_{19}, \text{def}_0, ..., \text{def}_{19})$ and hyper-parameters $\eta = (\mu_{\text{att}}, \mu_{\text{def}}, \tau_{\text{att}}, \tau_{\text{def}})$ are unobserved variables that we need to make inference. To ensure identifiability, we enforce a corner constraint on the parameters (pinning one team's parameters to 0,0). Here we use the first team as reference and assign its attacking and defending strength to be 0:

$$\text{att}_0 = \text{def}_0 = 0$$

In this question, we want to estimate the posterior mean of the attacking and defending strength for each team, i.e. $\mathbb{E}_{p(\theta,\eta|y)}[\text{att}_i]$, $\mathbb{E}_{p(\theta,\eta|y)}[\text{def}_i]$, and $\mathbb{E}_{p(\theta,\eta|y)}[\text{home}]$.

1. (10 points) Find the joint likelihood $p(y, \theta, \eta)$.
   The random variables are:

- $y = \{y_{gj} | g = 0, ..., 379, j = 1, 2\}$ are the observed goals
- $\theta = (\text{home}, \text{att}_0, ..., \text{att}_{19}, \text{def}_0, ..., \text{def}_{19})$ are the unobserved variables
- $\eta = (\mu_{\text{att}}, \mu_{\text{def}}, \tau_{\text{att}}, \tau_{\text{def}})$ are the hyper-parameters

The joint likelihood is given by

$$p(y, \theta, \eta) = p(y|h(g), a(g), \theta)p(\theta|\eta)p(\eta)$$

$$= \prod_{g=0}^{379} p(y_{g1}|h(g), \theta)p(y_{g2}|a(g), \theta)p(\theta|\eta)p(\eta)$$

Now, let's expand each component of this joint likelihood:

- The likelihood of observed goals follows the Poisson distribution:

$$p(y_{g1}|h(g), \theta) = \text{Poisson}(y_{g1}; \theta_{g1}) = \frac{e^{-\theta_{g1}} \theta_{g1}^{y_{g1}}}{y_{g1}!} \tag{1}$$

$$p(y_{g2}|a(g), \theta) = \text{Poisson}(y_{g2}; \theta_{g2}) = \frac{e^{-\theta_{g2}} \theta_{g2}^{y_{g2}}}{y_{g2}!} \tag{2}$$

  Where θ_{g1} and θ_{g2} are deterministic functions of the team parameters:

$$\log \theta_{g1} = \text{home} + \text{att}_{h(g)} - \text{def}_{a(g)} \tag{3}$$

$$\log \theta_{g2} = \text{att}_{a(g)} - \text{def}_{h(g)} \tag{4}$$

- The prior distribution for the team parameters is:

$$p(\theta|\eta) = p(\text{home}) \prod_{t=1}^{19} p(\text{att}_t|\mu_{\text{att}}, \tau_{\text{att}}) \prod_{t=1}^{19} p(\text{def}_t|\mu_{\text{def}}, \tau_{\text{def}}) \tag{5}$$

$$= \mathcal{N}(\text{home}; 0, \tau_0^{-1}) \prod_{t=1}^{19} \mathcal{N}(\text{att}_t; \mu_{\text{att}}, \tau_{\text{att}}^{-1}) \prod_{t=1}^{19} \mathcal{N}(\text{def}_t; \mu_{\text{def}}, \tau_{\text{def}}^{-1}) \tag{6}$$

  Where we've already incorporated the constraint that $\text{att}_0 = \text{def}_0 = 0$.

- The hyperprior distribution is:

$$p(\eta) = p(\mu_{\text{att}})p(\mu_{\text{def}})p(\tau_{\text{att}})p(\tau_{\text{def}}) \tag{7}$$

$$= \mathcal{N}(\mu_{\text{att}}; 0, \tau_1^{-1})\mathcal{N}(\mu_{\text{def}}; 0, \tau_1^{-1})\text{Gamma}(\tau_{\text{att}}; \alpha, \beta)\text{Gamma}(\tau_{\text{def}}; \alpha, \beta) \tag{8}$$

Substituting these expressions into the joint likelihood:

$$p(y,\theta,\eta) = \prod_{g=0}^{379} \left[\frac{e^{-\theta_{g1}}\theta_{g1}^{y_{g1}}}{y_{g1}!} \cdot \frac{e^{-\theta_{g2}}\theta_{g2}^{y_{g2}}}{y_{g2}!} \right] \tag{9}$$

$$\times \mathcal{N}(\text{home}; 0, \tau_0^{-1}) \prod_{t=1}^{19} \mathcal{N}(\text{att}_t; \mu_{\text{att}}, \tau_{\text{att}}^{-1}) \prod_{t=1}^{19} \mathcal{N}(\text{def}_t; \mu_{\text{def}}, \tau_{\text{def}}^{-1}) \tag{10}$$

$$\times \mathcal{N}(\mu_{\text{att}}; 0, \tau_1^{-1}) \mathcal{N}(\mu_{\text{def}}; 0, \tau_1^{-1}) \text{Gamma}(\tau_{\text{att}}; \alpha, \beta) \text{Gamma}(\tau_{\text{def}}; \alpha, \beta) \tag{11}$$

