STAT-221: Pset 5

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Abstract

In this homework we use an implementatin of the Expectation-Maximization (EM) algorithm to lead inference on non-observable origin-destination (OD) flows in a communication network where only link loads are measured. Measurements are taken every five minutes. Two implementation of EM are derived, replicating the two models described in Cao et al. (JASA, 2000).

question 1.1 We replicate figure 2 of the paper in figure 1, using link loads from `1router_allcount.dat`.

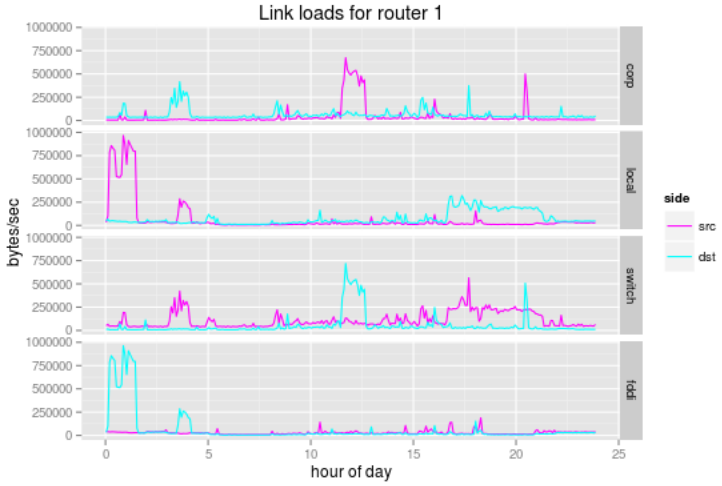

Figure 1: *Link loads on different node of router 1's subnetwork, replicating Cao et al. figure 2.*

question 1.2 We replicate figure 4 of the paper with `1router_allcount.dat`, of log variance against log mean in two time windows of 55 minutes. Linear fits are plotted for unfixed slope and slopes fixed at $c = 1$ and $c = 2$. From the plot $c = 2$ seems to give better regression results.

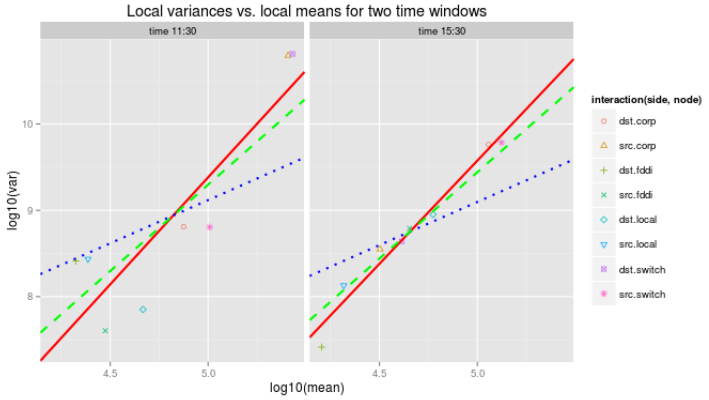

Figure 2: *Local variances versus local means on log scale for the first data set. Linear regression in red, $c = 1$ in dashed blue and $c = 2$ in dashed green.*

Same figure is plotted for `2router_linkcount.dat` on figure 3. In this dataset there are 8 different type of nodes, so 16 combinations of side (origin or destination) - node. Again $c = 2$ seems to give better results than $c = 1$.

