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# Fast Bayesian Non-Negative Matrix Factorisation and Tri-Factorisation

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## Abstract

We present a fast variational Bayesian algorithm for performing non-negative matrix factorisation and tri-factorisation. We show that our approach achieves faster convergence per iteration and timestep (wall-clock) than Gibbs sampling and non-probabilistic approaches, and do not require additional samples to estimate the posterior. We show that in particular for matrix tri-factorisation convergence is difficult, but our variational Bayesian approach offers a fast solution, allowing the tri-factorisation approach to be used more effectively.

## 1 Introduction

Non-negative matrix factorisation methods Lee and Seung [1999] have been used extensively in recent years to decompose matrices into latent factors, helping us reveal hidden structure and predict missing values. In particular we decompose a given matrix into two smaller matrices so that their product approximates the original one. The non-negativity constraint makes the resulting matrices easier to interpret, and is often inherent to the problem – such as in image processing or bioinformatics (Lee and Seung [1999], Wang et al. [2013]). Some approaches approximate a maximum likelihood (ML) or maximum a posteriori (MAP) solution that minimises the difference between the observed matrix and the decomposition of this matrix. This gives a single point estimate, which can lead to overfitting more easily and neglects uncertainty. Instead, we may wish to find a full distribution over the matrices using a Bayesian approach, where we define prior distributions over the matrices and then compute their posterior after observing the actual data.

Schmidt et al. [2009] presented a Bayesian model for non-negative matrix factorisation that uses Gibbs sampling to obtain draws of these posteriors, with exponential priors to enforce non-negativity. Markov chain Monte Carlo (MCMC) methods like Gibbs sampling rely on a sampling procedure to eventually converge to draws of the desired distribution – in this case the posterior of the matrices. This means that we need to inspect the values of the draws to determine when our method has converged (burn-in), and then take additional draws to estimate the posteriors.

We present a variational Bayesian approach to non-negative matrix factorisation, where instead of relying on random draws we obtain a deterministic convergence to a solution. We do this by introducing a new distribution that is easier to compute, and optimise it to be as similar to the true posterior as possible. We show that our approach gives faster convergence rates per iteration and timestep (wall-clock) than current methods, and is less prone to overfitting than the popular non-probabilistic approach of Lee and Seung [2000].

We also consider the problem of non-negative matrix tri-factorisation, first introduced by Ding et al. [2006], where we decompose the observed dataset into three smaller matrices, which again are constrained to be non-negative. Matrix tri-factorisation has been explored extensively in recent years, for example for collaborative filtering (Chen et al. [2009]) and clustering genes and phenotypes

(Hwang et al. [2012]). We present a fully Bayesian model for non-negative matrix tri-factorisation, extending the matrix factorisation model to obtain both a Gibbs sampler and a variational Bayesian algorithm for inference. We show that convergence is even harder, and that the variational approach provides significant speedups (roughly four times faster) compared to Gibbs sampling.

## 2 Non-Negative Matrix Factorisation

We follow the notation used by Schmidt et al. [2009] for non-negative matrix factorisation (NMF), which can be formulated as decomposing a matrix  $\mathbf{R} \in \mathbb{R}^{I \times J}$  into two latent (unobserved) matrices  $\mathbf{U} \in \mathbb{R}_+^{I \times K}$  and  $\mathbf{V} \in \mathbb{R}_+^{J \times K}$ . In other words, solving  $\mathbf{R} = \mathbf{UV}^T + \mathbf{E}$ , where noise is captured by matrix  $\mathbf{E} \in \mathbb{R}^{I \times J}$ . The dataset  $\mathbf{R}$  need not be complete – the indices of observed entries can be represented by the set  $\Omega = \{(i, j) \mid R_{ij} \text{ is observed}\}$ . These entries can then be predicted by  $\mathbf{UV}^T$ .

We take a probabilistic approach to this problem. We express a likelihood function for the observed data, and treat the latent matrices as random variables. As the likelihood we assume each value of  $\mathbf{R}$  comes from the product of  $\mathbf{U}$  and  $\mathbf{V}$ , with some Gaussian noise added,

$$R_{ij} \sim \mathcal{N}(R_{ij} \mid \mathbf{U}_i \cdot \mathbf{V}_j, \tau^{-1})$$

where  $\mathbf{U}_i, \mathbf{V}_j$  denote the  $i$ th and  $j$ th rows of  $\mathbf{U}$  and  $\mathbf{V}$ , and  $\mathcal{N}(x \mid \mu, \tau)$  is the density of the Gaussian distribution, with precision  $\tau$ . The full set of parameters for our model is denoted  $\boldsymbol{\theta} = \{\mathbf{U}, \mathbf{V}, \tau\}$ .

In the Bayesian approach to inference, we want to find the distributions over the parameters  $\boldsymbol{\theta}$  after observing the data  $D = \{R_{ij}\}_{i,j \in \Omega}$ . We can use Bayes' theorem for this,  $p(\boldsymbol{\theta} \mid D) \propto p(D \mid \boldsymbol{\theta})p(\boldsymbol{\theta})$ . We need priors over the parameters, allowing us to express beliefs for their values – such as constraining  $\mathbf{U}, \mathbf{V}$  to be non-negative. We can normally not compute the posterior  $p(\boldsymbol{\theta} \mid D)$  exactly, but some choices of priors allow us to obtain a good approximation. Schmidt et al. choose an exponential prior over  $\mathbf{U}$  and  $\mathbf{V}$ , so that each element in  $\mathbf{U}$  and  $\mathbf{V}$  is assumed to be independently exponentially distributed with rate parameters  $\lambda_{ik}^U, \lambda_{jk}^V > 0$ ,

$$U_{ik} \sim \mathcal{E}(U_{ik} \mid \lambda_{ik}^U) \quad V_{jk} \sim \mathcal{E}(V_{jk} \mid \lambda_{jk}^V)$$

where  $\mathcal{E}(x \mid \lambda)$  is the density of the exponential distribution. For the precision  $\tau$  we use a Gamma distribution with shape  $\alpha > 0$  and rate  $\beta > 0$ .

Schmidt et al. [2009] introduced a Gibbs sampling algorithm for approximating the posterior distribution, which relies on sampling new values for each random variable in turn from the conditional posterior distribution. Details on this method can be found in the supplementary materials (Section 1.1).