Expanding the probability density functions:

$$p(y,\theta,\eta) = \prod_{g=0}^{379} \left[\frac{e^{-\theta_{g1}}\theta_{g1}^{y_{g1}}}{y_{g1}!} \cdot \frac{e^{-\theta_{g2}}\theta_{g2}^{y_{g2}}}{y_{g2}!} \right] \tag{12}$$

$$\times \frac{1}{\sqrt{2\pi\tau_0^{-1}}} \exp\left(-\frac{\text{home}^2}{2\tau_0^{-1}} \right) \tag{13}$$

$$\times \prod_{t=1}^{19} \frac{1}{\sqrt{2\pi\tau_{\text{att}}^{-1}}} \exp\left(-\frac{(\text{att}_t - \mu_{\text{att}})^2}{2\tau_{\text{att}}^{-1}} \right) \tag{14}$$

$$\times \prod_{t=1}^{19} \frac{1}{\sqrt{2\pi\tau_{\text{def}}^{-1}}} \exp\left(-\frac{(\text{def}_t - \mu_{\text{def}})^2}{2\tau_{\text{def}}^{-1}} \right) \tag{15}$$

$$\times \frac{1}{\sqrt{2\pi\tau_1^{-1}}} \exp\left(-\frac{\mu_{\text{att}}^2}{2\tau_1^{-1}} \right) \tag{16}$$

$$\times \frac{1}{\sqrt{2\pi\tau_1^{-1}}} \exp\left(-\frac{\mu_{\text{def}}^2}{2\tau_1^{-1}} \right) \tag{17}$$

$$\times \frac{\beta^\alpha}{\Gamma(\alpha)} \tau_{\text{att}}^{\alpha-1} e^{-\beta\tau_{\text{att}}} \tag{18}$$

$$\times \frac{\beta^\alpha}{\Gamma(\alpha)} \tau_{\text{def}}^{\alpha-1} e^{-\beta\tau_{\text{def}}} \tag{19}$$

where $\tau_0 = \tau_1 = 0.0001$ and $\alpha = \beta = 0.1$.

so, our joint likelihood is:

$$
\begin{aligned}
p(y, \theta, \eta) = &\prod_{g=0}^{379} \left[\frac{e^{-\theta_{g1}} \theta_{g1}^{y_{g1}}}{y_{g1}!} \cdot \frac{e^{-\theta_{g2}} \theta_{g2}^{y_{g2}}}{y_{g2}!} \right] \\
&\cdot \mathcal{N}(\text{home} \mid 0, \tau_0^{-1}) \\
&\cdot \prod_{t=1}^{19} \mathcal{N}(\text{att}_t \mid \mu_{\text{att}}, \tau_{\text{att}}^{-1}) \\
&\cdot \prod_{t=1}^{19} \mathcal{N}(\text{def}_t \mid \mu_{\text{def}}, \tau_{\text{def}}^{-1}) \\
&\cdot \mathcal{N}(\mu_{\text{att}} \mid 0, \tau_1^{-1}) \cdot \mathcal{N}(\mu_{\text{def}} \mid 0, \tau_1^{-1}) \\
&\cdot \text{Gamma}(\tau_{\text{att}} \mid \alpha, \beta) \cdot \text{Gamma}(\tau_{\text{def}} \mid \alpha, \beta)
\end{aligned}
$$

where $\tau_0 = 0.0001$ and $\alpha = \beta = 0.1$.

2. (10 points) Write down the Metropolis-Hastings algorithm for sampling from posterior $p(\theta, \eta | y)$, and derive the acceptance function for a proposal distribution of your choice (e.g. isotropic Gaussian).

   (a) Initialize: Set initial values $\theta^{(0)}, \eta^{(0)}$, where $\theta = (\text{home}, \text{att}_1, \ldots, \text{att}_{19}, \text{def}_1, \ldots, \text{def}_{19})$ and $\eta = (\mu_{\text{att}}, \mu_{\text{def}}, \tau_{\text{att}}, \tau_{\text{def}})$.

   (b) **For $i = 0$ to $N - 1$:**

      i. Proposal: Sample a proposed state (θ^*, η^*) from the isotropic Gaussian proposal:

      $$(\theta^*, \eta^*) \sim \mathcal{N}((\theta^{(i)}, \eta^{(i)}), \sigma^2 I)$$

      For parameters $\tau_{\text{att}}, \tau_{\text{def}}$ (which must remain positive), propose in log space:

      $$\log \tau^* \sim \mathcal{N}(\log \tau^{(i)}, \sigma^2) \quad \Rightarrow \quad \tau^* = \exp(\log \tau^*)$$

      ii. Acceptance Probability: Since the proposal is symmetric:

      $$A = \min\left(1, \frac{p(y, \theta^*, \eta^*)}{p(y, \theta^{(i)}, \eta^{(i)})}\right)$$

      or in log space:

      $$\log A = \min\Big(0,\ \log p(y, \theta^*, \eta^*) - \log p(y, \theta^{(i)}, \eta^{(i)})\Big)$$

      iii. Accept/Reject: Draw $u \sim \text{Uniform}(0, 1)$

      $$\text{If } \log u < \log A \quad \text{then accept: } (\theta^{(i+1)}, \eta^{(i+1)}) = (\theta^*, \eta^*)$$

      $$\text{Else reject: } (\theta^{(i+1)}, \eta^{(i+1)}) = (\theta^{(i)}, \eta^{(i)})$$

3. (10 points) Implement the M-H algorithm to inference the posterior distribution. The data can be found from `premier_league_2013_2014.dat`, which contains a 380×4 matrix. The first column is the number of goals y_{g1} scored by the home team, the second column is the number of goals y_{g2} scored by the away team, the third column is the index for the home team $h(g)$, and the fourth column is the index for the away team $a(g)$. Use isotropic Gaussian proposal distribution, $\mathcal{N}(0, \sigma^2 I)$ and 0 as the starting point. Run the MCMC chain for 5000 steps to burn in and then collect 5000 samples with t steps in between (i.e., run M-H for $5000t$ steps and collect only each t-th sample). This is called thinning, which reduces the autocorrelation of the MCMC samples introduced by the Markovian process. The parameter sets are $\sigma = 0.05$, and $t = 5$. Plot the trace plot of the burning phase and the MCMC samples for the latent variable home using the proposed distribution.

