Hierarchical-block conditioning approximations for high-dimensional multivariate normal probabilities

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December 9, 2019

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Table of contents

Introduction

Introduction

- The computation of the multivariate normal (MVN) probability

$$\Phi_n(\mathbf{a}, \mathbf{b}; 0, \mathbf{\Sigma}) = \int_a^b \frac{1}{\sqrt{(2\pi)^n |\mathbf{\Sigma}|}} \exp\left(-\frac{1}{2}\mathbf{x}^T \mathbf{\Sigma}^{-1} \mathbf{x}\right) d\mathbf{x}, \qquad (1)$$

  where $\mathbf{a}$ and $\mathbf{b}$ are integration limits, the mean vector μ is assumed to be 0, $\mathbf{\Sigma}$ is a positive-definite covariance matrix, is required for a variety of applications.
- Various methods to compute MVN probability are suggested such as Richtmyer Quasi-Monte Carlo(QMC) (Genz and Bretz, 2009)
- However, In high-dimensional settings (large n), it is hard to compute (1) directly.
- We review new approaches proposed by Cao et al. (2019) to approximate high-dimensional multivariate normal probability (1) using the hierarchical matrix $\mathcal{H}$ (Hackbusch, 2015) for the covariance matrix $\mathbf{\Sigma}$.

Motivation

The methods are based on

1. the bivariate conditioning method (Trinh and Genz, 2015) and
2. the hierarchical QMC method (Genton et al., 2018).

Multidimensional Conditioning Approximations

Quasi Monte Carlo Method

- MonteCarlo Error bound : $O(N^{-1/2})$ for monte carlo(MC) method
- Genz and Bretz (2009) claimed independent sample points is the reason of slow convergence.
- Via employing low discrepancy sets for sequence, QMC is asymptotically efficient than MC.
- With $\mathbf{\Delta} \sim U[0,1]^n$,

$$L_N = \{\mathbf{z} + \mathbf{\Delta} \bmod 1 : \mathbf{z} \in K_N\}$$

$$K_N = \{i\mathbf{q} \bmod 1, i = 1, \cdots, N\}$$

  where $\mathbf{q} = \sqrt{\mathbf{p}}$ and $\mathbf{p}$ is set of prime numbers.
- Since square root of prime numbers is irrational and linear independent over the rational numbers,

Quasi Monte Carlo Method

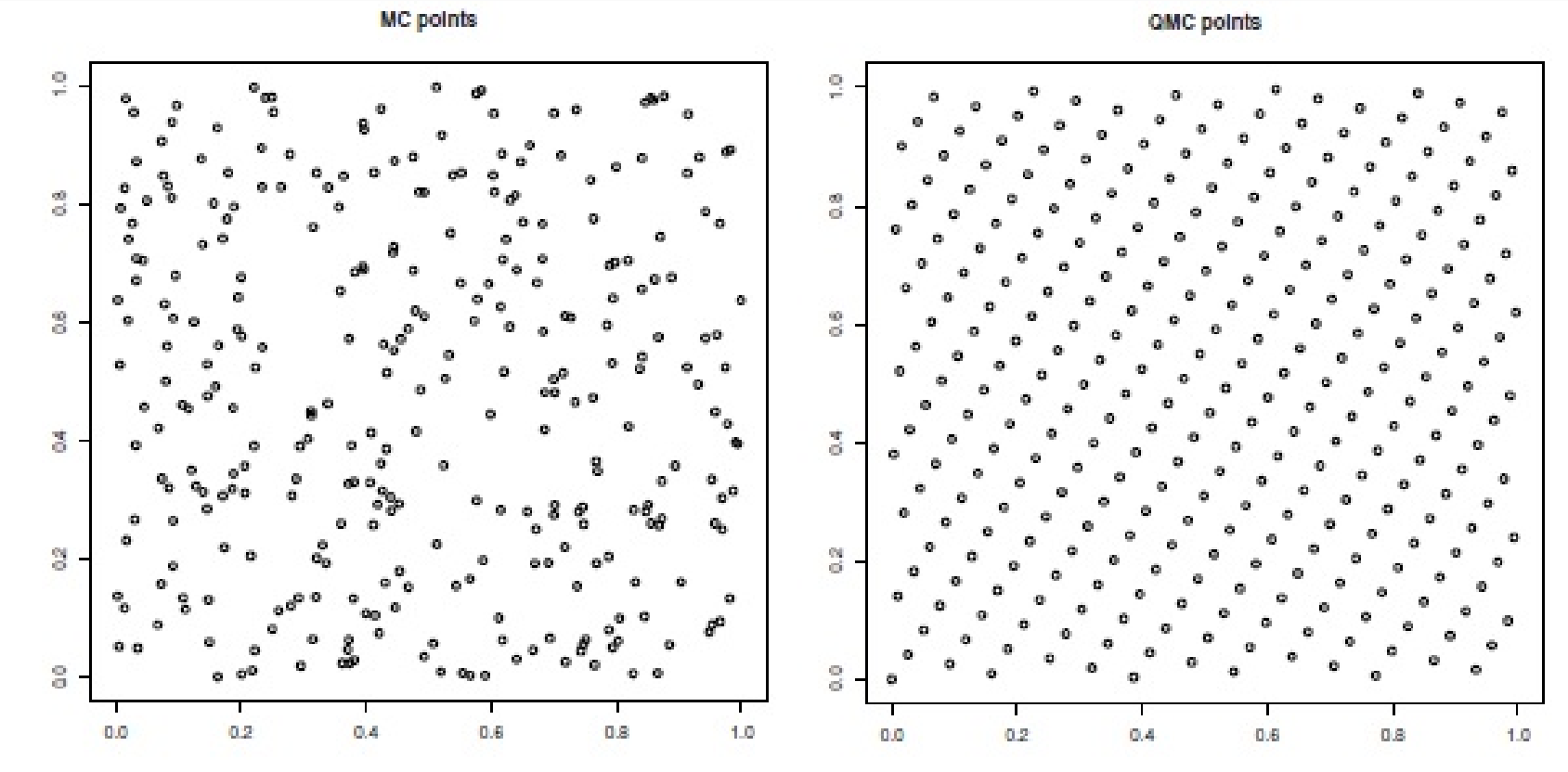


Figure 1: Comparison of MC and QMC sample points(Genz and Bretz, 2009)