**Variational Bayes for NMF** Like Gibbs sampling, variational Bayesian inference (VB) is a way to approximate the true posterior  $p(\boldsymbol{\theta} \mid D)$ . The idea behind VB is to introduce an approximation  $q(\boldsymbol{\theta})$  to the true posterior that is easier to compute, and to make our variational distribution  $q(\boldsymbol{\theta})$  as similar to  $p(\boldsymbol{\theta} \mid D)$  as possible (as measured by the KL-divergence). We assume the variational distribution  $q(\boldsymbol{\theta})$  factorises completely, so all variables are independent,  $q(\boldsymbol{\theta}) = \prod_{\theta_i \in \boldsymbol{\theta}} q(\theta_i)$ . This is called the mean-field assumption. We assume the same forms of  $q(\theta_i)$  as used in Gibbs sampling,

$$q(\tau) = \mathcal{G}(\tau \mid \alpha^*, \beta^*) \quad q(U_{ik}) = \mathcal{TN}(U_{ik} \mid \mu_{ik}^U, \tau_{ik}^U) \quad q(V_{jk}) = \mathcal{TN}(V_{jk} \mid \mu_{jk}^V, \tau_{jk}^V)$$

Beal and Ghahramani [2003] showed that the optimal distribution for the  $i$ th parameter,  $q^*(\theta_i)$ , can be expressed as follows (for some constant  $C$ ), allowing us to find the optimal updates for the variational parameters

$$\log q^*(\theta_i) = \mathbb{E}_{q(\boldsymbol{\theta}_{-i})} [\log p(\boldsymbol{\theta}, D)] + C.$$

Note that we take the expectation with respect to the distribution  $q(\boldsymbol{\theta}_{-i})$  over the parameters but excluding the  $i$ th one. This gives rise to an iterative algorithm: for each parameter  $\theta_i$  we update its distribution to that of its optimal variational distribution, and then update the expectation and variance with respect to  $q$ . This algorithm is guaranteed to maximise the Evidence Lower Bound (ELBO)

$$\mathcal{L} = \mathbb{E}_q [\log p(\boldsymbol{\theta}, D) - \log q(\boldsymbol{\theta})],$$

which is equivalent to minimising the KL-divergence. More details and updates for the approximate posterior distribution parameters are given in the supplementary materials (Section 1.2).

### 3 Non-Negative Matrix Tri-Factorisation

The problem of non-negative matrix tri-factorisation (NMTF) can be formulated similarly to that of non-negative matrix factorisation. We now decompose our dataset  $\mathbf{R} \in \mathbb{R}^{I \times J}$  into three matrices  $\mathbf{F} \in \mathbb{R}_+^{I \times K}$ ,  $\mathbf{S} \in \mathbb{R}_+^{K \times L}$ ,  $\mathbf{G} \in \mathbb{R}_+^{J \times L}$ , so that  $\mathbf{R} = \mathbf{F}\mathbf{S}\mathbf{G}^T + \mathbf{E}$ . We again use a Gaussian likelihood and Exponential priors for the latent matrices.

$$\begin{aligned} R_{ij} &\sim \mathcal{N}(R_{ij} | \mathbf{F}_i \cdot \mathbf{S} \cdot \mathbf{G}_j, \tau^{-1}) & \tau &\sim \mathcal{G}(\tau | \alpha, \beta) \\ F_{ik} &\sim \mathcal{E}(F_{ik} | \lambda_{ik}^F) & S_{kl} &\sim \mathcal{E}(S_{kl} | \lambda_{kl}^S) & G_{jl} &\sim \mathcal{E}(G_{jl} | \lambda_{jl}^G) \end{aligned}$$

A Gibbs sampling algorithm that can be derived similarly to before. Details can be found in the supplementary materials (Section 1.3).

#### 3.1 Variational Bayes for NMTF

Our VB algorithm for tri-factorisation follows the same steps as before, but now has an added complexity due to the term  $\mathbb{E}_q [(R_{ij} - \mathbf{F}_i \cdot \mathbf{S} \cdot \mathbf{G}_j)^2]$ . Before, all covariance terms for  $k' \neq k$  were zero due to the factorisation in  $q$ , but we now obtain some additional non-zero covariance terms. This leads to the more complicated variational updates given in the supplementary materials (Section 1.4).

$$\begin{aligned} \mathbb{E}_q [(R_{ij} - \mathbf{F}_i \cdot \mathbf{S} \cdot \mathbf{G}_j)^2] &= \left( R_{ij} - \sum_{k=1}^K \sum_{l=1}^L \widetilde{F}_{ik} \widetilde{S}_{kl} \widetilde{G}_{jl} \right)^2 + \sum_{k=1}^K \sum_{l=1}^L \text{Var}_q [F_{ik} S_{kl} G_{jl}] \\ &+ \sum_{k=1}^K \sum_{l=1}^L \sum_{k' \neq k} \text{Cov} [F_{ik} S_{kl} G_{jl}, F_{ik'} S_{k'l} G_{jl}] + \sum_{k=1}^K \sum_{l=1}^L \sum_{l' \neq l} \text{Cov} [F_{ik} S_{kl} G_{jl}, F_{ik} S_{kl'} G_{jl'}] \end{aligned}$$

## 4 Experiments

To demonstrate the performances of our proposed methods, we ran several experiments on a toy dataset, as well as several drug sensitivity datasets. For the toy dataset we generated the latent matrices using unit mean exponential distributions, and adding zero mean unit variance Gaussian noise to the resulting product. For the matrix factorisation model we use  $I = 100$ ,  $J = 80$ ,  $K = 10$ , and for the matrix tri-factorisation  $I = 100$ ,  $J = 80$ ,  $K = 5$ ,  $L = 5$ .

We also consider a drug sensitivity dataset, which detail the effectiveness of different drugs on cell lines for cancer and tissue types. The Genomics of Drug Sensitivity in Cancer (GDSC v5.0, Yang et al. [2013]) dataset contains 138 drugs and 622 cell lines, with 81% of entries observed.

We compare our methods against classic algorithms for matrix factorisation and tri-factorisation. Aside from the Gibbs sampler (G-NMF, G-NMTF) and VB algorithms (VB-NMF, VB-NMTF), we consider the non-probabilistic matrix factorisation (NP-NMF) and tri-factorisation (NP-NMTF) methods introduced by Lee and Seung [2000] and Yoo and Choi [2009], respectively. Schmidt et al. [2009] also proposed an Iterated Conditional Modes (ICM-NMF) algorithm for computing an MAP solution, where instead of using draws from the posteriors as updates we set their values to the mode. We also extended this method for matrix tri-factorisation (ICM-NMTF).

