Robust HMF Notes: proof/sketch of why there is an objective

Tom Hilder

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# Setup

Say we have measured data  $F_{ij}$  with known variances  $\sigma_{ij}^2$ . We model this with with lower rank matrices:

$$Y_{ij} = a_i^{\top} g_j, \tag{1}$$

where

$$Y: N \times M,$$
  
 $A: N \times K,$   
 $G: K \times M,$ 

and  $K \leq \min(N, M)$  such that

$$Y \approx AG.$$
 (2)

Assuming Gaussian (but independent) heteroskedastic noise gives the usual  $\chi^2$  objective:

$$\chi^{2}(A,G) = \sum_{ij} \frac{(Y_{ij} - a_{i}^{\top} g_{j})^{2}}{\sigma_{ij}^{2}}.$$
(3)

This is bilinear in (A, G) so solvable with alternating least squares.

a-step

$$A_i \leftarrow G_i F_i,$$

$$[G_i]_{kk'} = \sum_{j=1}^m \frac{g_{kj} g_{k'j}}{\sigma_{ij}^2},$$

$$[F_i]_k = \sum_{j=1}^m \frac{g_{kj} Y_{ij}}{\sigma_{ij}^2}.$$

g-step

$$G_j \leftarrow A_j^{\top} F_j,$$

$$[A_j]_{kk'} = \sum_{i=1}^{N} \frac{a_{ik} a_{ik'}}{\sigma_{ij}^2},$$

$$[F_j]_k = \sum_{i=1}^{N} \frac{a_{ik} Y_{ij}}{\sigma_{ij}^2}.$$

This is weighted least squares (WLS) for  $a_i$  or  $g_j$  given fixed G or A.

# **Adding Robustness**

Outliers are not dealt with well by  $\chi^2$  objective because the quadratic loss penalty is too chonky. Instead, define

$$r_{ij} = \frac{Y_{ij} - a_i^{\top} g_j}{\sigma_{ij}}, \qquad L(A, G) = \sum_{ij} \rho(r_{ij}). \tag{4}$$

If  $\rho(r) = \frac{1}{2}r^2$ , we recover the above. Switch to a Cauchy likelihood, taking the negative log likelihood as our loss function:

$$\rho(r) = \frac{Q^2}{2} \log \left( 1 + \left( \frac{r}{Q} \right)^2 \right). \tag{5}$$

The Cauchy distribution has large tails and so the loss penalty while quadratic for small r, tends to only  $\rho \propto \log r^2$  for large r. I think actually the nicest way to do this whole argument would be with student's t distribution, because the Cauchy and Gaussian distributions are special cases/limits of that. Anyway continuing with Cauchy.

# **Auxiliary Form**

Claim: the loss can be expressed for any r in the following way

$$\rho(r) = \min_{0 < w < 1} \left[ \frac{1}{2} w r^2 + \phi(w) \right], \tag{6}$$

where

$$\phi(w) = \frac{Q^2}{2} (w - 1 - \log w). \tag{7}$$

Let's prove that. Define

$$J(w;r) = \frac{1}{2}wr^2 + \frac{Q^2}{2}(w - 1 - \log w)$$
(8)

Differentiating with respect to w:

$$\frac{\partial J}{\partial w} = \frac{1}{2}r^2 + \frac{Q^2}{2}\left(1 - \frac{1}{w}\right),\tag{9}$$

and

$$\frac{\partial^2 J}{\partial w^2} = \frac{Q^2}{2} \frac{1}{w^2} > 0, \qquad \forall Q, w > 0.$$
 (10)

thus we know that the critical point minimises J. Setting  $\partial_w J = 0$  yields

$$\hat{w}(r) = \operatorname{argmin}_{w} J(w; r) \tag{11}$$

$$=\frac{1}{1+(r/Q)^2},\tag{12}$$

and note that  $\hat{w} \in (0,1]$  because  $(r/Q)^2 \ge 0$ . We now prove the claim. First set  $t = (r/Q)^2 \ge 0$ , then

$$\hat{w} = \frac{1}{1+t}, \qquad r^2 = Q^2 t, \tag{13}$$

such that

$$J(\hat{w};r) = \frac{1}{2}\hat{w}r^2 + \phi(\hat{w}),\tag{14}$$

substituting and simplifying one piece at a time:

$$\Rightarrow \frac{1}{2}\hat{w}r^2 = \frac{Q^2}{2} \frac{t}{1+t} \tag{15}$$

$$\Rightarrow \phi(\hat{w}) = \frac{Q^2}{2} \left( \hat{w} - 1 - \log \hat{w} \right) \tag{16}$$

$$= \frac{Q^2}{2} \left( -\frac{t}{1+t} + \log(1+t) \right) \tag{17}$$

$$\Rightarrow J(\hat{w};r) = \frac{Q^2}{2}\log\left(1 + \left(\frac{r}{Q}\right)^2\right). \tag{18}$$