Quasi Monte Carlo Method

$$\begin{aligned}
\mathbf{\Phi}_n(\mathbf{a} \le \mathbf{x} \le \mathbf{b}; \mathbf{\Sigma}) &= \mathbf{\Phi}_n(a \le \mathbf{L}\mathbf{y} \le \mathbf{b}; I_n) \\
&= \int_{a_1 \le l_{11} y_1 \le b_1} \phi(y_1) \cdots \int_{a_n \le \mathbf{l}_n^t \mathbf{y} \le b_n} \phi(y_n) d\mathbf{y} \\
&= \int_{\tilde{a}_1}^{\tilde{b}_1} \phi(y_1) \int_{\tilde{a}_2(y_1)}^{\tilde{b}_2(y_1)} \phi(y_2) \cdots \int_{\tilde{a}_n(y_1, \cdots, y_{n-1})}^{\tilde{b}_n(y_1, \cdots, y_{n-1})} \phi(y_n) d\mathbf{y}
\end{aligned}$$

$$\text{with } \tilde{a}_i(y_1, \cdots, y_{i-1}) = \frac{a_i - \sum_{j=1}^{i-1} l_{ij} y_j}{l_{ii}}$$

$$\text{and } (\tilde{b}_i(y_1, \cdots, y_{i-1})) = \frac{b_i - \sum_{j=1}^{i-1} l_{ij} y_j}{l_{ii}}$$

$$\begin{aligned}
&= \int_{\Phi(\tilde{a}_1)}^{\Phi(\tilde{b}_1)} \int_{\Phi(\tilde{a}_2(\Phi^{-1}(z_1)))}^{\Phi(\tilde{b}_2(\Phi^{-1}(z_1)))} \cdots \int_{\Phi(\tilde{a}_n(\Phi^{-1}(z_1), \cdots, \Phi^{-1}(z_{n-1})))}^{\Phi(\tilde{b}_n(\Phi^{-1}(z_1), \cdots, \Phi^{-1}(z_{n-1})))} d\mathbf{z} (y_i = \Phi^{-1}(z_i)) \\
&= (e_1 - d_1) \int_0^1 (e_2(w_1) - d_2(w_1)) \cdots \\
&\int_0^1 (e_n(w_1, \cdots, w_{n-1}) - d_n(w_1, \cdots, w_{n-1}))) \int_0^1 d\mathbf{w}
\end{aligned}$$

$$\text{with } z_i = d_i + (e_i - d_i) w_i \qquad (2)$$

Quasi Monte Carlo Method

procedure MVN($\boldsymbol{\mu}$, $\boldsymbol{\Sigma}$, $\mathbf{a}$, $\mathbf{b}$, ns, N)
  $\mathbf{L}$ = cholesky($\boldsymbol{\Sigma}$)
  $\mathbf{a} = \mathbf{a} - \boldsymbol{\mu}$; $\mathbf{b} = \mathbf{b} - \boldsymbol{\mu}$
  $T = 0$, $N = 0$, $V = 0$
  $\mathbf{p}$ = vector of primes less than $\frac{5n \log n+1}{4}$;$\mathbf{q} = \sqrt{\mathbf{p}}$
  $\mathbf{P} = \mathbf{1}_{ns}$
  $ans = 0$
  for $i = 1, \cdots, ns$ **do**
    $I_i = 0$, $\boldsymbol{\Delta} \sim U(0, 1)^n$
    for $j = 1, \cdots, N$ **do**
      $\mathbf{X}[1 : n, j] = (j + 1)\mathbf{q} + \boldsymbol{\Delta}$
      $\mathbf{X}[1 : n, j] = 2|\mathbf{X}[1 : n, j] - \text{floor}(\mathbf{X}[1 : n, j])| - 1$
    end for
    sample $= \mathbf{O}_{n,N}$
    $\mathbf{s}$, $\mathbf{c}$, $\mathbf{d}$, $\mathbf{dc}$, $\mathbf{P} = \mathbf{0}_N$
    for $j = 1, \cdots, n$ **do**
      if $j > 1$ **then**
        $c = \min(1, c + X[j - 1, :] \odot dc)$
        sample$[i - 1, 1 : N] = \Phi^{-1}(c)$
        $s = \mathbf{sample}[1 : i - 1, 1 : N]^T L[1 : i - 1, i]$
      end if
      $\mathbf{P}* = \Phi(\frac{b-s}{L[i,i]}) - \Phi(\frac{a-s}{L[i,i]})$
    end for
    ans+ = mean($\mathbf{P}$)
  end for
  return ans$/ns$
end procedure

Algorithm 1: Multivariate Normal Probability with Quasi Monte Carlo Method

Conditioning Approximation

Mendell and Elston (1974), Kamakura (1989), and Trinh and Genz (2015) exploit Cholesky factors from LDL decomposition rather than dealing with original covariance matrix. Biviarate example is follow.

$$\mathbf{\Sigma} = \begin{pmatrix} \mathbf{\Sigma}_{1,1} & \mathbf{R}^T \\ \mathbf{R} & \hat{\mathbf{\Sigma}} \end{pmatrix}, \text{ with } \mathbf{L} = \begin{pmatrix} \mathbf{I}_2 & \mathbf{O} \\ 1:\mathbf{M} & \mathbf{L} \end{pmatrix} \text{ and } \mathbf{D} = \begin{pmatrix} \mathbf{D}_1 & \mathbf{O} \\ \mathbf{O} & \widehat{\mathbf{D}} \end{pmatrix}$$

,where $\mathbf{\Sigma}_{1,1}, \mathbf{D}_1$ is a 2×2 matrix. From $\mathbf{D}_1 = \mathbf{\Sigma_{1,1}}$, $\mathbf{M} = \mathbf{R}\mathbf{D}_1^{-1}$, $\widehat{\mathbf{D}} = \hat{\mathbf{\Sigma}} - \mathbf{M}\mathbf{D}_1\mathbf{M}^T$

$$\begin{aligned} \mathbf{\Phi}_n(\mathbf{a}, \mathbf{b}; \mathbf{0}, \mathbf{\Sigma}) = \frac{1}{\sqrt{|\mathbf{D}|(2\pi)^n}} \int_{\alpha_1}^{\beta_1} \int_{\alpha_2}^{\beta_2} e^{-\frac{1}{2}\mathbf{x_2}^T \mathbf{D}_1^{-1} \mathbf{x}_2} \\ \cdots \int_{\alpha_{2k-1}}^{\beta_{2k-1}} \int_{\alpha_{2k}}^{\beta_{2k}} e^{-\frac{1}{2}\mathbf{x_{2k}}^T \mathbf{D}_1^{-1} \mathbf{x}_{2k}} \end{aligned} \tag{3}$$

Conditioning Approximation

Cao et al. (2019) generalizes bivariate method of Trinh and Genz (2015) to d-dimensional. Algorithms and details are following.