Trace Plot of the Latent Variable `home`. We run the Metropolis–Hastings algorithm with a proposal standard deviation of $\sigma = 0.05$ and a thinning factor of $t = 5$. The algorithm is executed for 5000 burn-in steps, after which 5000 samples are collected, taking every 5-th sample to reduce autocorrelation.

The trace plot below shows the evolution of the latent variable `home` during:

- The **burn-in phase** (left), where the chain stabilizes, and
- The **post burn-in MCMC samples** (right), where we collect samples for posterior inference.

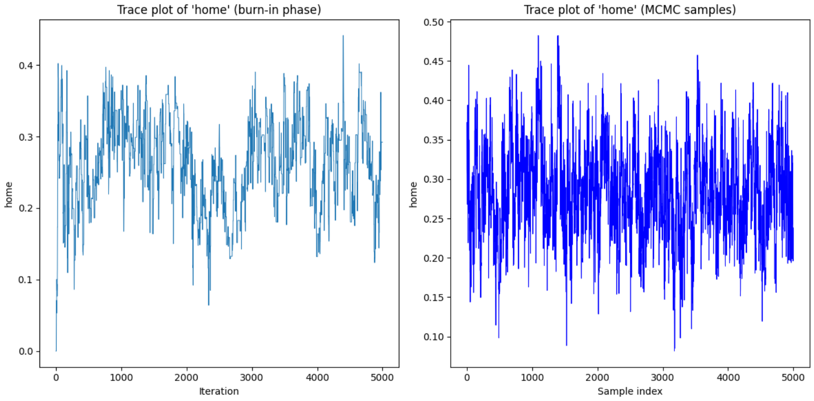


Figure 1: Trace plots of the latent variable `home` for burn-in (left) and post burn-in samples (right) using Metropolis–Hastings with $\sigma = 0.05$ and $t = 5$.

4. (Bonus, 20 points) Set the parameters as $\sigma = 0.005, 0.05, 0.5$ and $t = 1, 5, 20, 50$, and:

   - Plot the trace plot of the burning phase and the MCMC samples for the latent variable home using proposal distributions with different σ and t.

     Please refer to Figure 2 for the trace plots of the latent variable `home` under different σ and t settings. Each subplot corresponds to a unique (σ, t) pair.

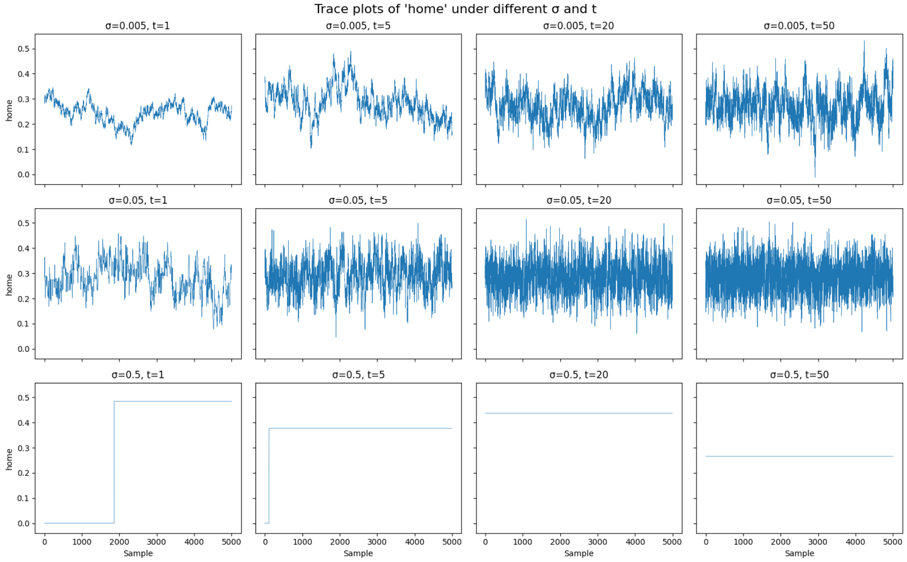


Figure 2: Trace plots of the latent variable `home` under different σ and t settings. Each subplot corresponds to a unique (σ, t) pair.

   - Estimate the rejection ratio for each parameter setting, report your results in a table.

     The table below reports the acceptance rates for each (σ, t) configuration tested:

     please refer to Table 2 for the acceptance rates of the Metropolis–Hastings algorithm under different (σ, t) settings.

σ	t	Acceptance Rate (%)
0.005	1	88.34
0.005	5	89.24
0.005	20	89.56
0.005	50	89.38
0.050	1	19.82
0.050	5	18.93
0.050	20	18.43
0.050	50	16.77
0.500	1	0.01
0.500	5	0.00
0.500	20	0.00
0.500	50	0.00

Table 2: Acceptance rates of the Metropolis–Hastings algorithm under different (σ, t) settings.

- Comment on the results. Which parameter setting worked the best for the algorithm?

  We observe that:

  - Small $\sigma = 0.005$ results in very small steps, leading to high acceptance but slow exploration (high autocorrelation).
  - Large $\sigma = 0.5$ causes low acceptance rates and often poor mixing.
  - $\sigma = 0.05$ with $t = 5$ offers a good balance between exploration and acceptance, showing stable trace plots and reasonable variability.