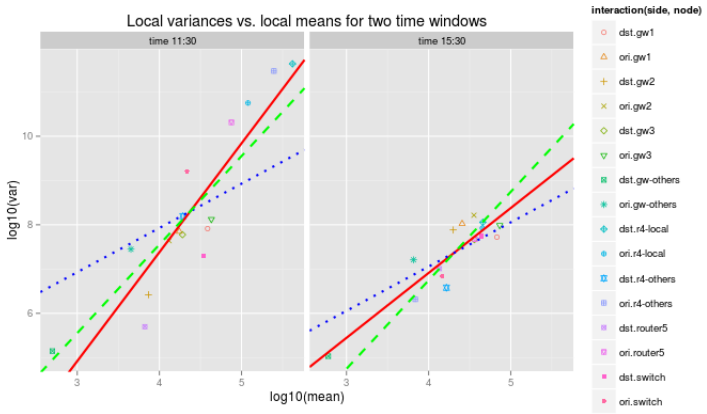

Figure 3: *Local variances versus local means on log scale for the second data set. Linear regression in red, $c = 1$ in dashed blue and $c = 2$ in dashed green.*

question 1.3 We model the I unobserved OD counts x_t at time t as a vector of independent normal random variables

$$x_t \sim Normal(\lambda, \Sigma)$$

with $\Sigma = \phi diag(\sigma^2(\lambda_1), ..., \sigma^2(\lambda_I))$, where $\sigma^2(\lambda) = \lambda^c$. And the observed link byte counts y_t as

$$y_t = Ax_t \sim Normal(A\lambda, A\Sigma A')$$

We base inference on maximum likelihood on iid measurement of this distribution. There is no closed form solution to the likelihood maximization, so that an EM algorithm is implemented to find the parameter solution.

We do not assume a particular value for c, and our parameter is $\theta = (\lambda, \phi)$ $(16 + 1 = 17$ dimensional).

The EM conditional expectation function Q is

$$Q(\theta, \theta^{(k)}) = E_q \left[log \left(p(y, x|\theta) \right) \right]$$

With $q = p(x|y, theta^{(k)})$, so that

$$\begin{aligned} Q(\theta, \theta^{(k)}) &= E \left[log \left(p(Y, X|\theta) \right) | Y, \theta^{(k)} \right] \\ &= E \left[log \left(p(X|\theta) \right) | Y, \theta^{(k)} \right] \\ &= E \left[l(\theta|X) | Y, \theta^{(k)} \right] \end{aligned}$$

With $l(\theta|X)$ latent variable likelihood. We have

$$\begin{aligned} l(\theta|X) &= -\frac{T}{2}log|\Sigma| - \frac{1}{2}\sum_{t=1}^{T}(x_t-\lambda)'\Sigma^{-1}(x_t-\lambda) \\ &= -\frac{T}{2}log|\Sigma| - \frac{1}{2}\sum_{t=1}^{T}x_t'\Sigma^{-1}x_t - \frac{1}{2}\sum_{t=1}^{T}x_t'\Sigma^{-1}\lambda - \frac{1}{2}\sum_{t=1}^{T}\lambda'\Sigma^{-1}x_t - \frac{1}{2}\sum_{t=1}^{T}\lambda'\Sigma^{-1}\lambda \end{aligned}$$

So that, taking expectation given $(Y, \theta^{(k)})$

$$\begin{aligned} Q(\theta,\theta^{(k)}) = &-\frac{T}{2}log|\Sigma| - \frac{1}{2}\sum_{t=1}^{T}\left(tr(\Sigma^{-1}var(x_t|Y,\theta^{(k)})) + E(x_t'|Y,\theta^{(k)})\Sigma^{-1}E(x_t|Y,\theta^{(k)})\right) \\ &- \frac{1}{2}\sum_{t=1}^{T}E(x_t'|Y,\theta^{(k)})\Sigma^{-1}\lambda - \frac{1}{2}\sum_{t=1}^{T}\lambda'\Sigma^{-1}E(x_t|Y,\theta^{(k)}) - \frac{1}{2}\sum_{t=1}^{T}\lambda'\Sigma^{-1}\lambda \end{aligned}$$

Using the variance formula for a quadratic form to compute the second term, $E(\epsilon'\Lambda\epsilon) = tr(\Lambda\epsilon) + \mu'\Lambda\mu$. As x_t is only dependent on y_t, the conditional expectation function simplifies to

$$Q(\theta,\theta^{(k)}) = -\frac{T}{2}\left(log|\Sigma| + tr(\Sigma^{-1}R^{(k)})\right) - \frac{1}{2}\sum_{t=1}^{T}(m_t^{(k)}-\lambda)'\Sigma^{-1}(m_t^{(k)}-\lambda)$$