#### 4.1 Convergence speed

We tested the convergence speed of the methods on both the toy data, giving the correct values for  $K$ ,  $L$ , and on the GDSC drug sensitivity dataset. We track the convergence rate of the error (mean square error) on the training data against the number of iterations taken. This can be found for the toy data in Figures 1a (MF) and 1b (MTF), and for the GDSC drug sensitivity dataset in Figures 1c and 1d. Below that (Figures 1e-1h) is the convergence in terms of time (wall-clock), timing each run 10 times and taking the average (using the same random seed).

We see that our VB methods takes the fewest iterations to converge to the best solution. This is especially the case in the tri-factorisation case, where the best solution is much harder to find (note that all methods initially find a worse solution and get stuck on that for a while), and our variational approach converges seven times faster in terms of iterations taken. We note that time wise, the ICM

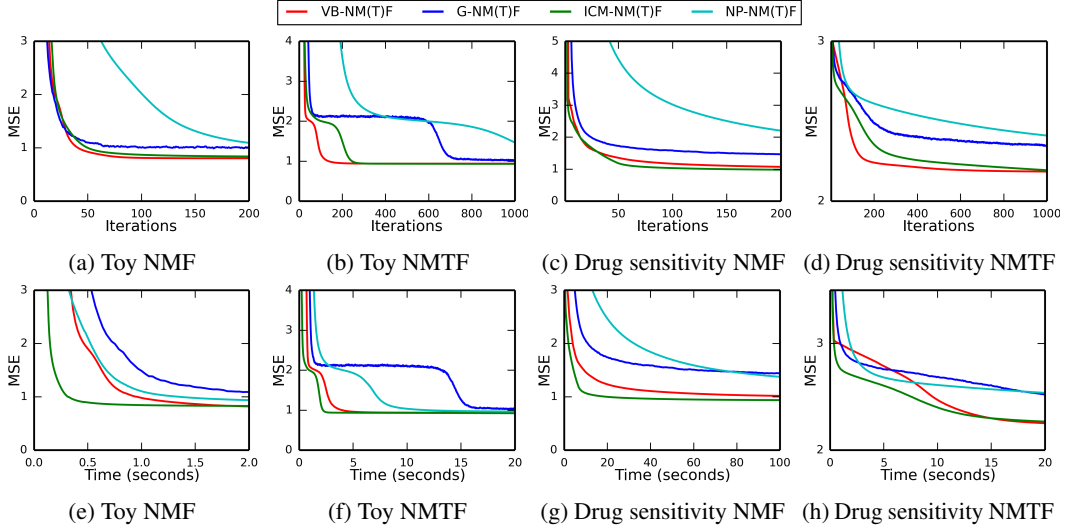


Figure 1: Convergence of algorithms on the toy and GDSC drug sensitivity datasets, measuring the training data fit (mean square error) across iterations (top row) and time (bottom row).

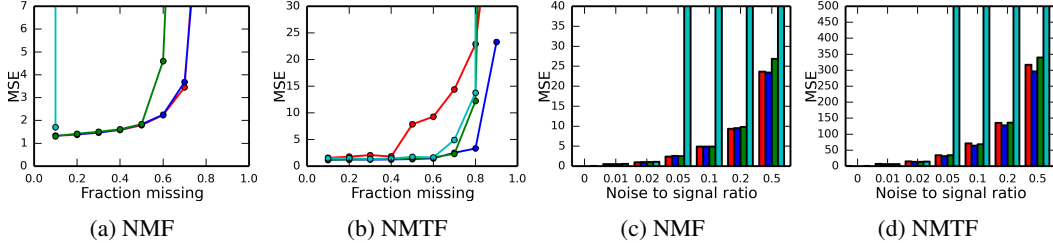


Figure 2: Missing values prediction performances (Figures 2a and 2b) and noise test performances (Figures 2c and 2d), measured by average predictive performance on test set (mean square error) for different fractions of unknown values and noise-to-signal ratios.

algorithms can be implemented more efficiently than the fully Bayesian approaches, but returns a MAP solution rather than the full posterior. Our VB method still converges four times faster than the other fully Bayesian approach, and twice as fast as the non-probabilistic method.

## 4.2 Other experiments

We conducted several other experiments, such as model selection on toy datasets, and cross-validation on three drug sensitivity datasets. Details and results for all experiments are given in the supplementary materials (Section 3), but here we highlight the results for missing value predictions and noise tests. In Figures 2a and 2b, we measure the ability of the models to predict missing values in a toy dataset as the fraction of missing values increases. Similarly, Figures 2c and 2d show the predictive performances as the amount of noise in the data increases. The figures show that the Bayesian models are more robust to noise, and perform better on sparse datasets than their non-probabilistic counterparts.

## 5 Conclusion

We have introduced a fast variational Bayesian algorithm for performing non-negative matrix factorisation and tri-factorisation. We have shown that this method gives us deterministic convergence that is faster than MCMC methods, without requiring additional samples to estimate the posterior distribution. We demonstrate that our variational approach is particularly useful for the tri-factorisation case, where convergence is even harder, and we obtain a four-fold time speedup. These speedups can open up the applicability of the models to larger datasets.

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## Supplementary Materials

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# 1 Model details

## 1.1 Gibbs sampling for matrix factorisation

In this section we offer an introduction to Gibbs sampling, and show how it can be applied to the Bayesian non-negative matrix factorisation model.

Gibbs sampling works by sampling new values for each parameter  $\theta_i$  from its marginal distribution given the current values of the other parameters  $\boldsymbol{\theta}_{-i}$ , and the observed data  $D$ . If we sample new values in turn for each parameter  $\theta_i$  from  $p(\theta_i|\boldsymbol{\theta}_{-i}, D)$ , we will eventually converge to draws from the posterior, which can be used to approximate the posterior  $p(\boldsymbol{\theta}|D)$ . We have to discard the first  $n$  draws because it takes a while to converge (*burn-in*), and since consecutive draws are correlated we only use every  $i$ th value (*thinning*).