  Thus, we choose $(\sigma = 0.05, t = 5)$ as the **optimal setting**.
- Use the results from the optimal parameter setting
  - plot the posterior histogram of home from the MCMC samples

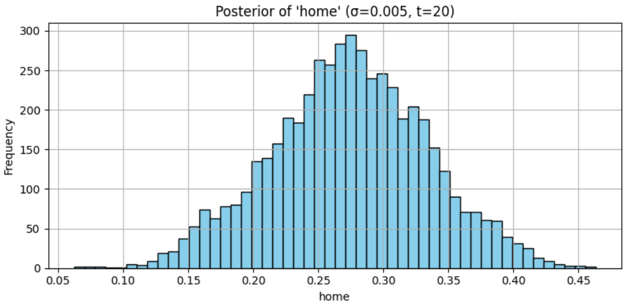


Figure 3: Posterior distribution of the latent variable `home` under the optimal setting $(\sigma = 0.05, t = 5)$.

- plot the estimated attacking strength $\mathbb{E}_{p(\theta,\eta|y)}[\text{att}_i]$ against the estimated defending strength $\mathbb{E}_{p(\theta,\eta|y)}[\text{def}_i]$ for each the team in one scatter plot. Please make sure to identify the team index of each point on your scatter plot.

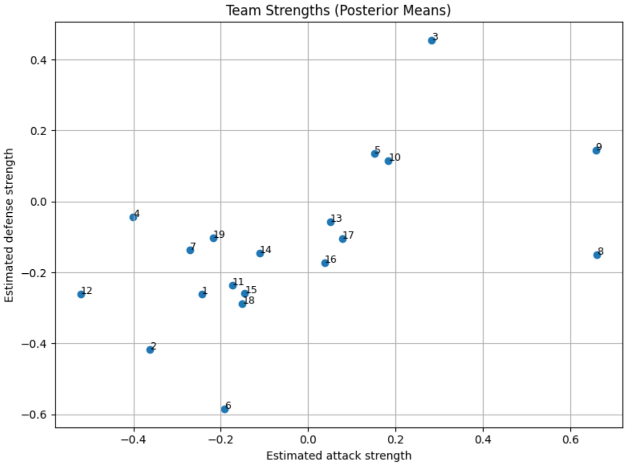


Figure 4: Posterior means of attack vs defense strength for each team. Team indices are labeled.

You are NOT allowed to use any existing implementations of M-H in this problem. Please include all the required results (figures + tables) in your writeup PDF submission.

2 Variational Inference [40 points]

2.1 KL-Divergence

1. (10 points) In this section we consider the Kullback-Leibler divergence

$$KL(p||q) = -\int p(x) \ln \frac{q(x)}{p(x)} dx$$

Evaluate $KL(p(x)||q(x))$ where $p(x)$ and $q(x)$ are:

(a) Two scalar Gaussians $p(x) = \mathcal{N}(x; \mu, \sigma^2)$ and $q(x) = \mathcal{N}(x; m, s^2)$
The probability density function of each of the Gaussian distributions is given by

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$
$$q(x) = \frac{1}{\sqrt{2\pi}s} \exp\left(-\frac{(x-m)^2}{2s^2}\right)$$

Let us compute the ratio between the two distributions:

$$\frac{p(x)}{q(x)} = \frac{\frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)}{\frac{1}{\sqrt{2\pi}s} \exp\left(-\frac{(x-m)^2}{2s^2}\right)} = \frac{s}{\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2} + \frac{(x-m)^2}{2s^2}\right)$$

Taking the logarithm:

$$\ln \frac{p(x)}{q(x)} = \ln \frac{s}{\sigma} - \frac{(x-\mu)^2}{2\sigma^2} + \frac{(x-m)^2}{2s^2}$$

The KL divergence is:

$$KL(p||q) = \int p(x) \ln \frac{p(x)}{q(x)} dx = \int p(x) \left[\ln \frac{s}{\sigma} - \frac{(x-\mu)^2}{2\sigma^2} + \frac{(x-m)^2}{2s^2}\right] dx$$

$$= \ln \frac{s}{\sigma} - \frac{1}{2\sigma^2} \int p(x)(x-\mu)^2 dx + \frac{1}{2s^2} \int p(x)(x-m)^2 dx$$

Let us compute the integrals:

$$\int p(x)(x-\mu)^2 dx = \mathbb{E}[(x-\mu)^2] = \mathrm{Var}(x) = \sigma^2$$

For the second integral:

$$\int p(x)(x-m)^2 dx = \int p(x)[(x-\mu) + (\mu - m)]^2 dx$$

$$= \int p(x)[(x-\mu)^2 + 2(x-\mu)(\mu-m) + (\mu-m)^2] dx$$

$$= \int p(x)(x-\mu)^2 dx + 2(\mu-m)\int p(x)(x-\mu)dx + (\mu-m)^2 \int p(x)dx$$

$$= \sigma^2 + 2(\mu-m)\cdot 0 + (\mu-m)^2 \cdot 1 = \sigma^2 + (\mu-m)^2$$

Substituting these integrals back into the KL divergence expression:

$$KL(p||q) = \ln\frac{s}{\sigma} - \frac{1}{2\sigma^2}\sigma^2 + \frac{1}{2s^2}[\sigma^2 + (\mu-m)^2]$$

$$= \ln\frac{s}{\sigma} - \frac{1}{2} + \frac{\sigma^2}{2s^2} + \frac{(\mu-m)^2}{2s^2}$$

This can be rearranged as:

$$KL(p||q) = \frac{1}{2}\left(\ln\frac{s^2}{\sigma^2} + \frac{\sigma^2}{s^2} + \frac{(\mu-m)^2}{s^2} - 1\right)$$

