

Description of algorithms implemented in the R package shrinkage

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Abstract

This document provides a detailed description of the algorithms implemented in the R package **shrinkage** available at github.com/gleday/shrinkage.

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1. Linear regression with global shrinkage priors

This section introduces linear regression models with global shrinkage priors, which are the simplest form of shrinkage priors, and yield ridge-type estimators (Hoerl and Kennard 1970).

1.1. Model and priors

Let y denote a n -dimensional response variable and X an n by p observation matrix. Then, the linear regression model with global shrinkage is:

$$y \mid \beta, \sigma^2 \sim N_n(X\beta, \sigma^2 I_n) \quad (1)$$

$$\beta \mid \sigma^2, \tau^2 \sim N_p(0, \tau^2 \sigma^2 I_p) \quad (2)$$

$$p(\sigma^2) \propto \sigma^{-2} \quad (3)$$

The R package **shrinkage** offers the following choices of priors for τ^2 :

1. $\tau^2 \sim \text{InvGamma}(a, b)$
2. $\tau^2 \sim \text{BetaPrime}(a, b)$
3. $\tau^2 \sim \text{InvGaussian}(a, b)$
4. $\tau^2 \sim \text{Gamma}(a, b)$
5. $\tau^2 = \hat{\tau}_{\text{ML}}^2$

1.2. Closed-form inference

When $\tau^2 = \hat{\tau}_{\text{ML}}^2$ the prior variance τ^2 is not endowed with a prior probability distribution but is instead set to the value that maximizes the marginal likelihood (ML) of the model (empirical Bayes). In such case, Bayesian inference is carried out analytically as the marginal

posterior distributions of β and σ^2 are available in closed-form:

$$\beta \mid y \sim T_p \left(\bar{\beta}, \frac{y^T y - \bar{\beta}^T \bar{\Sigma}^{-1} \bar{\beta}}{n} \bar{\Sigma}, n \right) \quad \text{and} \quad \sigma^2 \mid y \sim \text{InvGamma} \left(\frac{n}{2}, \frac{1}{2} [y^T y - \bar{\beta}^T \bar{\Sigma}^{-1} \bar{\beta}] \right).$$

Here

$$\bar{\Sigma} = \left(X^T X + \tau^{-2} I_p \right)^{-1} \quad \text{and} \quad \bar{\beta} = \bar{\Sigma} X^T y.$$

The marginal likelihood is also available in closed-form:

$$p(y) = \pi^{-\frac{n}{2}} \left(\tau^2 \right)^{-\frac{p}{2}} |X^T X + \tau^{-2} I_p|^{-\frac{1}{2}} \Gamma \left(\frac{n}{2} \right) \left(\frac{1}{2} y^T y - \frac{1}{2} \bar{\beta}^T \bar{\Sigma}^{-1} \bar{\beta} \right)^{-\frac{n}{2}},$$

and its maximizer,

$$\hat{\tau}_{\text{ML}}^2 = \arg \max_{\tau^2} \log p(y),$$

obtained very efficiently (Karabatsos 2018) when re-writing the log-marginal likelihood

$$\log p(y) = -\frac{n}{2} \log \pi - \frac{p}{2} \log \tau^2 - \frac{1}{2} \sum_{r=1}^q \log(d_r^2 + \tau^{-2}) + \log \Gamma \left(\frac{n}{2} \right) - \frac{n}{2} \log \left(\frac{1}{2} y^T y - \frac{1}{2} \sum_{r=1}^q \frac{\hat{\theta}_r^2 d_j^4}{d_r^2 + \tau^{-2}} \right),$$

in terms of the singular values d_r , $r = 1, \dots, q = \min(n, p)$, of $X = U D V^T = F V^T$ and the maximum likelihood estimate $\hat{\theta} = (F^T F)^{-1} F^T y = D^{-1} U^T y$ of $\theta = V^T y$.

1.3. Inference using a Gibbs sampler

The R package **shrinkage** provides approximate inference for priors 1-4 using a Gibbs sampler that samples very efficiently from the posterior conditional distributions of parameters, and provides closed-form inference for prior 5.