For the Bayesian non-negative matrix factorisation model this means that we need to be able to draw from the following distributions:

$$p(U_{ik}|\tau, \mathbf{U}_{-ik}, \mathbf{V}, D) \quad p(V_{jk}|\tau, \mathbf{U}, \mathbf{V}_{-jk}, D) \quad p(\tau|\mathbf{U}, \mathbf{V}, D)$$

where  $\mathbf{U}_{-ik}$  denotes all elements in  $\mathbf{U}$  except  $U_{ik}$ , and similarly for  $\mathbf{V}_{-jk}$ . Using Bayes theorem we can obtain the posterior distributions. For example, for  $p(U_{ik}|\tau, \mathbf{U}_{-ik}, \mathbf{V}, D)$ :

$$\begin{aligned} p(U_{ik}|\tau, \mathbf{U}_{-ik}, \mathbf{V}, D) &\propto p(D|\tau, \mathbf{U}, \mathbf{V}) \times p(U_{ik}|\lambda_{ik}^U) \\ &\propto \prod_{j \in \Omega_i} \mathcal{N}(R_{ij}|\mathbf{U}_i \cdot \mathbf{V}_j, \tau^{-1}) \times \mathcal{E}(U_{ik}|\lambda_{ik}^U) \\ &\propto \exp \left\{ \frac{\tau}{2} \sum_{j \in \Omega_i} (R_{ij} - \mathbf{U}_i \cdot \mathbf{V}_j)^2 \right\} \times \exp \{ -\lambda_{ik}^U U_{ik} \} \times u(x) \\ &\propto \exp \left\{ \frac{U_{ik}^2}{2} \left[ \tau \sum_{j \in \Omega_i} V_{jk}^2 \right] + U_{ik} \left[ -\lambda_{ik}^U + \tau \sum_{j \in \Omega_i} (R_{ij} - \sum_{k' \neq k} U_{ik'} V_{jk'}) V_{jk} \right] \right\} \times u(x) \\ &\propto \exp \left\{ \frac{\tau_{ik}^U}{2} (U_{ik} - \mu_{ik}^U)^2 \right\} \times u(x) \\ &\propto \mathcal{TN}(U_{ik}|\mu_{ik}^U, \tau_{ik}^U) \end{aligned}$$

where

$$\mathcal{TN}(x|\mu, \tau) = \begin{cases} \frac{\sqrt{\frac{\tau}{2\pi}} \exp \left\{ -\frac{\tau}{2} (x - \mu)^2 \right\}}{1 - \Phi(-\mu\sqrt{\tau})} & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases}$$

is a truncated normal: a normal distribution with zero density below  $x = 0$  and renormalised to integrate to one.  $\Phi(\cdot)$  is the cumulative distribution function of  $\mathcal{N}(0, 1)$ .

Applying the same technique to the other posteriors gives us:

$$\begin{aligned} p(\tau|\mathbf{U}, \mathbf{V}, D) &= \mathcal{G}(\tau|\alpha^*, \beta^*) \\ p(V_{jk}|\tau, \mathbf{U}, \mathbf{V}_{-jk}, D) &= \mathcal{TN}(V_{jk}|\mu_{jk}^V, \tau_{jk}^V) \end{aligned}$$

The parameters of these distributions are given in Table 1, where  $\Omega_i = \{j \mid (i, j) \in \Omega\}$  and  $\Omega_j = \{i \mid (i, j) \in \Omega\}$ .

Table 1: NMF variable update rules

	GIBBS SAMPLING	VARIATIONAL BAYES
$\alpha^*$	$\alpha + \frac{ \Omega }{2}$	$\alpha + \frac{ \Omega }{2}$
$\beta^*$	$\beta + \frac{1}{2} \sum_{(i,j) \in \Omega} (R_{ij} - \mathbf{U}_i \cdot \mathbf{V}_j)^2$	$\beta + \frac{1}{2} \sum_{(i,j) \in \Omega} \mathbb{E}_q \left[ (R_{ij} - \mathbf{U}_i \mathbf{V}_j)^2 \right]$
$\tau_{ik}^U$	$\tau \sum_{j \in \Omega_i} V_{jk}^2$	$\tilde{\tau} \sum_{j \in \Omega_i} \widetilde{V}_{jk}^2$
$\mu_{ik}^U$	$\frac{1}{\tau_{ik}^U} \left( -\lambda_{ik}^U + \tau \sum_{j \in \Omega_i} (R_{ij} - \sum_{k' \neq k} U_{ik'} V_{jk'}) V_{jk} \right)$	$\frac{1}{\tau_{ik}^U} \left( -\lambda_{ik}^U + \tilde{\tau} \sum_{j \in \Omega_i} (R_{ij} - \sum_{k' \neq k} \widetilde{U}_{ik'} \widetilde{V}_{jk'}) \widetilde{V}_{jk} \right)$
$\tau_{jk}^V$	$\tau \sum_{i \in \Omega_j} U_{ik}^2$	$\tau \sum_{i \in \Omega_j} \widetilde{U}_{ik}^2$
$\mu_{jk}^V$	$\frac{1}{\tau_{jk}^V} \left( -\lambda_{jk}^V + \tau \sum_{i \in \Omega_j} (R_{ij} - \sum_{k' \neq k} U_{ik'} V_{jk'}) U_{ik} \right)$	$\frac{1}{\tau_{jk}^V} \left( -\lambda_{jk}^V + \tilde{\tau} \sum_{i \in \Omega_j} (R_{ij} - \sum_{k' \neq k} \widetilde{U}_{ik'} \widetilde{V}_{jk'}) \widetilde{U}_{ik} \right)$

$$\mathbb{E}_q \left[ (R_{ij} - \mathbf{U}_i \mathbf{V}_j)^2 \right] = \left( R_{ij} - \sum_{k=1}^K \widetilde{U}_{ik} \widetilde{V}_{jk} \right)^2 + \sum_{k=1}^K \left( \widetilde{U}_{ik}^2 \widetilde{V}_{jk}^2 - \widetilde{U}_{ik}^2 \widetilde{V}_{jk}^2 \right)$$

## 1.2 Variational Bayes for matrix factorisation

For the Variational Bayes algorithm for inference, updates for the approximate posterior distributions are given in Table 1, and were obtained using the techniques described in the paper. We use  $f(\widetilde{X})$  as a shorthand for  $\mathbb{E}_q[f(X)]$ , where  $X$  is a random variable and  $f$  is a function over  $X$ . We make use of the identity  $\widetilde{X}^2 = \widetilde{X}^2 + \text{Var}_q[X]$ . The expectation and variance of the parameters with respect to  $q$  are given below, for random variables  $X \sim \mathcal{G}(a, b)$  and  $Y \sim \mathcal{TN}(\mu, \tau)$ .

$$\widetilde{X} = \frac{a}{b} \quad \widetilde{Y} = \mu + \frac{1}{\sqrt{\tau}} \lambda(-\mu\sqrt{\tau}) \quad \text{Var}[Y] = \frac{1}{\tau} [1 - \delta(-\mu\sqrt{\tau})]$$

where  $\psi(x) = \frac{d}{dx} \log \Gamma(x)$  is the digamma function,  $\lambda(x) = \phi(x)/[1 - \Phi(x)]$ , and  $\delta(x) = \lambda(x)[\lambda(x) - x]$ .  $\phi(x) = \frac{1}{\sqrt{2\pi}} \exp\{-\frac{1}{2}x^2\}$  is the density function of  $\mathcal{N}(0, 1)$ .