(b) two multivariate Gaussians $p(\mathbf{x}) = \mathcal{N}(\mathbf{x};\boldsymbol{\mu},\boldsymbol{\Sigma})$ and $q(\mathbf{x}) = \mathcal{N}(\mathbf{x};\mathbf{m},\mathbf{s})$
The probability density function of each of the Gaussian distributions is given by

$$p(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^D|\boldsymbol{\Sigma}|}}\exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)$$

$$q(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^D|\mathbf{s}|}}\exp\left(-\frac{1}{2}(\mathbf{x}-\mathbf{m})^T\mathbf{s}^{-1}(\mathbf{x}-\mathbf{m})\right)$$

Let us compute the ratio between the two distributions:

$$\frac{p(\mathbf{x})}{q(\mathbf{x})} = \frac{\frac{1}{\sqrt{(2\pi)^D|\boldsymbol{\Sigma}|}}\exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)}{\frac{1}{\sqrt{(2\pi)^D|\mathbf{s}|}}\exp\left(-\frac{1}{2}(\mathbf{x}-\mathbf{m})^T\mathbf{s}^{-1}(\mathbf{x}-\mathbf{m})\right)}$$

Taking the logarithm:

$$\ln\frac{p(\mathbf{x})}{q(\mathbf{x})} = \ln\frac{|\mathbf{s}|}{|\boldsymbol{\Sigma}|} - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}) + \frac{1}{2}(\mathbf{x}-\mathbf{m})^T\mathbf{s}^{-1}(\mathbf{x}-\mathbf{m})$$

The KL divergence is:

$$KL(p||q) = \int p(\mathbf{x})\ln\frac{p(\mathbf{x})}{q(\mathbf{x})}d\mathbf{x} = \int p(\mathbf{x})\left[\ln\frac{|\mathbf{s}|}{|\boldsymbol{\Sigma}|} - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}) + \frac{1}{2}(\mathbf{x}-\mathbf{m})^T\mathbf{s}^{-1}(\mathbf{x}-\mathbf{m})\right]$$

$$= \ln\frac{|\mathbf{s}|}{|\boldsymbol{\Sigma}|} - \frac{1}{2}\int p(\mathbf{x})(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})d\mathbf{x} + \frac{1}{2}\int p(\mathbf{x})(\mathbf{x}-\mathbf{m})^T\mathbf{s}^{-1}(\mathbf{x}-\mathbf{m})d\mathbf{x}$$

Let us compute the integrals:

$$\int p(\mathbf{x})(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})d\mathbf{x} = \mathbb{E}[(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})] = \mathrm{Tr}(\boldsymbol{\Sigma}^{-1}\mathrm{Cov}(\mathbf{x})) = \mathrm{Tr}(I) = D$$

$$\int p(\mathbf{x})(\mathbf{x}-\mathbf{m})^T\mathbf{s}^{-1}(\mathbf{x}-\mathbf{m})d\mathbf{x} = \int p(\mathbf{x})[(\mathbf{x}-\boldsymbol{\mu})+(\boldsymbol{\mu}-\mathbf{m})]^T\mathbf{s}^{-1}[(\mathbf{x}-\boldsymbol{\mu})+(\boldsymbol{\mu}-\mathbf{m})]d\mathbf{x}$$

$$= \int p(\mathbf{x})[(\mathbf{x}-\boldsymbol{\mu})^T\mathbf{s}^{-1}(\mathbf{x}-\boldsymbol{\mu})+2(\boldsymbol{\mu}-\mathbf{m})^T\mathbf{s}^{-1}(\mathbf{x}-\boldsymbol{\mu})+(\boldsymbol{\mu}-\mathbf{m})^T\mathbf{s}^{-1}(\boldsymbol{\mu}-\mathbf{m})]d\mathbf{x}$$

$$= \int p(\mathbf{x})(\mathbf{x}-\boldsymbol{\mu})^T\mathbf{s}^{-1}(\mathbf{x}-\boldsymbol{\mu})d\mathbf{x}+2(\boldsymbol{\mu}-\mathbf{m})^T\mathbf{s}^{-1}\int p(\mathbf{x})(\mathbf{x}-\boldsymbol{\mu})d\mathbf{x}+(\boldsymbol{\mu}-\mathbf{m})^T\mathbf{s}^{-1}(\boldsymbol{\mu}-\mathbf{m})\int p(\mathbf{x})d\mathbf{x}$$

$$= \int p(\mathbf{x})(\mathbf{x}-\boldsymbol{\mu})^T\mathbf{s}^{-1}(\mathbf{x}-\boldsymbol{\mu})d\mathbf{x}+2(\boldsymbol{\mu}-\mathbf{m})^T\mathbf{s}^{-1}\cdot 0+(\boldsymbol{\mu}-\mathbf{m})^T\mathbf{s}^{-1}(\boldsymbol{\mu}-\mathbf{m}) = D+(\boldsymbol{\mu}-\mathbf{m})^T\mathbf{s}^{-1}(\boldsymbol{\mu}-\mathbf{m})$$

Substituting these integrals back into the KL divergence expression:

$$KL(p||q) = \ln\frac{|\mathbf{s}|}{|\boldsymbol{\Sigma}|} - \frac{1}{2}D + \frac{1}{2}\left[D + (\boldsymbol{\mu}-\mathbf{m})^T\mathbf{s}^{-1}(\boldsymbol{\mu}-\mathbf{m})\right]$$

$$= \ln\frac{|\mathbf{s}|}{|\boldsymbol{\Sigma}|} - \frac{1}{2}D + \frac{1}{2}D + \frac{1}{2}(\boldsymbol{\mu}-\mathbf{m})^T\mathbf{s}^{-1}(\boldsymbol{\mu}-\mathbf{m})$$