1: **procedure** LDL($\mathbf{\Sigma}$)
2: $\mathbf{L} \leftarrow \mathbf{I}_m$, $\mathbf{D} \leftarrow \mathbf{O}_m$
3: **for** $i = 1 : d : m - d + 1$ **do**
4: $\mathbf{D}[i : i + d - 1, i : i + d - 1] \leftarrow \mathbf{\Sigma}[i : i + d - 1, i : i + d - 1]$
5: $\mathbf{L}[i + d : m, i : i + d - 1] \leftarrow \mathbf{\Sigma}[i + d : m, i : i + d - 1]\mathbf{D}^{-1}[i : i + d - 1, i : i + d - 1]$
6: $\mathbf{\Sigma}[i + d : m, i + d : m] \leftarrow \mathbf{\Sigma}[i + d : m, i + d : m] - \mathbf{L}[i + d : m, i : i + d - 1]\mathbf{D}^{-1}[i : i + d - 1, i : i + d - 1]\mathbf{L}[i : i + d - 1, i + d : m]$
7: **if** $i + d < m$ **then**
8: $\mathbf{D}[i + d : m, i + d : m] \leftarrow \mathbf{\Sigma}[i + d : m, i + d : m]$
9: **end if**
10: **end for**
11: **return** $\mathbf{L}$ and $\mathbf{D}$
12: **end procedure**

Algorithm 2: LDL decomposition

Conditioning Approximation

When $s = \frac{m}{d}$ is integer, results of Algorithm 2, $\mathbf{L}, \mathbf{D}$ can be written as

$$\mathbf{L} = \begin{pmatrix} \mathbf{I}_d & \mathbf{O}_d & \cdots & \mathbf{O}_d \\ \mathbf{L}_{2,1} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \mathbf{I}_d & \mathbf{O}_d \\ \mathbf{L}_{s,1} & \cdots & \mathbf{L}_{s,s-1} & \mathbf{I}_d \end{pmatrix}, \mathbf{D} = \begin{pmatrix} \mathbf{D}_1 & \mathbf{O}_d & \cdots & \mathbf{O}_d \\ \mathbf{O}_d & \ddots & \ddots & \vdots \\ \vdots & \ddots & \mathbf{D}_{s-1} & \mathbf{O}_d \\ \mathbf{O}_d & \cdots & \mathbf{O}_d & \mathbf{D}_s \end{pmatrix}$$

with d-dimensional identitiy matrix $\mathbf{I}_d$ and d-dimensional zero matrix $\mathbf{O}_d$ and d-dimensional positive-definite matrix $\mathbf{D}_1, \cdots, \mathbf{D}_s$. As in (3), tranformation, $Y = LX$ provides m-dimensional multivariate normal prabability as the product of s d-dimensional multivariate normal probabilities as below.

$$\mathbf{\Phi}_{\boldsymbol{m}}(\mathbf{a}, \mathbf{b}; \mathbf{0}, \mathbf{\Sigma}) = \int_{\alpha_1}^{\beta_1} \phi_d(\mathbf{y}_1; \mathbf{D}_1) \int_{\alpha_2}^{\beta_2} \phi_d(\mathbf{y}_2; \mathbf{D}_2) \cdots \int_{\alpha_s}^{\beta_s} \phi_d(\mathbf{y}_s; \mathbf{D}_s) d\mathbf{y}_s \cdots d\mathbf{y}_2 d\mathbf{y}_1 \quad (4)$$

,where $\alpha_i = \mathbf{a}_i - \sum_{j=1}^{i-1} \mathbf{L}_{ij}\mathbf{y}_j, \beta_i = \mathbf{b}_i - \sum_{j=1}^{i-1} \mathbf{L}_{ij}\mathbf{y}_j$

Conditioning Approximation

procedure CMVN($\mathbf{\Sigma}, \mathbf{a}, \mathbf{b}, d$)
  $\mathbf{y} \leftarrow \mathbf{0}, P \leftarrow 1$
  for $i = 1 : s$ **do**
    $j \leftarrow (i-1)d$
    $\mathbf{g} \leftarrow \mathbf{L}[j+1 : j+d, 1 : j]\mathbf{y}[1 : j]$
    $\boldsymbol{\alpha} \leftarrow \mathbf{a}[j+1 : j+d] - \mathbf{g}$
    $\boldsymbol{\beta} \leftarrow \mathbf{b}[j+1 : j+d] - \mathbf{g}$
    $\mathbf{D}' \leftarrow \mathbf{D}[j+1 : j+d, j+1 : j+d]$
    $P \leftarrow P \cdot \mathbf{\Phi}_d(\boldsymbol{\alpha}, \boldsymbol{\beta}; \mathbf{0}, \mathbf{D}')$
    $\mathbf{y}[j+1 : j+d] \leftarrow E[\mathbf{Y}']$
  end for
  return P and $\mathbf{y}$
end procedure

Algorithm 3: d-dimensional conditioning algorithm

Multidimensional Truncated Expectations

The truncated expectation is expressed as

$$E(X^{e_j}) = \frac{1}{\Phi(\mathbf{a}, \mathbf{b}; \boldsymbol{\mu}, \boldsymbol{\Sigma})} \int_{\mathbf{a}}^{\mathbf{b}} x_j \phi_d(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{x} = \frac{1}{\Phi(\mathbf{a}, \mathbf{b}; \boldsymbol{\mu}, \boldsymbol{\Sigma})} F_j^d(\mathbf{a}, \mathbf{b}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

Theorem
(Kan and Robotti, 2017)

$$F_j^d(\mathbf{a}, \mathbf{b}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \mu_j \Phi_d(\mathbf{a}, \mathbf{b}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) + \mathbf{e}_j^T \boldsymbol{\Sigma} \mathbf{c}$$