Where we have conditional mean and variance of x_t

$$\begin{aligned} m_t^{(k)} &= E\left(x_t|y_t,\theta^{(k)}\right) \\ &= \lambda^{(k)} + \Sigma^{(k)}A'(A\Sigma^{(k)}A')^{-1}\left(y_t - A\lambda^{(k)}\right) \\ R^{(k)} &= var\left(x_t|y_t,\theta^{(k)}\right) \\ &= \Sigma^{(k)} - \Sigma^{(k)}A'(A\Sigma^{(k)}A')^{-1}A\Sigma^{(k)} \end{aligned}$$

Those expression are derived by considering the multivariate normal vector (x_t, y_t), and apply formulas for projected multivariate normals given that $cov(x_t, y_t) = cov(x_t, Ax_t) = A\Sigma^{(k)}$ and $cov(y_t, y_t) = A\Sigma^{(k)}A'$ given $\theta^{(k)}$.

Expanding the expression of Q, we have

$$\begin{aligned} Q(\theta,\theta^{(k)}) = &-\frac{T}{2}\sum_{i=1}^{I}clog(\lambda_i) - \frac{T}{2}\sum_{i=1}^{I}\frac{r_{ii}^{(k)}}{\phi\lambda_i^c} - \frac{1}{2}\sum_{t=1}^{T}\sum_{i=1}^{I}\frac{(m_{t,i}^{(k)})^2}{\phi\lambda_i^c} \\ &+ \sum_{t=1}^{T}\sum_{i=1}^{I}\frac{\lambda_i m_{t,i}^{(k)}}{\phi\lambda_i^c} - \frac{1}{2}\sum_{t=1}^{T}\sum_{i=1}^{I}\frac{\lambda_i^2}{\phi\lambda_i^c} \end{aligned}$$

So that taking $\frac{\partial Q}{\partial\theta}$ gives us the system of equations (first I ones due to λ, last one to ϕ)

$$c\phi\lambda_i^c + (2-c)\lambda_i^2 - 2(1-c)\lambda_i b_i^{(k)} - ca_i^{(k)} = 0 \qquad i = 1...I \tag{1}$$

$$\sum_{i=1}^{I}\lambda_i^{-c+1}(\lambda_i - b_i^{(k)}) = 0 \tag{2}$$

Where we have defined

$$a_i^{(k)} = r_{ii}^{(k)} + \frac{1}{T}\sum_{t=1}^{T}(m_{t,i}^{(k)})^2$$

$$b_i^{(k)} = \frac{1}{T}\sum_{t=1}^{T} m_{t,i}^{(k)}$$

We hence derive the steps of the EM algorithm for our iid model.

Data: Observed link loads Y.
Result: MLE of parameter θ.
initialization: $\theta = \theta_0$ positive parameter.
while $|Q(\theta^{(k+1)}, \theta^{(k)}) - Q(\theta^{(k)}, \theta^{(k-1)})| > \epsilon$ **do**
- Update step: k = k + 1
- E-step: Compute $m_t^{(k)}, R^{(k)}, a_i^{(k)}, b_i^{(k)}$.
- M-step **if** *c = 1 or c = 2* **then**
  1. Solve (1) for λ analytically given ϕ (positive solution).
  2. Solve for ϕ using fractional steps Newton-Raphson or constrained `optim` optimization (ensures ϕ positive).

else
  Update θ using constrained `optim` optimization (ensures parameters positive).