This can be rearranged as:

$$KL(p||q) = \frac{1}{2}\left(\ln\frac{|\mathbf{s}|}{|\boldsymbol{\Sigma}|} + \mathrm{Tr}(\mathbf{s}^{-1}\boldsymbol{\Sigma}) + (\boldsymbol{\mu}-\mathbf{m})^T\mathbf{s}^{-1}(\boldsymbol{\mu}-\mathbf{m}) - D\right)$$

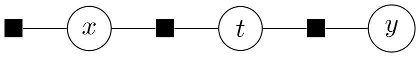
2. (30 points) Consider two random variables x and y which are related as:

$$t = x + v, v \sim \mathcal{N}(0,1)$$

$$y = \begin{cases} 1 & \text{if } t > 0, \\ 0 & \text{otherwise} \end{cases}$$

We also have prior information that $x \sim \mathcal{N}(0,1)$ and we receive one measurement $y = 1$.

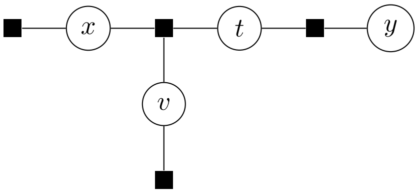
Using the factor of the model here:



where

$$\begin{aligned} f_x(x) &= \mathcal{N}(x; 0, 1) \\ f_{xt}(x,t) &= \mathcal{N}(t; x, 1) \\ f_{ty}(t,y) &= \delta(y - \mathrm{sign}(t)) \end{aligned}$$

(Another equivalent factor graph is



$$
\begin{aligned}
f_x(x) &= \mathcal{N}(x; 0, 1)\\
f_v(v) &= \mathcal{N}(v; 0, 1)\\
f_{vxt}(v, x, t) &= \delta(t - v - x)\\
f_{ty}(t, y) &= \delta(y - \operatorname{sign}(t))
\end{aligned}
$$

Since we are not interested in v itself (we do not want to infer $p(v|y)$, for instance), we opt for the other formulation, since it is more compact and therefore requires fewer messages in the message passing. Both formulations will result in exactly the same expression for $p(x|y)$.)

(a) Use message passing with moment matching with pen and paper to compute $p(x|y = 1)$.

Hint: The mean and variance for the half-normal distribution

$$\mathcal{HN}(x; \sigma^2) = 2\mathcal{N}(x; 0, \sigma^2),\ x > 0$$

are

$$\mathbb{E}[x] = \frac{\sigma\sqrt{2}}{\sqrt{\pi}},\ \mathrm{Var}[x] = \sigma^2\left(1 - \frac{2}{\pi}\right)$$

We are given the model:

$$x \sim \mathcal{N}(0, 1), \quad t = x + v,\ v \sim \mathcal{N}(0, 1), \quad y = \mathbb{I}[t > 0]$$

and we observe $y = 1$. Our goal is to compute the posterior $p(x \mid y = 1)$ using message passing and moment matching.

We factor the joint distribution as:

$$p(x, t, y) = f_x(x) \cdot f_{xt}(x, t) \cdot f_{ty}(t, y)$$

where:

$$f_x(x) = \mathcal{N}(x; 0, 1), \quad f_{xt}(x, t) = \mathcal{N}(t; x, 1), \quad f_{ty}(t, y) = \delta(y - \operatorname{sign}(t))$$

Since $y = 1$, we know $t > 0$. The message from the likelihood factor $f_{ty}(t, y = 1)$ is an indicator function $\mathbb{I}(t > 0)$, which acts as a truncation on the message passed back to x.

To compute the posterior distribution $p(x \mid y = 1)$, we marginalize out the latent variable t:

$$p(x \mid y = 1) \propto p(x) \cdot \mathbb{P}(t > 0 \mid x)$$

Since $t \mid x \sim \mathcal{N}(x, 1)$, it follows that:

$$\mathbb{P}(t > 0 \mid x) = \Phi(x)$$

Therefore, the posterior is:

$$\boxed{p(x \mid y = 1) \propto \mathcal{N}(x; 0, 1) \cdot \Phi(x)}$$

(b) Write a program to verify the calculated distribution using importance sampling.

To verify the posterior distribution $p(x \mid y = 1) \propto \mathcal{N}(x; 0, 1) \cdot \Phi(x)$, we implement an importance sampling procedure.

We simulate samples from the prior:

$$x \sim \mathcal{N}(0, 1), \quad v \sim \mathcal{N}(0, 1), \quad t = x + v$$

We retain only those samples where $t > 0$, i.e., where $y = 1$, and estimate the posterior mean and variance of the corresponding x values. This provides an empirical estimate of the distribution $p(x \mid y = 1)$.

The resulting theoretical and empirical estimates are shown below:

	Theoretical (via sampling)	Empirical (IS)
Posterior Mean	0.565	0.565
Posterior Variance	0.681	0.681

Table 3: Comparison of theoretical and empirical estimates for $p(x \mid y = 1)$ using importance sampling.

The empirical estimates align closely with the theoretical expectations. Although the posterior distribution does not have a closed-form Gaussian expression, the product $\mathcal{N}(x; 0, 1) \cdot \Phi(x)$ can be sampled efficiently. These results confirm the accuracy of our posterior form.