,where c is a vector with lth component defined as

$$c_l = \phi_1(a_l; \mu_l, \sigma_l^2) \Phi_{d-1}(\mathbf{a}_{-l}, \mathbf{b}_{-l}; \hat{\boldsymbol{\mu}}^1, \hat{\boldsymbol{\Sigma}}_l) - \phi_1(b_l; \mu_l, \sigma_l^2) \Phi_{d-1}(\mathbf{a}_{-l}, \mathbf{b}_{-l}; \hat{\boldsymbol{\mu}}^2, \hat{\boldsymbol{\Sigma}}_l)$$

$$\hat{\boldsymbol{\mu}}_l^1 = \mu_{-l} + \boldsymbol{\Sigma}_{-l,l} \frac{a_l - \mu_l}{\sigma_l^2}, \hat{\boldsymbol{\mu}}_l^2 = \mu_{-l} + \boldsymbol{\Sigma}_{-l,l} \frac{b_l - \mu_l}{\sigma_l^2},$$

$$\hat{\boldsymbol{\Sigma}}_l = \boldsymbol{\Sigma}_{-l,-l} - \frac{1}{\sigma_l^2} \boldsymbol{\Sigma}_{-l,l} \boldsymbol{\Sigma}_{l,-l}$$

Theorem 1 has same form with bivariate version of Trinh and Genz (2015) with $d = 2$ and it allows us to calculate $E[Y']$ in Algorithm 3 with $\boldsymbol{\Phi}$ which can be obtained with quasi monte calro method proposed by Genz (1992)

Multidimensional Conditioning Approximation with Univariate Reordering

Appropriate integration order on conditioning algorithm possibly improves estiation accuracy

- Schervish (1984) : integral with shortest integration interval widths be the outermost integration variables
- Gibson et al. (1994) : variables which have smallest expected values be the outermost integration variables.
  Since innermost integrals which have smaller variation have the most influence with this order, overall variance reduces.
- Trinh and Genz (2015) also employs this ordering, and Cao et al. (2019) generalized it to d-dimensional problem.

Multidimensional Conditioning Approximation with Univariate Reordering

1: **procedure** RCMVN($\mathbf{\Sigma}$, $\mathbf{a}$, $\mathbf{b}$, d)
2: $\mathbf{y} \leftarrow \mathbf{0}$, $\mathbf{C} \leftarrow \mathbf{\Sigma}$
3: **for** $i = 1 : m$ **do**
4: **if** $i > 1$ **then**
5: $\mathbf{y}[i-1] \leftarrow \frac{\phi(a') - \phi(b')}{\Phi(b') - \Phi(a')}$
6: **end if**
7: $j \leftarrow \text{argmin}_{i \le j \le m}\{\Phi(\frac{\mathbf{b}[j] - \mathbf{C}[j,1:i-1]\mathbf{y}[1:i-1]}{\sqrt{\mathbf{\Sigma}[j,j] - \mathbf{C}[j,1:i-1]\mathbf{C}^T[j,1:i-1]}}) - \Phi(\frac{\mathbf{a}[j] - \mathbf{C}[j,1:i-1]\mathbf{y}[1:i-1]}{\sqrt{\mathbf{\Sigma}[j,j] - \mathbf{C}[j,1:i-1]\mathbf{C}^T[j,1:i-1]}})\}$
8: $\mathbf{\Sigma}[:,(i,j)] \leftarrow \mathbf{\Sigma}[:,(j,i)]; \mathbf{\Sigma}[(i,j),:] \leftarrow \mathbf{\Sigma}[(j,i),:]$
9: $\mathbf{C}[:,(i,j)] \leftarrow \mathbf{C}[:,(j,i)]; \mathbf{C}[(i,j),:] \leftarrow \mathbf{C}[(j,i),:]$
10: $\mathbf{a}[(i,j)] = \mathbf{a}[(j,i)]$
11: $\mathbf{b}[(i,j)] = \mathbf{b}[(j,i)]$
12: $\mathbf{C}[i,i] \leftarrow \sqrt{\mathbf{\Sigma}[i,i] - \mathbf{C}[i,1:i-1]\mathbf{C}^T[i,1:i-1]}$
13: $\mathbf{C}[j,i] \leftarrow \frac{\mathbf{\Sigma}[j,i] - \mathbf{C}[i,1:i-1]\mathbf{C}^T[j,1:i-1]}{\mathbf{C}[i,i]}$, for $j = i+1, \cdots, m$
14: $a' = \frac{\mathbf{a}[i] - \mathbf{C}[i,1:i-1]y[1:i-1]}{\mathbf{C}[\mathbf{i},\mathbf{i}]}$
15: $b' = \frac{\mathbf{b}[i] - \mathbf{C}[i,1:i-1]y[1:i-1]}{\mathbf{C}[\mathbf{i},\mathbf{i}]}$
16: **end for**
17: **return** CMVN($\mathbf{\Sigma}$, $\mathbf{a}$, $\mathbf{b}$, d) as in Algorithm 3
18: **end procedure**

Algorithm 4: d-dimensional conditioning algorithm with univariate reordering

Hierarchical-Block Approximation

Hierarchical Cholesky Decomposition

Hackbusch (2015) proposed hiarchical matrix and its cholesky decomposition method. $A = LU$ have the structure

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} L_{11} & O \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} L_{11}^T & L_{12}^T \\ O & L_{22}^T \end{pmatrix}$$

with lower triangular matrix L_{11}, L_{22}. It leads to four tasks:

(a) compute L_{11} via Cholesky decomposition of A_{11}

(b) compute L_{12} from $L_{21}L_{11}^T = A_{21}$

(c) low rank approximation of $L_{12} = UV^T$

(d) compute L_{22} via Cholesky decomposition of $A_{22} - L_{21}L_{21}^T$

We have applied low rank approximation with svd to (c) each block of its decomposition to make implementation efficiently and save storage while accuracy is preserved. : i.e. $A = UDV^T = \sum_{i=1}^{n} d_i u_i v_i^T \approx \sum_{i=1}^{k} d_i u_i v_i^T$.