end
end

Algorithm 1: EM algorithm for iid model

question 1.4 We fix the variance and window frame parameters to be $c = 2$ (most appropriate according to exploratory data analysis), $w = 11$. The MLE equations (1) then becomes

$$\phi\lambda_i^2 + \lambda_i b_i^{(k)} - a_i^{(k)} = 0 \quad i = 1...I$$

Which gives us a positive solution (the biggest of the two roots of the equation) for λ_i given ϕ

$$\lambda_i^{(k+1)} = \frac{\sqrt{(b_i^{(k)})^2 + 4\phi^{(k)} a_i^{(k)}} - b_i^{(k)}}{2\phi^{(k)}}$$

Setting λ to those values, we have $f_i(\theta) = 0$ for $i = 1..I$ where $f(\theta)$ is the left hand-side of equations (1) and (2), so that the one-step Newton-Raphson algorithm

$$\theta^{(k+1)} = \theta^{(k)} - \left[F(\theta^{(k)})\right]^{-1} f(\theta^{(k)})$$

Reduces to

$$\phi^{(k+1)} = \phi^{(k)} - \left(\left[F(\theta^{(k)})\right]^{-1}\right)_{I+1,I+1} f_{I+1}(\theta^{(k)})$$

With

$$f_{I+1}(\theta^{(k)}) = \sum_{i=1}^{I} \frac{\lambda_i - b_i^{(k)}}{\lambda_i}$$

And the Jacobian $F(\theta^{(k)})$ defined by

$$\frac{\partial f_i}{\partial \lambda_j} = \delta_{ij}\left(\frac{4\phi}{\lambda_i} + 2b_i^{(k)}\right)$$
$$\frac{\partial f_{I+1}}{\partial \lambda_j} = \frac{b_j^{(k)}}{\lambda_j}$$
$$\frac{\partial f_i}{\partial \phi} = 2\lambda_i^2$$
$$\frac{\partial f_{I+1}}{\partial \phi} = 0$$

To solve the M-step of our EM algorithm, we adopt an iterative fractional Newton-Raphson method, by dividing the step in the former udpate of ϕ by bigger and bigger integer if the update is negative. However this approach failed to converge fast enough (steps are too small), and we falled back on an `optim` optimization method. We extend the basic iid model to a local idd model,

by setting time moving windows in which observations are treated iid.

$$y_{t-h}, ..., y_{t+h} \sim Normal(A\lambda_t, A\Sigma_t A')$$

With $\Sigma_t = \phi_t diag(\lambda_t^2)$. On each of those windowed data set, the MLE parameter θ_t is fitted using the previously derived iid model EM.