Thus

$$\rho(r) = J(\hat{w}; r) \tag{19}$$

$$= \min_{0 < w < 1} \left[ \frac{1}{2} w r^2 + \phi(w) \right], \tag{20}$$

as claimed.

# Three-Step Algorithm

Define new objective:

$$J(A, G, W) = \frac{1}{2} \sum_{ij} \left[ w_{ij} r_{ij}^2 + \phi(w_{ij}) \right], \tag{21}$$

with  $r_{ij} = (Y_{ij} - a_i^{\top} g_j) / \sigma_{ij}$ . By construction,

$$L(A,G) = \min_{W} J(A,G,W), \tag{22}$$

and if

$$\hat{W} = \operatorname{argmin}_{w} J(A, G, W), \tag{23}$$

then

$$\left[\hat{W}\right]_{ij} = \hat{w}(r_{ij}) \tag{24}$$

$$=\frac{1}{1+(r_{ij}/Q)^2}. (25)$$

This immediately yield's Hogg's procedure

w-step:  $w_{ij} \leftarrow \hat{w}(r_{ij})$ ,

a-step: solve WLS for A with new weights, g-step: solve WLS for G with new weights.

where the a-step optimises the quadratic

$$Q(A \mid G, W) = \frac{1}{2} \sum_{ij} w_{ij} r_{ij}^{2}, \tag{26}$$

and the g-step optimises Q(G | A, W). It should be pretty apparent now that the procedure gives the MLE with a Cauchy likelihood.

# Extra convincing (showing that the procedure optimises L)

Consider one outer cycle starting at  $(A^{(t)}, G^{(t)})$ . Choose  $W^{(t)} = \hat{w}(r(A^{(t)}, G^{(t)}))$ . Then

$$L(A^{(t)}, G^{(t)}) = J(A^{(t)}, G^{(t)}, W^{(t)}).$$
(27)

With frozen  $W^{(t)}$ , the a- and g-steps minimize  $Q(\cdot | W^{(t)})$ . Since our total objective is  $J = Q + \sum \phi(W^{(t)})$ , this implies

$$J(A^{(t+1)}, G^{(t+1)}, W^{(t)}) \le J(A^{(t)}, G^{(t)}, W^{(t)}).$$
(28)

We're guaranteed to be helped by the w-step again now, so setting

$$W^{(t+1)} = \hat{w}\left(r(A^{(t+1)}, G^{(t+1)})\right),\tag{29}$$

and using our result from the previous section gives

$$J(A^{(t+1)}, G^{(t+1)}, W^{(t+1)}) \le J(A^{(t+1)}, G^{(t+1)}, W^{(t)}). \tag{30}$$

Thus chaining the inequalities and  $L(A, G) = \min_{W} J(A, G, W)$  gives

$$L(A^{(t+1)}, G^{(t+1)}) \le L(A^{(t)}, G^{(t)}).$$
 (31)

This is enough to guarantee that robust HMF with Hogg's w-step converges to the Cauchy MLE.

#### Extra Notes

- The update  $w_{ij} \leftarrow \hat{w}(r_{ij})$  is exactly Hogg's update rule if one combines  $\sigma_{ij}$  into the weights:  $\tilde{w}_{ij} = w_{ij}/\sigma_{ij}^2$ . I kept the updated weights separate to the data variances since it makes the connection to the MLE clearer (in my mind).
- Different  $\rho$  losses (negative log likelihoods) yield different w-step rules.
- This is basically the standard argument for IRLS (iteratively reweighted least squares), didn't require much extra.
- $\bullet$  I accidentally overloaded my notation a bit (Q is two things). Sorry about that.
- This view gives a very natural interpretation for any regularisation, priors or constraints.
- I ignored the re-orienting step (via SVD) in this discussion. I think actually one can leave it until the end, rather than doing it every iteration.
- In theory, we could also just directly optimise the objective with something like stochastic gradient descent, which could be really good when the data set gets large.