Hierarchical Cholesky Decomposition

Hierachical cholesky decomposition of $n \times n$ matrix into $m \times m$ blocks is implemented like below.

```
1:  procedure HCHOL(A, n,m,rank)
2:      for i = 1 : log_2(n/m) do
3:          nb = n/2^i
4:          x = 0, y = nb
5:          for j = 1 : 2^(i-1) do
6:              U, D, V = lowrankSVD(A[xbegin + 1 : xbegin + nb, ybegin + 1 : ybegin + nb], rank)
7:              A[x + 1 : x + nb, y + 1 : y + rank] = UD
8:              A[x + 1 : x + nb, y + rank + 1 : y + nb] = O
9:              A[y + 1 : y + nb, x + 1 : x + rank] = VD
10:             A[y + 1 : y + nb, x + rank + 1 : x + nb] = O
11:             x+ = 2nb, y+ = 2nb
12:         end for
13:     end for
14: end procedure
```

Algorithm 5: Hierachical cholesky decomposition

The Hierarchical-Block Conditioning Method

Let $\phi_m(\mathbf{x}; \mathbf{\Sigma})$ be a pdf of the m-dimensional normal distribution $N(\mathbf{0}, \mathbf{\Sigma})$ and $(\mathbf{B}, \mathbf{U}\mathbf{V}^T)$ be the hierarchical Cholesky decompostion of the covariance matrix $\mathbf{\Sigma}$. Then,

$$\Phi_n(\mathbf{a}, \mathbf{b}; \mathbf{0}, \mathbf{\Sigma}) = \int_{\mathbf{a}_1'}^{\mathbf{b}_1'} \phi_m(\mathbf{x}_1; \mathbf{B}_1\mathbf{B}_1^T) \cdots \int_{\mathbf{a}_r'}^{\mathbf{b}_r'} \phi_r(\mathbf{x}_r; \mathbf{B}_r\mathbf{B}_r^T) d\mathbf{x}_r \cdots d\mathbf{x}_1. \tag{5}$$

,where $\mathbf{a}'$, $\mathbf{b}'$, $i = 1, \cdots, r$, are the corresponding segments of the updated $\mathbf{a}$ and $\mathbf{b}$.

Note the probabilities $\Phi_m(\mathbf{a}_i, \mathbf{b}_i; \mathbf{0}, \mathbf{B}_i\mathbf{B}_i^T)$ can be computed using

1. Quasi-Monte Carlo method (`HMVN`, Method 1 in Cao et al. (2019))
2. d-dimensional conditioning algorithm (`HCMVN`, Method 2 in Cao et al. (2019))
3. d-dimensional conditioning algorithm with univariate reordering (`HRCMVN`, Method 3 in Cao et al. (2019)).

These methods are more effective and easily parallelizable than the classical methods.

The Hierarchical-Block Conditioning Method

1: **procedure** HMVN(a, b, $\mathbf{\Sigma}$, d)
2: $\mathbf{x} \leftarrow \mathbf{0}$ and $P \leftarrow 1$
3: $[\mathbf{B}, \mathbf{UV}] \leftarrow$ choldecomp_hmatrix($\mathbf{\Sigma}$)
4: **for** $i = 1 : r$ **do**
5: $j \leftarrow (i-1)m$
6: **if** $i > 1$ **then**
7: $o_r \leftarrow$ row offset of $\mathbf{U}_{i-1}\mathbf{V}_{i-1}^T$
8: $o_c \leftarrow$ column offset of $\mathbf{U}_{i-1}\mathbf{V}_{i-1}^T$
9: $l \leftarrow \dim(\mathbf{U}_{i-1}\mathbf{V}_{i-1}^T)$
10: $\mathbf{g} \leftarrow \mathbf{U}_{i-1}\mathbf{V}_{i-1}^T\mathbf{x}[o_c + 1 : o_c + l]$
11: $\mathbf{a}[o_r + 1 : o_r + l] = \mathbf{a}[o_r + 1 : o_r + l] - \mathbf{g}$
12: $\mathbf{b}[o_r + 1 : o_r + l] = \mathbf{a}[o_r + 1 : o_r + l] - \mathbf{g}$
13: **end if**
14: $\mathbf{a}_i \leftarrow \mathbf{a}[j + 1 : j + m]$
15: $\mathbf{b}_i \leftarrow \mathbf{b}[j + 1 : j + m]$
16: $P = P * \Phi_m(\mathbf{a}_i, \mathbf{b}_i; \mathbf{0}, \mathbf{B}_i\mathbf{B}_i^T)$
17: $\mathbf{x}[j + 1 : j + m] \leftarrow \mathbf{B}_i^{-1}E(\mathbf{X}_i)$
18: **end for**
19: **end procedure**

Algorithm 6: Hierarchical-block conditioning algorithm

Computational Complexity

$M(\cdot)$ denotes the complexity of the QMC simulation in the given dimension. Table 1 shows that the time efficiency of the d-dimensional conditioning algorithm mainly comes from lowering the dimension in which the QMC simulation is performed.

	MVN prob	Trunc exp	Upd limits
`HMVN`	$\frac{n}{m}M(m)$	$2nM(m) + O(nm^2)$	$O(mn + knlog(n/m))$
`HCMVN`	$\frac{n}{d}M(d) + O(m^2 n)$	$2nM(d) + O(nd^2)$	$O(mn + knlog(n/m))$
`HRCMVN`	$\frac{n}{d}M(d) + O(m^2 n)$	$2nM(d) + O(nd^2)$	$O(mn + knlog(n/m))$

Table 1: Complexity decomposition of the `HMVN`, `HCMVN`, and `HRCMVN`

- The updating cost is independent of the method.
- The complexity of the univariate reordering is $O(m^2 n)$, the same as the complexity of computing the MVN probabilities in `HCMVN`
- Since `HCMVN` and `HRCMVN` perform the QMC simulation in d-dimensions, these two methods are not greatly affected by the choice of m.

Block Reordering

Block Reordering

- The cdf value for n-dimensioned multivariate normal variable comprises of m multiplications of d-dimensional integrals.
- Recall the `RCMVN` algorithm(3) : as computing each d-dimensional integral values, integration variables were arranged in order of increasing order of `CMVN` probability values, from outer to inner
- Permutes the block of LDL-decomposed covariance matrix, in order of `RCMVN` probability values of each blocks
- Result accuracy and time cost is compared among `HMVN`, `HCMVN`, `HRCMVN` with/without block reordering.