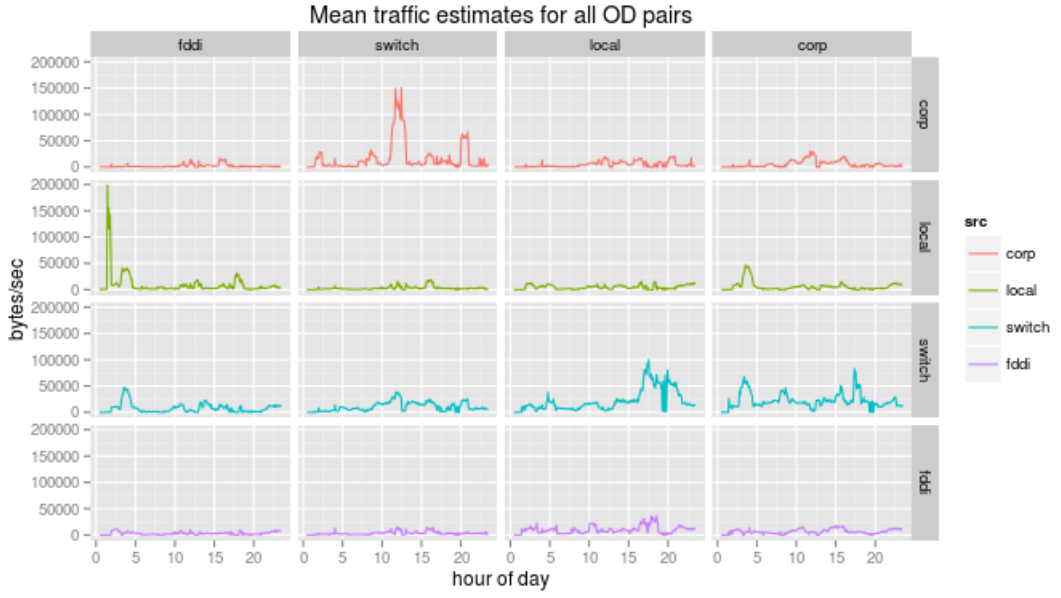

Figure 4: *Mean Traffic estimates $\hat{\lambda}_t$ for all OD pairs, reproducing figure 5 of the paper.*

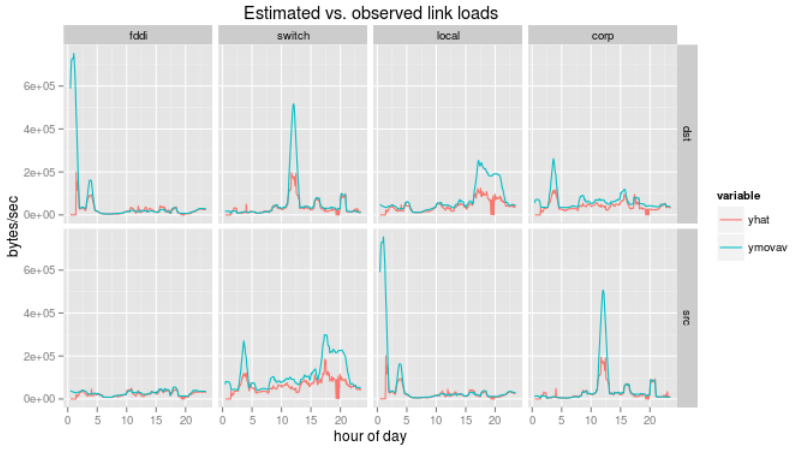

Figure 5: *Estimated and observed link loads (marginal plots on figure 5 of the paper). We observe that we underestimate the traffic at pick times.*

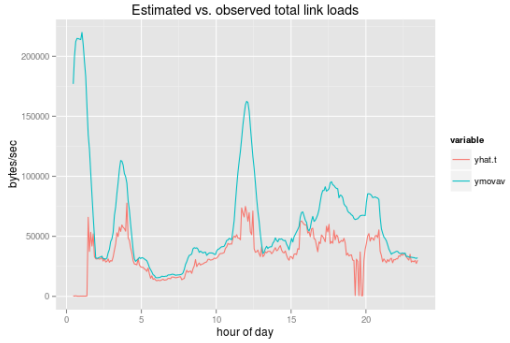

Figure 6: *Total estimated and observed link loads (top rightmarginal plots on figure 5 of the paper).*

question 1.5 We derive the EM algorithm for the refined model of the paper's fourth section. This refined model adds smoothing to the estimates by considering the parameters as following hidden markov model, resulting in an algorithm similar to the Kalman Filter.

$\eta_t = (log(\lambda_t), log(\phi_t))$ is modeled as a random walk state

$$\eta_t = \eta_{t-1} + v_t$$

With $v_t \sim Normal(0, V)$, and V fixed variance matrix. We denote all the current information until time $t+h$ by $\tilde{Y}_t = (y_1, ..., y_{t+h})$, and the window data set at time t Y_t. The goal of our EM algorithm is to find the MAP estimator, ie. the mode of the posterior distribution $p(\eta_t|\tilde{Y}_t)$.

We actually have

$$p(\eta_t|\tilde{Y}_t) = p(\eta_t|\tilde{Y}_{t-1}, Y_t) \propto p(\eta_t|\tilde{Y}_{t-1})p(Y_t|\eta_t)$$

Using Baye's rule. Hence we now want to maximize the log posterior distribution (removing additive constants)

$$g(\eta_t) = log\left(\pi_t(\eta_t)\right) + log\left(p(Y_t|\eta_t)\right)$$

Where $\pi_t(\eta_t) = p(\eta_t|\tilde{Y}_{t-1})$ prior at time t, and $log\left(p(Y_t|\eta_t)\right) = log\left(p(Y_t|\theta_t)\right)$ is what we were trying to maximize in the previous local EM algorithm.