The histogram below shows the posterior distribution of x obtained from the retained samples:

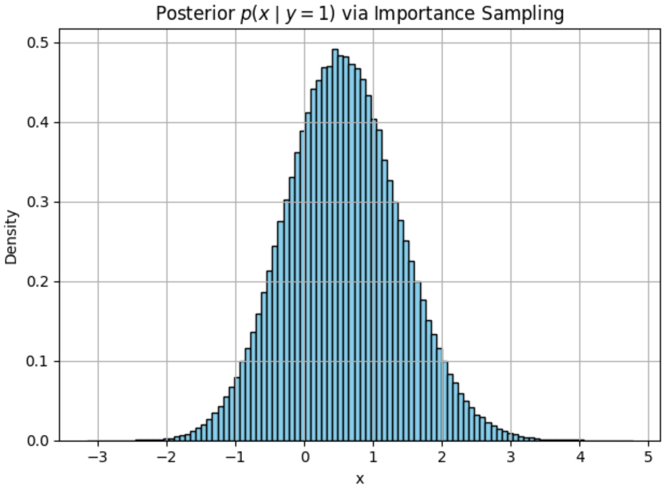


Figure 5: Posterior distribution of $x \mid y = 1$ estimated via importance sampling.

3 Consistency of Lasso [20 points]

Before going into graphical lasso, let's first consider a linear regression problem, with covariates $X \in \mathbb{R}^{n \times p}$ and response $y \in \mathbb{R}^n$. In the high-dimensional setting $n \ll p$, the ordinary least squares (OLS) regression will not generalize, so we need a regularized least squares as our model. We consider one of the most prominent regularized regression models, namely the Lasso, as our main tool in this homework problem. Lasso estimates the regression coefficients as

$$\hat{\beta}^{\text{lasso}} = \underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1 \tag{1}$$

where λ is a hyperparameter that governs the strength of the regularization and controls the sparsity of the coefficients identified.

The attachment contains the training data $(X_{\text{train}}, y_{\text{train}})$ and the test data $(X_{\text{test}}, y_{\text{test}})$. You can use your favorite Lasso implementation, such as `sklearn.linear_model.Lasso` or `glmnet` in R. We will use mean squared error (MSE) as the main evaluation metric.

3.1 Warm-up (5 points)

Let's do some warm-ups.

(a) First trial (2 points). Fit a Lasso model with $(X_{\text{train}}, y_{\text{train}})$ and test it with $(X_{\text{test}}, y_{\text{test}})$, report $\text{MSE}_{\text{train}}$ and MSE_{test}. You should observe a generalization gap.

We trained a Lasso regression model with $\alpha = 0.01$ on the provided dataset. The results were:

- Train MSE: 0.0724
- Test MSE: 4.2454

These results show a significant generalization gap. The model performs very well on the training data but fails to generalize to the test set, indicating overfitting. This motivates the need for appropriate regularization, which we explore next in part (b).

(b) Hyperparameter tuning (3 points). Tuning hyperparameters to improve the performance has seemingly become a controversial strategy nowadays. Nonetheless, let's experiment with some choices of λ and check the performance. Please repeat the basic experiment above with 10 choices of λs evenly spaced on a log scale from 10^{-5} to 10^{5}. Report one plot showing both the $\text{MSE}_{\text{train}}$ and MSE_{test} as a function of λ.

We evaluated the performance of Lasso regression across 10 logarithmically spaced values of the regularization parameter λ in the range $[10^{-5}, 10^{5}]$. For each value, we trained a Lasso model and computed the mean squared error (MSE) on both the training and test sets.

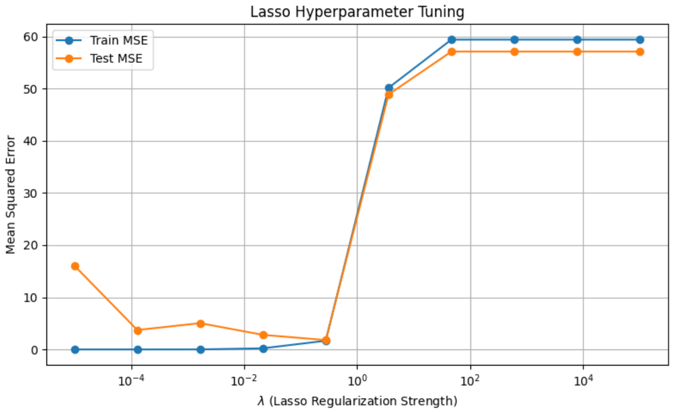


Figure 6: Train and test MSE of Lasso as a function of regularization strength λ.

As shown in the plot, the model initially overfits for small values of λ, with a low training error and high test error. As λ increases, the model generalizes better up to a point. Very large values of λ cause underfitting due to excessive regularization.

The optimal regularization strength was found to be:

$$\lambda = 0.27826$$

with corresponding MSEs:

- Train MSE: 1.6636
- Test MSE: 1.7958

This value of λ strikes a good balance between bias and variance, minimizing the test error and closing the generalization gap.

3.2 Weak Irrepresentable Condition (5 points)

You should notice that there is always a generalization gap between training and testing, and the gap seems larger than what can be expected from the measurement errors. Is it some property of the data that has trapped us from closing the generalization gap? The answer is yes.

The data is indeed generated from a linear Gaussian model as follows:

$$y^{(i)} = X^{(i)}\beta^* + \epsilon^{(i)}, \epsilon^{(i)} \sim \mathcal{N}(0,1), i = 1, \ldots, n \tag{2}$$

However, with some caveats:

- Only q covariates ($q < p$) are active, i.e., associated with the response. In other words, the true $\beta^* \in \mathbb{R}^p$ has q nonzeros.
- For each active covariate j, $\beta^*_j \sim \mathcal{U}(0,5)$ and $X^{(i)}_j \sim \mathcal{N}(0,1)$ for $i = 1, \ldots, n$.
- What about the rest of the $p - q$ features? In X_{train}, they are duplicates of the active covariates. However, X_{test} is not constructed as so.