## 1.3 BNMFTF Gibbs sampling parameter values

For the BNMFTF Gibbs sampling algorithm, we sample from the following posteriors:

$$\begin{aligned} p(\tau | \mathbf{F}, \mathbf{S}, \mathbf{G}, D) &= \mathcal{G}(\tau | \alpha^*, \beta^*) \\ p(F_{ik} | \tau, \mathbf{F}_{-ik}, \mathbf{S}, \mathbf{G}, D) &= \mathcal{TN}(F_{ik} | \mu_{ik}^F, \tau_{ik}^F) \\ p(S_{kl} | \tau, \mathbf{F}, \mathbf{S}_{-kl}, \mathbf{G}, D) &= \mathcal{TN}(S_{kl} | \mu_{kl}^S, \tau_{kl}^S) \\ p(G_{jl} | \tau, \mathbf{F}, \mathbf{S}, \mathbf{G}_{-jl}, D) &= \mathcal{TN}(G_{jl} | \mu_{jl}^G, \tau_{jl}^G) \end{aligned}$$



The updates for the parameters are given in Table 2 below.

Table 2: NMTF Gibbs Update Rules

GIBBS SAMPLING	
$\alpha^*$	$\alpha + \frac{ \Omega }{2}$
$\beta^*$	$\beta + \frac{1}{2} \sum_{(i,j) \in \Omega} (R_{ij} - \mathbf{F}_i \cdot \mathbf{S} \cdot \mathbf{G}_j)^2$
$\tau_{ik}^F$	$\tau \sum_{j \in \Omega_i} (\mathbf{S}_k \cdot \mathbf{G}_j)^2$
$\mu_{ik}^F$	$\frac{1}{\tau_{ik}^F} \left( -\lambda_{ik}^F + \tau \sum_{j \in \Omega_i} \left( R_{ij} - \sum_{k' \neq k} \sum_{l=1}^L F_{ik'} S_{k'l} G_{jl} \right) (\mathbf{S}_k \cdot \mathbf{G}_j) \right)$
$\tau_{kl}^S$	$\tau \sum_{(i,j) \in \Omega} F_{ik}^2 G_{jl}^2$
$\mu_{kl}^S$	$\frac{1}{\tau_{kl}^S} \left( -\lambda_{kl}^S + \tau \sum_{(i,j) \in \Omega} \left( R_{ij} - \sum_{(k',l') \neq (k,l)} F_{ik'} S_{k'l'} G_{jl'} \right) F_{ik} G_{jl} \right)$
$\tau_{jl}^G$	$\tau \sum_{i \in \Omega_j} (\mathbf{F}_i \cdot \mathbf{S}_{\cdot,l})^2$
$\mu_{jl}^G$	$\frac{1}{\tau_{jl}^G} \left( -\lambda_{jl}^G + \tau \sum_{i \in \Omega_j} \left( R_{ij} - \sum_{k=1}^K \sum_{l' \neq l} F_{ik} S_{kl'} G_{jl'} \right) (\mathbf{F}_i \cdot \mathbf{S}_{\cdot,l}) \right)$

#### 1.4 BNMTF Variational Bayes parameter updates

As discussed in the paper, the term  $\mathbb{E}_q [(R_{ij} - \mathbf{F}_i \cdot \mathbf{S} \cdot \mathbf{G}_j)^2]$  adds extra complexity to the matrix tri-factorisation case.

$$\begin{aligned} \mathbb{E}_q [(R_{ij} - \mathbf{F}_i \cdot \mathbf{S} \cdot \mathbf{G}_j)^2] &= \\ & \left( R_{ij} - \sum_{k=1}^K \sum_{l=1}^L \widetilde{F}_{ik} \widetilde{S}_{kl} \widetilde{G}_{jl} \right)^2 \\ & + \sum_{k=1}^K \sum_{l=1}^L \text{Var}_q [F_{ik} S_{kl} G_{jl}] \end{aligned} \quad (1)$$

$$+ \sum_{k=1}^K \sum_{l=1}^L \sum_{k' \neq k} \text{Cov} [F_{ik} S_{kl} G_{jl}, F_{ik'} S_{k'l} G_{jl}] \quad (2)$$

$$+ \sum_{k=1}^K \sum_{l=1}^L \sum_{l' \neq l} \text{Cov} [F_{ik} S_{kl} G_{jl}, F_{ik} S_{kl'} G_{jl'}] \quad (3)$$

The above variance and covariance terms are equal to the following, respectively:

$$\widetilde{F}_{ik}^2 \widetilde{S}_{kl}^2 \widetilde{G}_{jl}^2 - \widetilde{F}_{ik}^2 \widetilde{S}_{kl}^2 \widetilde{G}_{jl}^2 \quad (1)$$

$$\text{Var}_q [F_{ik}] \widetilde{S}_{kl} \widetilde{G}_{jl} \widetilde{S}_{kl'} \widetilde{G}_{j'l'} \quad (2)$$

$$\widetilde{F}_{ik} \widetilde{S}_{kl} \text{Var}_q [G_{jl}] \widetilde{F}_{ik'} \widetilde{S}_{k'l} \quad (3)$$

The updates for the variational parameters of the Variational Bayes algorithm for the Bayesian non-negative matrix tri-factorisation are given in Table 3 below.