This modifies our EM algorithm by adding a constant (in that it does not depend on the data) prior component to the Q expectation function, ie.

$$Q(\theta, \theta_t^{(k)}) = Q_{local}(\theta, \theta_t^{(k)}) + log\left(\pi_t(log(\theta))\right)$$

Hence we just need to come up with the expression of $log\left(\pi_t(\eta_t)\right)$ to modify our E-step, and optimize the new Q for our M-step.

Integrating on all values of former step states, we have

$$\pi_t(\eta_t) = \int p(\eta_{t-1}|\tilde{Y}_{t-1}) p(\eta_t|\eta_{t-1}) d\eta_{t-1}$$

With $\eta_t|\eta_{t-1} \sim Normal(\eta_{t-1}, V)$. The paper approximates the former state posterior as a normal distribution, ie. $\eta_{t-1}|\tilde{Y}_{t-1} \sim Normal(\hat{\eta}_{t-1}, \hat{\Sigma}_{t-1})$, where $\hat{\eta}_{t-1}$ is the previous state posterior mode and $\hat{\Sigma}_{t-1} = -\ddot{g}(\hat{\eta}_t)^{-1}$ (local normal approximation, there seems to be a mistake in the paper, which forgets the minus sign before the Hessian). So the integral for the prior gives us

$$\pi_t(\eta_t) = Normal(\hat{\eta}_{t-1}, \hat{\Sigma}_{t-1} + V)$$

So that we obtain a Q expectation function

$$Q(\theta, \theta_t^{(k)}) = Q_{local}(\theta, \theta_t^{(k)}) + log\left(dnorm\left(log(\theta), \hat{\eta}_{t-1}, \hat{\Sigma}_{t-1} + V\right)\right) \tag{3}$$

And the refined model EM algorithm proceeds as follows:

Data: Observed link loads Y.
Result: MAP of parameters θ_t.
for *t=1* **to** T **do**
  initialization: $\theta_t = \theta_0$ positive parameter.
  while $|Q(\theta_t^{(k+1)}, \theta_t^{(k)}) - Q(\theta_t^{(k)}, \theta_t^{(k-1)})| > \epsilon$ **do**
    - Update step: k = k + 1
    - E-step: Compute $m_t^{(k)}, R^{(k)}, a_i^{(k)}, b_i^{(k)}, \hat{\eta}_{t-1}, \hat{\Sigma}_{t-1}$ (using numerical methods for the Hessian).
    - M-step: Update θ_t using constrained `optim` optimization (ensures parameters positive) on the Q function defined in (3).
  end
end

Algorithm 2: EM algorithm for refined model

question 1.6 We fit the refined EM model as described in the previous question. To implement the update of $\hat{\Sigma}_t$ we use the hessian numerical approximation function from the `numDeriv` package.

The implementation of the algorithm is implemented in `kuatefodouop_functions.R`. Unfortunately the optimization ran into numerical issues, and the smoothed estimates could not be computed.

question 1.8 The model of Tabaldi and West uses a Bayesian perspective and use an MCMC implementation to solve the defined OD model. However it only deals with a single y interval, and does not use the shifted time windows introduced by Cao et al. Hence Cao's model will perform better when there is strong time local structure to the variation of the packet traffic.

On the other side, Tebaldi et al.'s model makes good use of informative prior and hence avoids overestimating low flows on OD routes that share links with OD routes experiencing high flows. It will hence perform better in configuration where for example two edges going to (or coming from) a node have very different traffic.

question 1.9 We run the same models as before (local idd and refined), on the second data set.

The code to be run on Odyssey is implemented in `kuatefodouop_2router.R`, but unfortunately numerical error in the optimization involved in the EM were encountered.