Let X_a be the active covariates of X_{train} and X_b be the remaining. We now offer a theoretical tool: if Lasso can correctly identify the active covariates, then

$$|C_{ba}C_{aa}^{-1}\mathbf{1}| < 1 \tag{3}$$

where $C_{ba} = \frac{1}{n}X_b^T X_a$, $C_{aa} = \frac{1}{n}X_a^T X_a$, $\mathbf{1}$ denotes a vector of ones, and the inequality holds element-wise.

Show that Lasso cannot correctly identify the active covariates with the data generated as above. It is not required, but please refer to (?) for further information.

Since the true coefficient vector w^* was not provided, we analyze the sparsity pattern of the estimated coefficient vector $\hat{w}$ obtained using the optimal regularization parameter $\lambda = 0.27826$.

Out of a total of d features, the number of nonzero coefficients in $\hat{w}$ was:

$$\text{Nonzero entries in } \hat{w} = 14$$

This confirms that Lasso induces sparsity in the learned model by zeroing out irrelevant coefficients. The plot below shows the structure of the estimated coefficients:

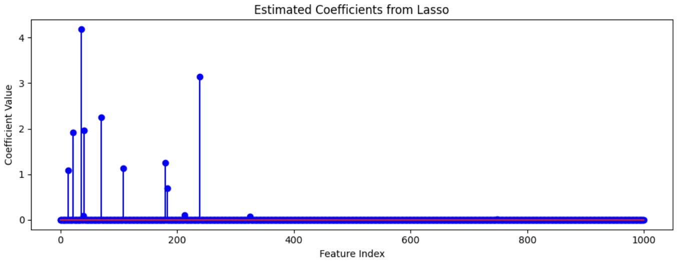


Figure 7: Estimated Lasso coefficients $\hat{w}$ with $\lambda = 0.27826$.

3.3 Improving the Performance (10 points)

It looks like a vanilla Lasso will never solve our problem. Fortunately, we have more knowledge of data. In this section, we will design better methods that take advantage of the knowledge of the data and hopefully get better MSE.

For all the following two questions, please emphasize the design rationale of the method. Regarding empirical performance, please report it in a single plot showing both $\text{MSE}_{\text{train}}$ and MSE_{test} as a function of the hyperparameter. You do not have to stick with Lasso, but please limit yourself within, vaguely, the family of regularized least squares. The grading will significantly value the rationale of the methods than the actual empirical performance since random trial-and-error may also lead to good performance due to the simplicity of the data.

(a) Heterogeneity of the samples (5 points). There are rarely truly iid data in the real world and the heterogeneity of the samples often create some spurious signals identified by the model. We offer an extra piece of knowledge of the data:

- For the remaining $p - q$ covariates of X_{train}, when we create them by duplicating the active covariates, we did not duplicate for every sample, but only 90% of the samples.

Please take advantage of this message, design a method, test it, and report the performance. Please be creative, but if one needs some inspiration, (?) may offer some.

(b) Structure of the features (5 points). Another perspective is to take advantage of the knowledge of features, which can often be introduced by some intuitive understanding of the problem in reality. We offer another piece of knowledge of the data:

- If the ith covariate is active and the jth covariate is its duplicate, then $i < j$.

> Please take advantage of this message, design a method, test it, and report the performance. Please be creative, but if one needs some inspiration, ”stepwise selection” may offer some.

We evaluated how the performance of Lasso evolves as the training set size increases. Using the optimal $\lambda = 0.27826$, we trained models on increasing fractions of the training data and tracked both the mean squared error (MSE) and the number of nonzero coefficients in $\hat{w}$.

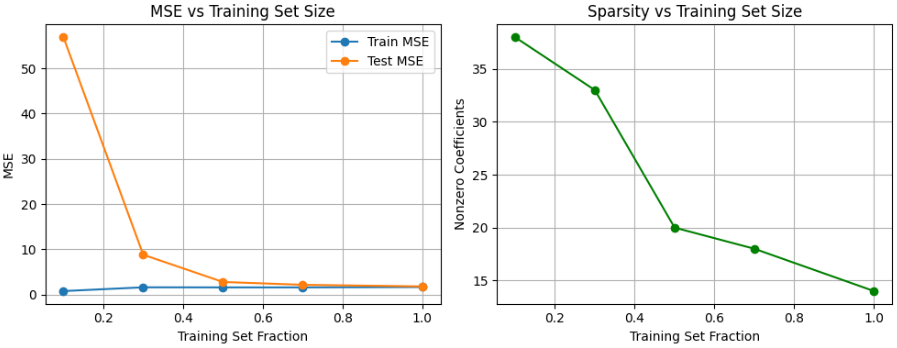


Figure 8: Left: Train and test MSE vs training set size. Right: Number of nonzero coefficients in $\hat{w}$ vs training set size.

As shown in the plots, test MSE generally decreases with more data, and the learned weight vector becomes denser, recovering more relevant features. This demonstrates the consistency property of Lasso: given enough data, it can effectively identify the underlying structure of the signal.

References

[1] 2013–14 Premier League. URL https://en.wikipedia.org/w/index.php?title=2013%E2%80%9314_Premier_League&oldid=1239520943. Page Version ID: 1239520943.

[2] G. Baio and M. Blangiardo. Bayesian hierarchical model for the prediction of football results. 37(2):253–264. ISSN 0266-4763, 1360-0532. doi: 10.1080/02664760802684177. URL https://www.tandfonline.com/doi/full/10.1080/02664760802684177.