Table 3: NMTF VB Update Rules

VARIATIONAL BAYES	
$\alpha^*$	$\alpha + \frac{ \Omega }{2}$
$\beta^*$	$\beta + \frac{1}{2} \sum_{(i,j) \in \Omega} \mathbb{E}_q [(R_{ij} - \mathbf{F}_i \cdot \mathbf{S} \cdot \mathbf{G}_j)^2]$
$\tau_{ik}^F$	$\tilde{\tau} \sum_{j \in \Omega_i} \left( \left( \sum_{l=1}^L \widetilde{S}_{kl} \widetilde{G}_{jl} \right)^2 + \sum_{l=1}^L \left( \widetilde{S}_{kl}^2 \widetilde{G}_{jl}^2 - \widetilde{S}_{kl}^2 \widetilde{G}_{jl}^2 \right) \right)$
$\mu_{ik}^F$	$\frac{1}{\tau_{ik}^F} \left( -\lambda_{ik}^F + \tilde{\tau} \sum_{j \in \Omega_i} \left( \left( R_{ij} - \sum_{k' \neq k} \sum_{l=1}^L \widetilde{F}_{ik'} \widetilde{S}_{k'l} \widetilde{G}_{jl} \right) \sum_{l=1}^L \widetilde{S}_{kl} \widetilde{G}_{jl} - \sum_{l=1}^L \widetilde{S}_{kl} \text{Var}_q [G_{jl}] \sum_{k' \neq k} \widetilde{F}_{ik'} \widetilde{S}_{k'l} \right) \right)$
$\tau_{kl}^S$	$\tilde{\tau} \sum_{(i,j) \in \Omega} \widetilde{F}_{ik}^2 \widetilde{G}_{jl}^2$
$\mu_{kl}^S$	$\frac{1}{\tau_{kl}^S} \left( -\lambda_{kl}^S + \tilde{\tau} \sum_{(i,j) \in \Omega} \left( \left( R_{ij} - \sum_{(k',l') \neq (k,l)} \widetilde{F}_{ik'} \widetilde{S}_{k'l'} \widetilde{G}_{jl'} \right) \widetilde{F}_{ik} \widetilde{G}_{jl} - \widetilde{F}_{ik} \text{Var}_q [G_{jl}] \sum_{k' \neq k} \widetilde{F}_{ik'} \widetilde{S}_{k'l} - \text{Var}_q [F_{ik}] \widetilde{G}_{jl} \sum_{l' \neq l} \widetilde{S}_{kl'} \widetilde{G}_{j'l'} \right) \right)$
$\tau_{jl}^G$	$\tilde{\tau} \sum_{i \in \Omega_j} \left( \left( \sum_{k=1}^K \widetilde{F}_{ik} \widetilde{S}_{kl} \right)^2 + \sum_{k=1}^K \left( \widetilde{F}_{ik}^2 \widetilde{S}_{kl}^2 - \widetilde{F}_{ik}^2 \widetilde{S}_{kl}^2 \right) \right)$
$\mu_{jl}^G$	$\frac{1}{\tau_{jl}^G} \left( -\lambda_{jl}^G + \tilde{\tau} \sum_{i \in \Omega_j} \left( \left( R_{ij} - \sum_{k=1}^K \sum_{l' \neq l} \widetilde{F}_{ik} \widetilde{S}_{k'l'} \widetilde{G}_{jl'} \right) \sum_{k=1}^K \widetilde{F}_{ik} \widetilde{S}_{kl} - \sum_{k=1}^K \text{Var}_q [F_{ik}] \widetilde{S}_{kl} \sum_{l' \neq l} \widetilde{S}_{k'l'} \widetilde{G}_{j'l'} \right) \right)$

## 2 Model discussion

### 2.1 Complexity

The updates for the Gibbs samplers and VB algorithms can be implemented efficiently using matrix operations. The time complexity per iteration for Bayesian non-negative matrix factorisation is  $\mathcal{O}(IJK^2)$  for both Gibbs and VB, and  $\mathcal{O}(IJ(K^2L + KL^2))$  per iteration for tri-factorisation. However, the updates in each column of  $\mathbf{U}$ ,  $\mathbf{V}$ ,  $\mathbf{F}$ ,  $\mathbf{G}$  are independent of each other and can therefore be updated in parallel.

For the Gibbs sampler, this means we can draw these values in parallel, but for the VB algorithm we can jointly update the columns using a single matrix operation. Modern computer architectures can exploit this using vector processors, leading to a great speedup.

Furthermore, after the VB algorithm converges we have our approximation to the posterior distributions immediately, whereas with Gibbs we need to obtain further draws after convergence and use a thinning rate to obtain an accurate estimate of the posterior. This deterministic behaviour of VB makes it easier to use. Although additional variables need to be stored to represent the posteriors, this does not result in a worse space complexity, as the Gibbs sampler needs to store draws over time.

### 2.2 Model selection

In practice we do not know the optimal model dimensionality of our data, and we need to estimate its value. In our case, we want to find the best value of  $K$  for matrix factorisation, and  $K, L$  for tri-factorisation.

The log probability of the data,  $\log p(D|\boldsymbol{\theta})$ , is a good measure for the quality of the fit to the data. As  $K$  increases we expect the log likelihood to improve as we give the model more freedom for fitting to the data, but this can lead to overfitting. Therefore, we need to penalise the model's performance by its complexity. We use the Akaike information criterion (AIC) Akaike [1974] defined as

$$AIC = 2k - 2 \log p(D|\boldsymbol{\theta})$$

where  $k$  is the number of free parameters in our model. For matrix factorisation this is  $IK + JK$  and for tri-factorisation  $IK + KL + JL$ .

Another popular measure is the Bayesian information criterion (BIC) Schwarz [1978]. BIC tends to penalise complicated models more heavily than AIC. We found that AIC peaked closer to the true model dimensionality on synthetic data than BIC, especially for matrix tri-factorisation, and we therefore use the former.

For matrix factorisation we then try different values for  $K$  in a given range and pick the  $K$  that gives the lowest AIC. Similarly for matrix tri-factorisation, we can perform a **grid search** for a range of values for  $K$  and  $L$ , trying each possible  $(K, L)$  pair, but this results in training  $K \times L$  different models. Instead, we can perform a **greedy search** on the grid, as illustrated in Figure 1.

- We are given a grid of values  $(K_i, L_i)$ .
- We start with the lowest values,  $(K_1, L_1)$ , train a model, and measure the model quality.
- For each of the three points above it –  $(K_i, L_{i+1})$ ,  $(K_{i+1}, L_i)$ ,  $(K_{i+1}, L_{i+1})$  – we train a model and measure the model quality.
- The model that gives the best improvement is selected as our next value on the grid. If no improvement is made, the current point  $(K_i, L_i)$  gives the best values for  $K$  and  $L$ .