Block Reordering

```
procedure BLOCKREORDER(G, ρ, a, b, m, ind)
    G, ρ, a, b, m, ind given, P ← 0
    for i = 1 : m : n − m + 1 do
        s ← ind[i : i + m − 1]
        A ← ρ(G, s)
        a′ ← a[s]
        b′ ← b[s]
        P ← [P, RCMVN(A, a′, b′, 1).P]
    end for
    sort(ind, P, m)
    return ind
end procedure
```

Algorithm 7: Blockwise reordering

Block Reordering

procedure HCMVN_BRO(a, b, Σ, d)
  $\mathbf{x} \leftarrow \mathbf{0}$, $P \leftarrow 1$, ind $\leftarrow [1, \ldots, n]$
  $[\mathbf{B}, \mathbf{UV}] \leftarrow$ choldecomp_hmatrix(Σ)
  $\mathbf{B} \leftarrow$ Blockreorder(G, ρ, a, b, m, ind)
  for $i = 1 : r$ **do**
    $j \leftarrow (i-1)m$
    if $i > 1$ **then**
      $o_r \leftarrow$ row offset of $\mathbf{U}_{i-1}\mathbf{V}_{i-1}^T$
      $o_c \leftarrow$ column offset of $\mathbf{U}_{i-1}\mathbf{V}_{i-1}^T$
      $l \leftarrow \dim(\mathbf{U}_{i-1}\mathbf{V}_{i-1}^T)$
      $\mathbf{g} \leftarrow \mathbf{U}_{i-1}\mathbf{V}_{i-1}^T \mathbf{x}[o_c + 1 : o_c + l]$
      $\mathbf{a}[o_r + 1 : o_r + l] = \mathbf{a}[o_r + 1 : o_r + l] - \mathbf{g}$
      $\mathbf{b}[o_r + 1 : o_r + l] = \mathbf{a}[o_r + 1 : o_r + l] - \mathbf{g}$
    end if
    $\mathbf{a}_i \leftarrow \mathbf{a}[j + 1 : j + m]$
    $\mathbf{b}_i \leftarrow \mathbf{b}[j + 1 : j + m]$
    $P = P * \Phi_m(\mathbf{a}_i, \mathbf{b}_i; \mathbf{0}, \mathbf{B}_i\mathbf{B}_i^T)$
    $\mathbf{x}[j + 1 : j + m] \leftarrow \mathbf{B}_i^{-1} E[\mathbf{X}_i]$
  end for
end procedure

Algorithm 8: Hierarchical-block conditioning algorithm with Block Reordering

Numerical Examples

Cholesky Factorization

- The *chol* function from **LinearAlgebra** package
- The *dpotrf* from **LAPACK** package
- Hierarchical cholesky decomposition which suggested by Hackbusch (2015) are implemented.

Exponential covariance matrix, $\mathbf{\Sigma}_{ij} = exp(-\|\mathbf{s}_i - \mathbf{s}_j\|/\beta)$ is set with $\beta = 0.3$. n points, $\mathbf{s}_1, \cdots, \mathbf{s}_n$ is evenly distributed over unique square with Morton's order which defined recursively as described in figure 2.

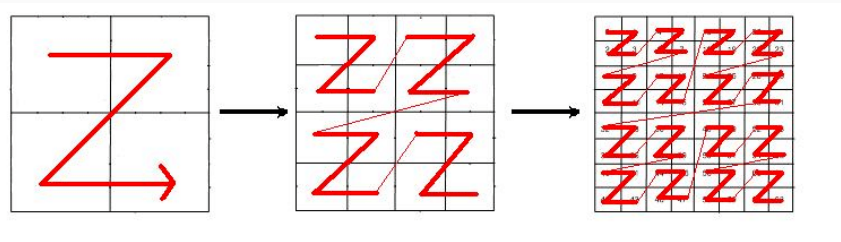


Figure 2: Morton's order(Salem and Arab, 2016)

Cholesky Factorization

With various n, three Cholesky methods are applied and results are below table 2. In low rank approximation at algorithm 5, rank is about $n^{1/4}$.

n	256	1024	4096	16384
chol	0.001s	0.0097s	0.414s	156.3s
dpotrf	0.0007s	0.0132s	0.431s	154.1s
hierarchical cholesky	0.153s	0.076s	0.916s	37.3s
Error of hierarchical cholesky	1.06e-7	9.97e-7	1.11e-3	1.87e-3

Table 2: Excution times for Cholesky factorization

- Hierarchical cholesky decomposition is more efficient than other classical cholesky method with large dimension.
- Hierarchical cholesky decomposition provides $\mathbf{\Sigma} \approx L_H L_H^T$. Its relative error is defined as $\frac{\|\mathbf{\Sigma} - L_H L_H^T\|_2}{\|\mathbf{\Sigma}\|_2}$
- Table 2 ensures accuracy of hierarchical cholesky decomposition proposed by Hackbusch (2015).

Multivariate Normal Probabilities

d-dimensional Conditioning Algorithm without/with Reordering

Theorem

Stewart (1980) Let the independent vectors $x_1, \cdots, x_n$ *be distributed* $N(0, \sigma^2 \mathbf{I})$. *For* $j = 1, 2, \cdots, n-1$, *let* $\mathbf{H}_{x_j}$ *be the Householder transformation that reduces* x_j *to* $r_{jj} e_1$, *where* r_{ij} *is obtained in QR decomposition of* $[x_1, \cdots, x_n]$ *Let* $\mathbf{H}_j = diag(\mathbf{I}_{j-1}, \bar{\mathbf{H}}_j)$. *Let* $\mathbf{D} = diag(sign(r_{11}), \cdots, sign(r_{nn}))$. *Then the product* $\mathbf{Q} = \mathbf{D}\mathbf{H_1} \cdots \mathbf{H_{n-1}}$ *follows Haar Distribution.*