Posterior conditional distributions

Regardless of the prior on τ^2 , the posterior conditional distributions of β and σ^2 are:

$$\begin{aligned} \beta \mid y, \tau^2, \sigma^2 &\sim N_p \left(\bar{\beta}, \sigma^2 \bar{\Sigma} \right), \\ \sigma^2 \mid y, \beta, \tau^2 &\sim \text{InvGamma} \left(\frac{n+p}{2}, \frac{1}{2} \left[\tau^{-2} \beta^T \beta + (y - X\beta)^T (y - X\beta) \right] \right). \end{aligned}$$

In contrast, the posterior conditional distribution of τ^2 depends on the choice of prior distribution, namely:

1. when $\tau^2 \sim \text{InvGamma}(a, b)$, the posterior conditional distribution of τ^2 is:

$$\tau^2 \mid \beta, \sigma^2 \sim \text{InvGamma} \left(a + \frac{p}{2}, \frac{1}{2} \sigma^{-2} \beta^T \beta + b \right).$$

2. when $\tau^2 \sim \text{BetaPrime}(a, b)$ two parametrizations can be used:

- the Gamma-Gamma representation of the beta prime distribution (Zhang, Reich, and Bondell 2016):

$$\tau^2 \sim \text{BetaPrime}(a, b) \Leftrightarrow \tau^2 \mid \gamma^2 \sim \text{Gamma}(a, \gamma^2), \gamma^2 \sim \text{Gamma}(b, 1),$$

yields the posterior conditional distributions:

$$\begin{aligned} \tau^2 \mid \beta, \sigma^2, \gamma^2 &\sim \text{GIG} \left(\sigma^{-2} \beta^T \beta, 2\gamma^2, a - \frac{p}{2} \right), \\ \gamma^2 \mid \tau^2 &\sim \text{Gamma} \left(a + b, \tau^2 + 1 \right). \end{aligned}$$

- the inverse-Gamma-inverse-Gamma representation of the beta prime distribution (Schmidt and Makalic 2019, Proposition 1):

$$\tau^2 \sim \text{BetaPrime}(a, b) \Leftrightarrow \tau^2 \mid \gamma^2 \sim \text{InvGamma}(b, 1/\gamma^2), \gamma^2 \sim \text{InvGamma}(a, 1),$$

yields the posterior conditional distributions:

$$\begin{aligned} \tau^2 \mid \beta, \gamma^2, \sigma^2 &\sim \text{InvGamma} \left(b + \frac{p}{2}, \frac{\beta^T \beta}{2\sigma^2} + \frac{1}{\gamma^2} \right) \\ \gamma^2 \mid \tau^2 &\sim \text{InvGamma} \left(a + b, 1 + \frac{1}{\tau^2} \right) \end{aligned}$$

3. when $\tau^2 \sim \text{InvGaussian}(a, b)$ the posterior conditional distribution of τ^2 is:

$$\tau^2 \mid \beta, \sigma^2 \sim \text{GIG} \left(b + \sigma^{-2} \beta^T \beta, \frac{b}{a^2}, -\frac{1}{2} - \frac{p}{2} \right).$$

4. when $\tau^2 \sim \text{Gamma}(a, b)$ the posterior conditional distribution of τ^2 is:

$$\tau^2 \mid \beta, \sigma^2 \sim \text{GIG} \left(\sigma^{-2} \beta^T \beta, 2b, a - \frac{p}{2} \right).$$

Algorithm

Algorithm 1 describes a very fast Gibbs sampler, obtained from the conditional distributions described above, that is used in the R package **shrinkage** to fit linear regression models with global shrinkage priors 1-4. Note that the algorithm is different than standard Gibbs samplers on the following aspect: instead of sampling β at iteration i from

$$\beta^{(i)} \sim N_p \left(\left(X^T X + \frac{I_p}{\tau^{2(i-1)}} \right)^{-1} X^T y, \sigma^2 \left(X^T X + \frac{I_p}{\tau^{2(i-1)}} \right)^{-1} \right),$$

using the procedures of Rue (2001) (when $n > p$) or Bhattacharya, Chakraborty, and Mallick (2016) (when $n \leq p$), Algorithm 1 uses the singular value decomposition of X to sample

$$\theta_j^{(i)} \sim N \left(\frac{d_j u_j^T y}{d_j^2 + \tau^{2(i-1)}}, \frac{\sigma^2}{d_j^2 + \tau^{2(i-1)}} \right), \quad \text{for } j = 1, \dots, q,$$

and substitute $\beta^{(i)T} \beta^{(i)}$ and $X \beta^{(i)}$ with $\theta^{(i)T} \theta^{(i)}$ and $F \theta^{(i)}$, respectively. Samples of β are then obtained upon convergence (i.e. when $i = n_{\text{iter}}$) using $\beta^{(i)} = V \theta^{(i)}$, for $i = 1, \dots, n_{\text{iter}}$.