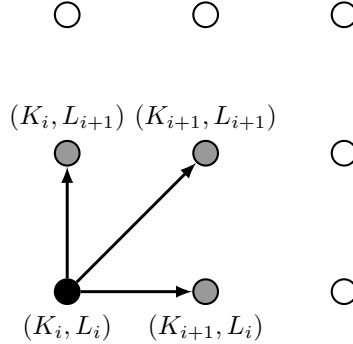


Figure 1: Greedy search procedure for model selection

Since we are looking for the best fitting model, we can train multiple models with random initialisations for each  $K, L$  and use the one with the highest log likelihood (we denote *restarts*).

### 2.3 Initialisation

Initialising the parameters of the models can vastly influence the quality of convergence. This can be done for example by using the hyperparameters  $\lambda_{ik}^U, \lambda_{jk}^V, \lambda_{ik}^F, \lambda_{kl}^S, \lambda_{jl}^G, \alpha, \beta$  to set the initial values to the mean of the priors of the model. Alternatively, we can use random draws of the priors as the initial values. We found that random draws tend to give faster and better convergence than the expectation.

For matrix tri-factorisation we can also initialise  $\mathbf{F}$  by running the K-means clustering algorithm on the rows as datapoints, and similarly  $\mathbf{G}$  for the columns, as suggested by Ding et al. [2006]. For the VB algorithm we then set the  $\mu$  parameters to the cluster indicators, and for Gibbs we set the matrices to the cluster indicators, plus 0.2 for smoothing. We found that this improved the convergence as well, with  $\mathbf{S}$  initialised using random draws.

### 2.4 Implementation

All algorithms mentioned were implemented using the Python language. The *numpy* package was used for fast matrix operations, and for random draws of the truncated normal distribution we used the Python package *rtnorm* by C. Lassner (<http://miv.u-strasbg.fr/mazet/rtnorm/>), giving more efficient draws than the standard libraries and dealing with rounding errors.

The mean and variance of the truncated normal involve operations prone to numerical errors when  $\mu \ll 0$ . To deal with this we observe that when  $\mu\sqrt{\tau} \ll 0$  the truncated normal distribution approximates an exponential one with rate  $\mu\sqrt{\tau}$ , and therefore has mean  $1/(\mu\sqrt{\tau})$  and variance  $1/(\mu\sqrt{\tau})^2$ .

All experiments were run on a Medion Erazer laptop with an Intel i7-3610QM CPU (4 cores of 2.30GHz each), GeForce GTX 670M graphics card, and 16GB memory.

## 2.5 Code

Implementations of all discussed methods are available online, via <https://github.com/ThomasBrouwer/BNMTF/>.

### 3 Additional experiments

#### 3.1 Model selection

To demonstrate our proposed model selection framework (see section 2.2) we use the toy dataset described earlier, using our VB algorithms. We let each model train for 1000 iterations with 5 restarts.

As can be seen in Figure 2a, the mean square error on the training data for matrix factorisation converges after  $K = 10$ , whereas Figure 2b shows that using the Akaike information criterion gives a clear peak at the true  $K$ . The ELBO also provides a good heuristic for model selection, as seen in figure 2c.

Figure 2e shows the full grid search for matrix tri-factorisation, and gives a peak at  $K = 4, L = 4$ . This is slightly lower than the true  $K, L$ , but shows that a good enough fit can be achieved using fewer factors. The proposed greedy search in Figure 2f finds the same solution but only trying 13 of the 100 possible combinations, suggesting that this model selection procedure can offer a significant speedup with similar performance.

We also ran the model selection frameworks on the drug sensitivity dataset, where the true number of latent factors are unknown. Figure 3 shows that for matrix factorisation the best value for  $K$  is around 25, and for matrix tri-factorisation  $K = L = 5$ .

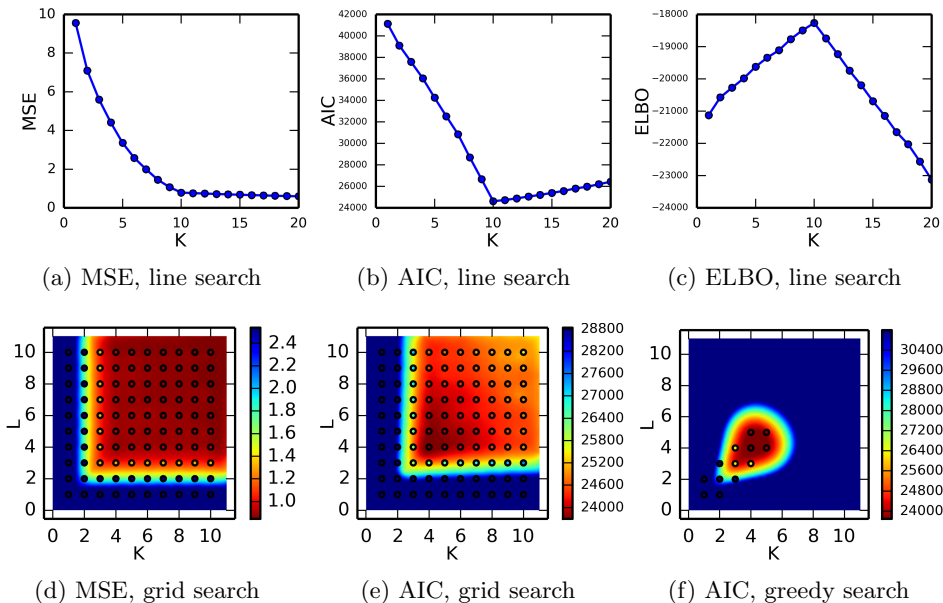


Figure 2: Model selection for VB-NMF (top row) and VB-NMTF (bottom row). We measure the model quality for different values of  $K$  (and  $L$ ) on the toy datasets. The true  $K$  for NMF is 10, and the true  $K, L$  for NMTF is 5, 5. Figures 2a–2c show that the MSE cannot find the right model dimensionality for NMF, but the AIC and ELBO can. The same applies to NMTF, as shown in Figures 2d–2f, where we additionally see that the proposed greedy search model selection method finds the same solution as the full grid one, but trying only 13 of the 100 possible values.

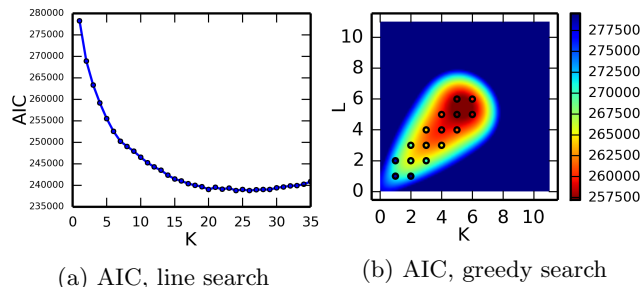


Figure 3: Model selection for VB-NMF (top row) and VB-NMTF (bottom row) on the GDSC drug sensitivity dataset. We see that the found optimal model dimensionalities are  $K = 25$  for NMF, and  $K = 5, L = 5$  for NMTF.