- 250 MVN problems with various values of m and d
- $\mathbf{\Sigma} = \mathbf{Q}\mathbf{J}\mathbf{Q}^T$ is simulated with $\mathbf{Q} \sim$ *Haardistribution* and $J = diag(j_i)$ where $j_1, \cdots, j_m \sim U(0, 1)$
- Integration limits $a_i = -\infty$ and $b_i \sim (U, m)$ for $i = 1 \cdots, m$
- Estimated value is compared with approximated value obtained via quasi monte carlo method with a sample size of 10^4, which ensures error below 10^{-4}

d-dimensional Conditioning Algorithm without/with Reordering

(m, d)	1	2	4	8	16
Without univariate reordering					
16	3.7% 0.029ms	3.5% 0.201ms	3.6% 0.431ms	3.8% 0.676ms	2.9% 1.372ms
32	2.4% 0.001ms	2.9% 0.390ms	2.9% 0.833ms	3.3% 1.283ms	2.7% 2.545ms
64	1.9% 0.004ms	2.1% 0.762ms	2.1% 1.686ms	1.8% 2.545ms	1.9% 5.004ms
128	1.3% 0.024ms	1.5% 1.505ms	1.3% 3.333ms	1.2% 5.146ms	1.4% 10.548ms
With univariate reordering					
16	3.3% 0.007ms	3.1% 0.203ms	3.3% 0.439ms	3.6% 0.680ms	2.7% 1.363ms
32	2.3% 0.004ms	2.6% 0.393ms	2.6% 0.841ms	3.2% 1.289ms	2.6% 2.544ms
64	2.0% 0.014ms	2.1% 0.773ms	2.1% 1.695ms	1.9% 2.552ms	1.9% 5.022ms
128	1.2% 0.097ms	1.5% 1.593ms	1.4% 3.462ms	1.2% 5.268ms	1.4% 10.7861ms

Table 3: Errors and execution times of the d-dimensional conditioning method

Estimation error tended to decrease as d increases with each m since lager d implers less discarded correlation information. Spent time grows to a linear fashion with m while it grows exponentially with d.

Elements

Typography

```
The theme provides sensible defaults to
\emph{emphasize} text, \alert{accent} parts
or show \textbf{bold} results.
```

becomes

The theme provides sensible defaults to *emphasize* text, accent parts or show **bold** results.

Font feature test

- Regular
- *Italic*
- SmallCaps
- **Bold**
- ***Bold Italic***
- **Bold SmallCaps**
- `Monospace`
- *`Monospace Italic`*
- **`Monospace Bold`**
- ***`Monospace Bold Italic`***

Lists

Items

- Milk
- Eggs
- Potatos

Enumerations

1. First,
2. Second and
3. Last.

Descriptions

PowerPoint Meeh.

Beamer Yeeeha.

Animation

- This is important

Animation

- This is important
- Now this

Animation

- This is important
- Now this
- And now this

Animation

- This is really important
- Now this
- And now this

Figures

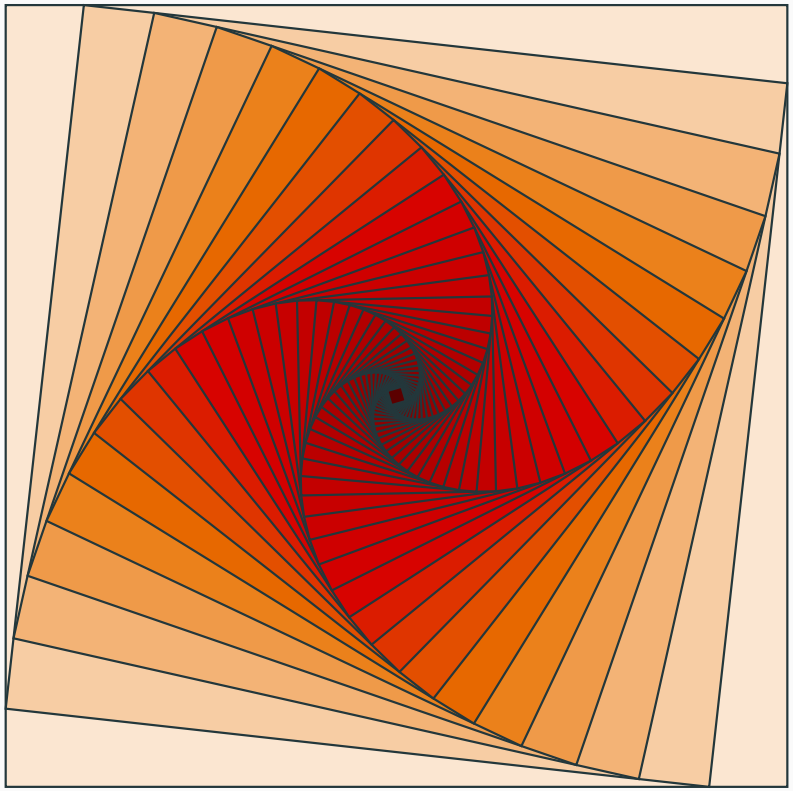


Figure 3: Rotated square from texample.net.

Tables

Table 4: Largest cities in the world (source: Wikipedia)

City	Population
Mexico City	20,116,842
Shanghai	19,210,000
Peking	15,796,450
Istanbul	14,160,467

Blocks

Three different block environments are pre-defined and may be styled with an optional background color.

Default
Block content.

Alert
Block content.

Example
Block content.

Default

Block content.

Alert

Block content.