In our experience, the SVD decomposition provides considerable computational speed-ups while giving similar results to standard samplers.

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1 Initialize:
2    $a = b = 0.5, \tau^{2(0)} = \gamma^{2(0)} = 1, n_{\text{mcmc}} = 1000, n_{\text{burnin}} = 1000, n_{\text{iter}} = n_{\text{mcmc}} + n_{\text{burnin}}$ 
3 for  $i = 1$  to  $n_{\text{iter}}$  do
4   for  $j = 1$  to  $q$  do
5      $\text{sample } \theta_j^{(i)} \sim N\left(\frac{d_j u_j^T y}{d_j^2 + \tau^{2(i-1)}}, \frac{\sigma^2}{d_j^2 + \tau^{2(i-1)}}\right)$ 
6   end
7   if  $\tau^2 \sim \text{InvGamma}(a, b)$  then
8      $\text{sample } \tau^{2(i)} \sim \text{InvGamma}\left(a + \frac{p}{2}, \frac{\theta^{(i)T} \theta^{(i)}}{2\sigma^{2(i-1)}} + b\right)$ 
9   end
10  if  $\tau^2 \sim \text{BetaPrime}(a, b)$  then
11     $\text{sample } \tau^{2(i)} \sim \text{GIG}\left(\frac{\theta^{(i)T} \theta^{(i)}}{\sigma^{2(i-1)}}, 2\gamma^{2(i-1)}, a - \frac{p}{2}\right)$ 
12     $\text{sample } \gamma^{2(i)} \sim \text{Gamma}(a + b, \tau^{2(i)} + 1)$ 
13  end
14  if  $\tau^2 \sim \text{InvGaussian}(a, b)$  then
15     $\text{sample } \tau^{2(i)} \sim \text{GIG}\left(b + \frac{\theta^{(i)T} \theta^{(i)}}{\sigma^{2(i-1)}}, \frac{b}{a^2}, -\frac{1}{2} - \frac{p}{2}\right)$ 
16  end
17  if  $\tau^2 \sim \text{Gamma}(a, b)$  then
18     $\text{sample } \tau^{2(i)} \sim \text{GIG}\left(\frac{\theta^{(i)T} \theta^{(i)}}{\sigma^{2(i-1)}}, 2b, a - \frac{p}{2}\right)$ 
19  end
20   $\text{sample } \sigma^{2(i)} \sim \text{InvGamma}\left(\frac{n+p}{2}, \frac{1}{2} \left[ \frac{\theta^{(i)T} \theta^{(i)}}{\tau^{2(i)}} + (y - F\theta^{(i)})^T (y - F\theta^{(i)}) \right]\right)$ 
21 end

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Algorithm 1: Gibbs algorithm for linear regression models with global shrinkage priors.

2. Linear regression with local shrinkage priors

Local shrinkage priors provide more flexibility than global shrinkage priors by allowing the prior variance of the regression parameters to differ between (groups of) variables. Models with local shrinkage priors yield generalized ridge estimators and some sparse estimators.

2.1. Model and priors

Given a partition of the set of p variables into K groups, denote by G_k the set of indexes of the variables that belong to group k and $p_k = \text{card}(G_k)$. (Thus, $\cup_{k=1}^K G_k = \{1, \dots, p\}$ and $\sum_{k=1}^K p_k = p$.) Then, the linear regression model with local shrinkage priors is

$$y \mid \beta, \sigma^2 \sim N_n(X\beta, \sigma^2 I_n), \quad (4)$$

$$\beta \mid \tau^2, \sigma^2 \sim N_p(0, \sigma^2 D_\tau) \quad (5)$$

$$p(\sigma^2) \propto \sigma^{-2}. \quad (6)$$

where $\tau^2 = (\tau_1^2, \dots, \tau_K^2)$ and the diagonal matrix D_τ is such that $(D_\tau)_{jj} = \tau_k^2$ if variable

$j = 1, \dots, p$ belongs to group $k = 1, \dots, K$.