### 3.2 Missing values

We furthermore tested the ability of our model to recover missing values as the fraction of unknown entries increases (more sparse datasets). We run each algorithm on the same dataset for 1000 iterations (burn-in 800, thinning rate 5) to give the algorithms enough time to converge, splitting the data randomly ten times each into test and training data, and computing the average mean square error of the predictions on the test data.

High errors are indicative of overfitting or not converging to a good solution. We can see in Figure 4a that the fully Bayesian methods for matrix factorisation obtain good predictive power even at 70% missing values, whereas ICM starts failing there. The non-probabilistic method starts overfitting from 20% missing values, leading to very high prediction errors.

For matrix tri-factorisation we notice that our VB method sometimes does not converge to the best solution for 50% or more missing values. This is shown in Figure 4b. As a result, the average error is higher than the other methods in those cases.

### 3.3 Noise test

We conducted a noise test to measure the robustness of the different methods. Our experiment works in a similar manner to the missing values test, but now adding different levels of Gaussian noise to the data, and with 10% test data. The noise-to-signal ratio is given by the ratio of the variance of the Gaussian noise we add, to the variance of the generated data. We see in Figures 4c and 4d that the non-probabilistic approach starts overfitting heavily at low levels of noise, whereas the fully Bayesian approaches achieve the best possible predictive powers even at high levels of noise.

### 3.4 Drug sensitivity predictions

Finally, we performed cross-validation experiments on three different drug sensitivity experiments. Firstly, the Genomics of Drug Sensitivity in Cancer (GDSC v5.0, Yang et al. [2013]) dataset contains 138 drugs and 622 cell lines, with 81% of entries observed (as introduced in the paper). Secondly, the Cancer Cell Line Encyclopedia (CCLE, Barretina et al. [2012]) has 504 drugs and 22 cell lines. There are two versions: one detailing  $IC_{50}$  drug sensitivity

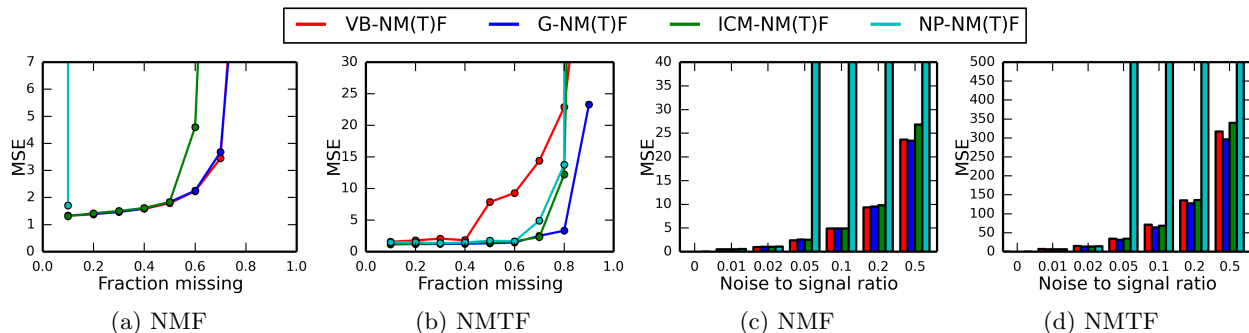


Figure 4: Missing values prediction performances (Figures 4a and 4b) and noise test performances (Figures 4c and 4d), measured by average predictive performance on test set (mean square error) for different fractions of unknown values and noise-to-signal ratios.

values (96% observed) and another giving  $EC_{50}$  values (63% observed).

We compare our methods against classic algorithms for matrix factorisation and tri-factorisation. Aside from the Gibbs sampler (G-NMF, G-NMTF) and VB algorithms (VB-NMF, VB-NMTF), we consider the non-probabilistic matrix factorisation (NP-NMF) and tri-factorisation (NP-NMTF) methods introduced by Lee and Seung [2000] and Yoo and Choi [2009], respectively. Schmidt et al. [2009] also proposed an Iterated Conditional Modes (ICM-NMF) algorithm for computing an MAP solution, where instead of using draws from the posteriors as updates we set their values to the mode. We also extended this method for matrix tri-factorisation (ICM-NMTF).

For the GDSC dataset we also compare with a recent paper by Ammad-ud din et al. [2014] which uses a method called Kernelised Bayesian Matrix Factorisation (KBMF), leveraging similarity kernels of the drugs and cell lines. We reconstructed the drug kernels using targets, PaDeL fingerprints, and 1D and 2D descriptors. Similarly for the cell lines we used gene expression, copy-number variation, and cancer mutation data. For the other datasets we only compared the matrix factorisation models.

The results of running 10-fold cross-validation can be found in Table 4. For KBMF and non-probabilistic NMF and NMTF we use nested cross-validation to find the best value for  $K$  (and  $L$ ). For the other methods we use cross-validation with the model selection detailed in the supplementary materials (Section 2.2).

We can see the Gibbs sampling NMF model performs the best in two of the three datasets, outperforming even the KBMF model which uses side information. The ICM models tend to overfit to the data, and often led to very high predictive errors. The non-probabilistic models do well on the large GDSC dataset, but less so on the small CCLE datasets with only 24 rows. The Bayesian models do significantly better on these two.

The matrix tri-factorisation models generally perform as well as its matrix factorisation counterpart. For matrix factorisation, the fast VB version does worse than the Gibbs sampling variant. However, for matrix tri-factorisation VB outperforms Gibbs on two of the three datasets.



Table 4: 10-fold cross-validation drug sensitivity prediction results (mean squared error). Very high predictive errors are replaced by  $\infty$ , and the best performances are highlighted in bold.

	KBMF	NMF				NMTF			
		NP	ICM	G	VB	NP	ICM	G	VB
GDSC $IC_{50}$	2.144	2.251	$\infty$	<b>2.055</b>	2.282	2.258	2.199	2.402	2.321
CCLC $IC_{50}$	-	4.683	$\infty$	<b>3.719</b>	3.984	4.664	4.153	3.745	4.107
CCLC $EC_{50}$	-	8.047	$\infty$	7.807	7.805	8.076	$\infty$	7.857	<b>7.790</b>

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