The R package **shrinkage** offers the following choices of priors for τ^2 :

1. $\tau_k^2 \sim \text{InvGamma}(a, b)$
2. $\tau_k^2 \sim \text{BetaPrime}(a, b)$
3. $\tau_k^2 \sim \text{InvGaussian}(a, b)$
4. $\tau_k^2 \sim \text{Gamma}(a, b)$

Several models proposed in the literature can be seen as models with local shrinkage priors, e.g.:

- [Bai and Ghosh \(2018\)](#), when $K = p$ and $\tau_k^2 \sim \text{BetaPrime}(a, b)$
- [Caron and Doucet \(2008\)](#), when $K = p$ and $\tau_k^2 \sim \text{InvGaussian}(a, b)$
- [Brown and Griffin \(2010\)](#) and [Caron and Doucet \(2008\)](#), when $K = p$ and $\tau_k^2 \sim \text{Gamma}(a, b)$

2.2. Closed-form inference

When $\tau^2 = \hat{\tau}_{\text{ML}}^2$ the prior variance τ^2 is not endowed with a prior probability distribution but is instead set to the value that maximizes the marginal likelihood (ML) of the model (empirical Bayes). In such case, Bayesian inference is carried out analytically as the marginal posterior distributions of β and σ^2 are available in closed-form:

$$\beta \mid y \sim \text{Tp} \left(\tilde{\beta}, \frac{y^T y - \tilde{\beta}^T \tilde{\Sigma}^{-1} \tilde{\beta}}{n} \tilde{\Sigma}, n \right) \quad \text{and} \quad \sigma^2 \mid y \sim \text{InvGamma} \left(\frac{n}{2}, \frac{1}{2} [y^T y - \tilde{\beta}^T \tilde{\Sigma}^{-1} \tilde{\beta}] \right).$$

Here

$$\tilde{\Sigma} = (X^T X + D_\tau^{-1})^{-1} \quad \text{and} \quad \tilde{\beta} = \tilde{\Sigma} X^T y.$$

The marginal likelihood is also available in closed-form:

$$p(y) = \pi^{-\frac{n}{2}} \left(\prod_{k=1}^K (\tau_k^2)^{-\frac{p}{2}} \right) |X^T X + D_\tau^{-1}|^{-\frac{1}{2}} \Gamma \left(\frac{n}{2} \right) \left(\frac{1}{2} y^T y - \frac{1}{2} \tilde{\beta}^T \tilde{\Sigma}^{-1} \tilde{\beta} \right)^{-\frac{n}{2}},$$

and its maximizer,

$$\hat{\tau}_{\text{ML}}^2 = \arg \max_{\tau^2} \log p(y),$$

obtained very efficiently ([Karabatsos 2018](#)) when re-writing the log-marginal likelihood

$$\log p(y) = -\frac{n}{2} \log \pi - \frac{p}{2} \log \tau^2 - \frac{1}{2} \sum_{r=1}^q \log(d_r^2 + \tau^{-2}) + \log \Gamma \left(\frac{n}{2} \right) - \frac{n}{2} \log \left(\frac{1}{2} y^T y - \frac{1}{2} \sum_{r=1}^q \frac{\hat{\theta}_r^2 d_j^4}{d_r^2 + \tau^{-2}} \right),$$

in terms of the singular values d_r , $r = 1, \dots, q = \min(n, p)$, of $X = U D V^T = F V^T$ and the maximum likelihood estimate $\hat{\theta} = (F^T F)^{-1} F^T y = D^{-1} U^T y$ of $\theta = V^T \beta$.

2.3. Inference using a Gibbs sampler

Inference for linear models with local shrinkage priors is carried out using a Gibbs sampler.

Posterior conditional distributions

Regardless of the prior on τ_k^2 , the posterior conditional distributions for β and σ^2 are:

$$\begin{aligned}\beta \mid \tau^2, \sigma^2 &\sim N_p(\tilde{\beta}, \sigma^2 \tilde{\Sigma}), \\ \sigma^2 \mid \beta, \tau^2 &\sim \text{InvGamma}\left(\frac{n+p}{2}, \frac{1}{2} \left[\beta^T D_\tau^{-1} \beta + (y - X\beta)^T (y - X\beta) \right]\right).\end{aligned}$$

The posterior conditional distribution of τ_k^2 , for $k = 1, \dots, K$, depends on the choice of prior distribution:

1. when $\tau_k^2 \sim \text{InvGamma}(a, b)$, the posterior conditional distribution of τ_k^2 is:

$$\tau_k^2 \mid \beta_k, \sigma^2 \sim \text{InvGamma}\left(a + \frac{p_k}{2}, \frac{1}{2} \sigma^{-2} \beta_k^T \beta_k + b\right),$$

where β_k denotes the sub-vector of β consisting of the regression parameters of variables in group k .

2. when $\tau_k^2 \sim \text{BetaPrime}(a, b)$ two parametrizations can be used:

- the Gamma-Gamma representation of the beta prime distribution ([Zhang et al. 2016](#)):

$$\tau_k^2 \sim \text{BetaPrime}(a, b) \quad \Leftrightarrow \quad \tau_k^2 \sim \gamma_k^2 \sim \text{Gamma}(a, \gamma_k^2), \quad \gamma_k^2 \sim \text{Gamma}(b, 1),$$

yields the posterior conditional distributions:

$$\begin{aligned}\tau_k^2 \mid \beta_k, \gamma_k^2, \sigma^2 &\sim \text{GIG}\left(\sigma^{-2} \beta_k^T \beta_k, 2\gamma_k^2, a - \frac{p_k}{2}\right), \\ \gamma_k^2 \mid \tau_k^2 &\sim \text{Gamma}\left(a + b, \tau_k^2 + 1\right).\end{aligned}$$

- the inverse-Gamma-inverse-Gamma representation of the beta prime distribution ([Schmidt and Makalic 2019](#), Proposition 1):

$$\tau_k^2 \sim \text{BetaPrime}(a, b) \quad \Leftrightarrow \quad \tau_k^2 \mid \gamma_k^2 \sim \text{InvGamma}(b, 1/\gamma_k^2), \quad \gamma_k^2 \sim \text{InvGamma}(a, 1)$$

yields the posterior conditional distributions:

$$\begin{aligned}\tau_k^2 \mid \beta_{j \in G_k}, \gamma_k^2, \sigma^2 &\sim \text{InvGamma}\left(b + \frac{p_k}{2}, \frac{\beta_k^T \beta_k}{2\sigma^2} + \frac{1}{\gamma_k^2}\right), \\ \gamma_k^2 \mid \tau_k^2 &\sim \text{InvGamma}\left(a + b, 1 + \frac{1}{\tau_k^2}\right).\end{aligned}$$

3. when $\tau_k^2 \sim \text{InvGaussian}(a, b)$ the posterior conditional distribution of τ_k^2 is

$$\tau_k^2 \mid \beta_k, \sigma^2 \sim \text{GIG}\left(b + \sigma^{-2} \beta_k^T \beta_k, \frac{b}{a^2}, -\frac{1}{2} - \frac{p_k}{2}\right)$$

4. when $\tau_k^2 \sim \text{Gamma}(a, b)$ the posterior conditional distribution for τ_k is

$$\tau_k^2 \mid \beta_k, \sigma^2 \sim \text{GIG} \left(\sigma^{-2} \beta_k^T \beta_k, 2b, a - \frac{p_k}{2} \right).$$

Algorithm

Algorithm 2 describes the Gibbs sampler for linear regression models with local shrinkage priors. Note that to sample β at iteration i the R package **shrinkage** uses the method of Rue (2001) when $n > p$ and the method of Bhattacharya *et al.* (2016) when $n \leq p$.

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1 Initialize:
2  $a = b = 0.5, \tau_1^{2(0)} = \dots = \tau_K^{2(0)} = \gamma^{2(0)} = 1, n_{\text{mcmc}} = 1000, n_{\text{burnin}} = 1000,$ 
    $n_{\text{iter}} = n_{\text{mcmc}} + n_{\text{burnin}}$ 
3 for  $i = 1$  to  $n_{\text{iter}}$  do
4   sample  $\beta^{(i)} \sim N_p \left( \left( X^T X + D_\tau^{(i-1)-1} \right)^{-1} X^T y, \sigma^2 \left( X^T X + D_\tau^{(i-1)-1} \right)^{-1} \right)$ 
5   for  $k = 1$  to  $K$  do
6     if  $\tau_k^2 \sim \text{InvGamma}(a, b)$  then
7       sample  $\tau_k^{2(i)} \sim \text{InvGamma} \left( a + \frac{p_k}{2}, \frac{\beta_k^{(i)T} \beta_k^{(i)}}{2\sigma^{2(i-1)}} + b \right)$ 
8     end
9     if  $\tau_k^2 \sim \text{BetaPrime}(a, b)$  then
10      sample  $\tau_k^{2(i)} \sim \text{GIG} \left( \frac{\beta_k^{(i)T} \beta_k^{(i)}}{\sigma^{2(i-1)}}, 2\gamma_k^{2(i-1)}, a - \frac{p_k}{2} \right)$ 
11      sample  $\gamma_k^{2(i)} \sim \text{Gamma} \left( a + b, \tau_k^{2(i)} + 1 \right)$ 
12    end
13    if  $\tau_k^2 \sim \text{InvGaussian}(a, b)$  then
14      sample  $\tau_k^{2(i)} \sim \text{GIG} \left( b + \frac{\beta_k^{(i)T} \beta_k^{(i)}}{\sigma^{2(i-1)}}, \frac{b}{a^2}, -\frac{1}{2} - \frac{p_k}{2} \right)$ 
15    end
16    if  $\tau_k^2 \sim \text{Gamma}(a, b)$  then
17      sample  $\tau_k^{2(i)} \sim \text{GIG} \left( \frac{\beta_k^{(i)T} \beta_k^{(i)}}{\sigma^{2(i-1)}}, 2b, a - \frac{p_k}{2} \right)$ 
18    end
19  end
20  sample  $\sigma^{2(i)} \sim \text{InvGamma} \left( \frac{n+p}{2}, \frac{1}{2} \left[ \beta^{(i)T} D_\tau^{(i)} \beta^{(i)} + (y - X\beta^{(i)})^T (y - X\beta^{(i)}) \right] \right)$ 
21 end

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Algorithm 2: Gibbs algorithm for linear regression models with local shrinkage priors.

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A. Distributions

The following table provides notation of distributions used throughout the document.

notation	domain	name	density
$x \sim \text{InvGamma}(a, b)$	$x > 0$	inverse-Gamma	$p(x \mid a, b) \propto x^{-a-1} \exp \left\{ -\frac{b}{x} \right\}$
$x \sim \text{Gamma}(a, b)$	$x > 0$	Gamma	$p(x \mid a, b) \propto x^{a-1} \exp \{-bx\}$
$x \sim \text{BetaPrime}(a, b)$	$x > 0$	beta prime	$p(x \mid a, b) \propto x^{a-1} (1+x)^{-a-b}$
$x \sim \text{GIG}(a, b, c)$	$x > 0$	generalized inverse-Gaussian	$p(x \mid a, b, c) \propto x^{c-1} \exp \left\{ -\frac{a/x+bx}{2} \right\}$
$x \sim \text{InvGaussian}(a, b)$	$x > 0$	inverse-Gaussian	$p(x \mid a, b) \propto x^{-\frac{3}{2}} \exp \left\{ -\frac{b(x-a)^2}{2a^2x} \right\}$
$x \sim \text{N}_p(m, V)$	$x \in \mathbb{R}^p$	Multivariate Normal	$p(x \mid m, V) \propto V ^{-\frac{1}{2}} \exp \left\{ -\frac{1}{2} (x-m)^T V^{-1} (x-m) \right\}$
$x \sim \text{T}_p(m, V, d)$	$x \in \mathbb{R}^p$	Multivariate T	$p(x \mid m, V, d) \propto [1 + \frac{1}{d} (x-m)^T V^{-1} (x-m)]^{-\frac{d+p}{2}}$

Table 1: List of probability distributions.

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