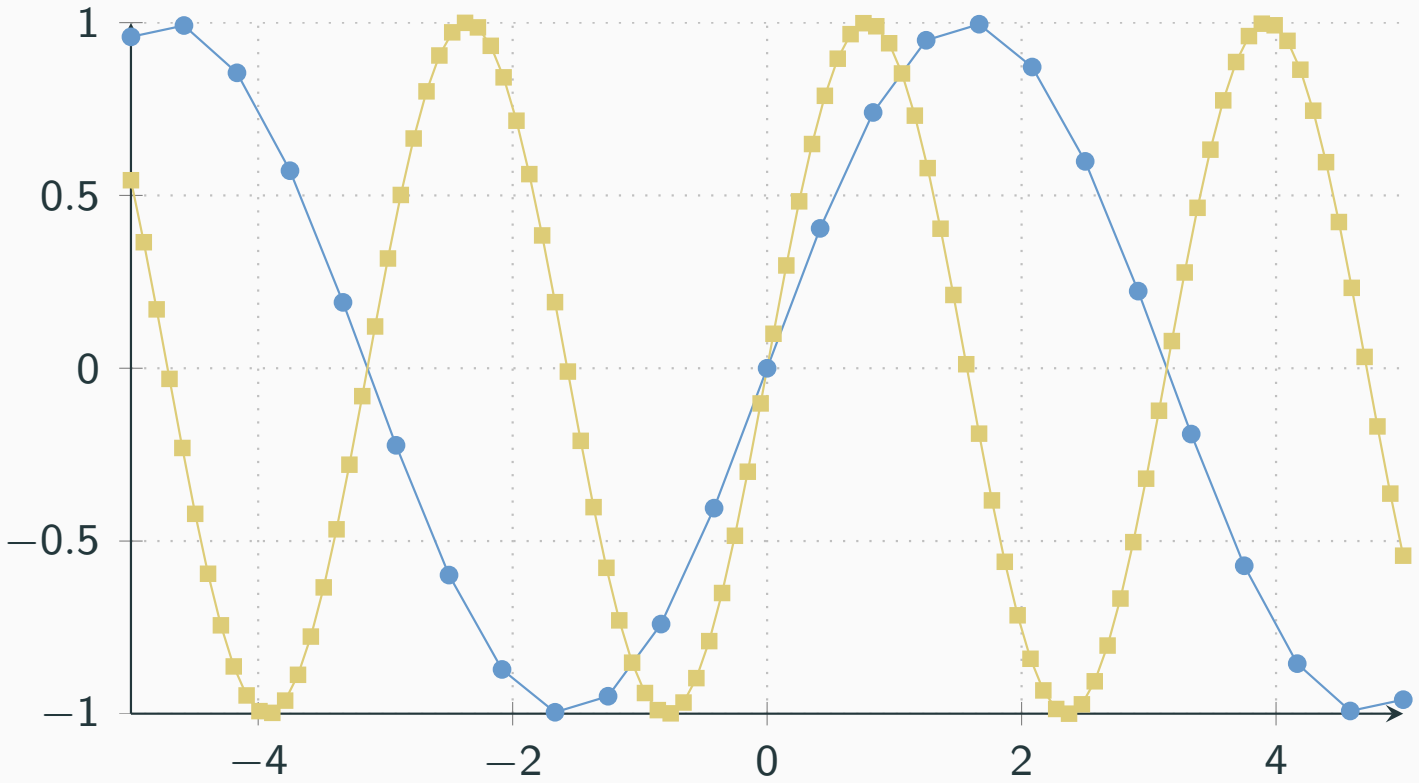
Example

Block content.

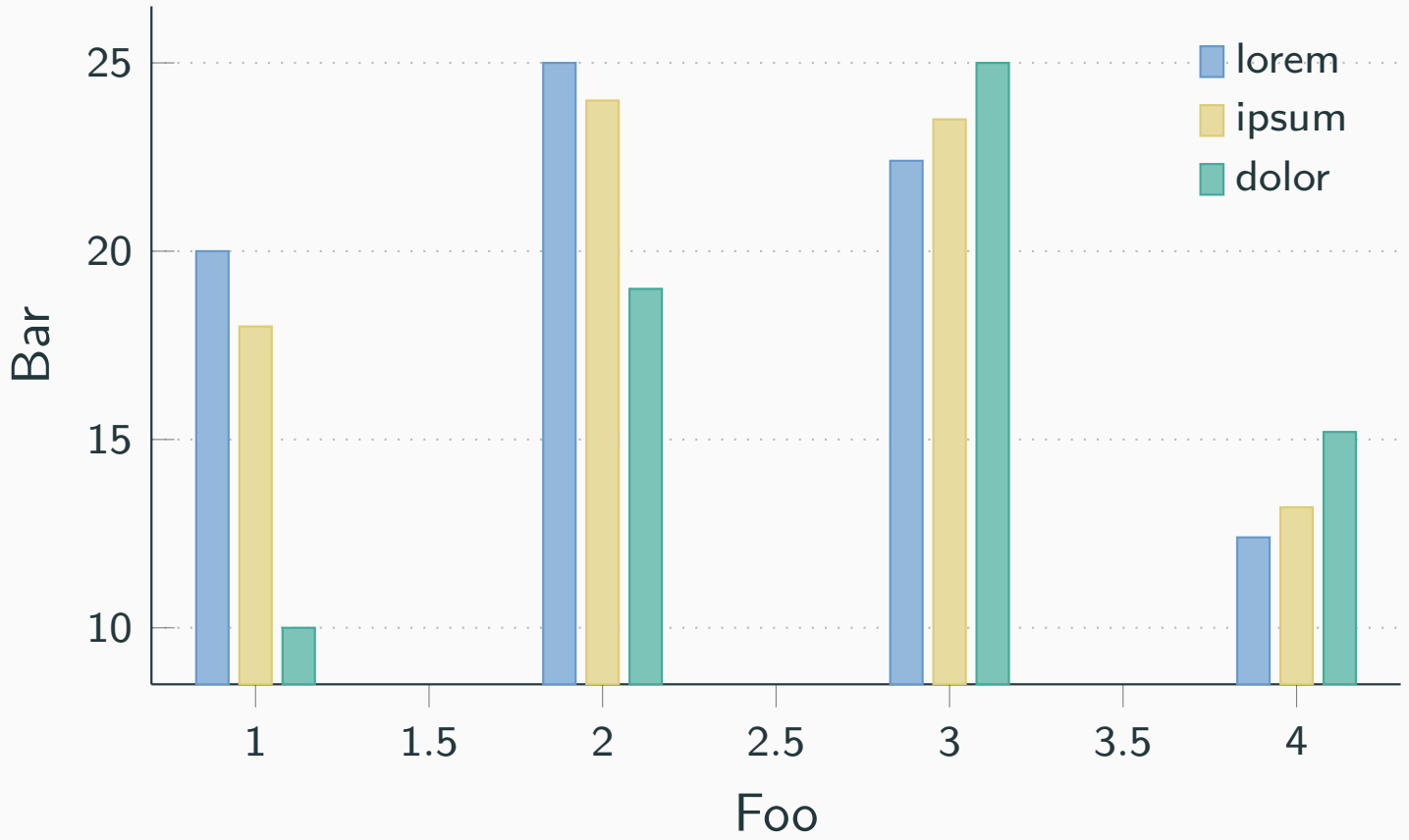
Math

$$e = \lim_{n \to \infty} \left(1 + \frac{1}{n}\right)^n$$

Line plots



Bar charts



Quotes

Veni, Vidi, Vici

Frame footer

metropolis defines a custom beamer template to add a text to the footer. It can be set via

```
\setbeamertemplate{frame footer}{My custom footer}
```

References

Some references to showcase [allowframebreaks] **?????**

Conclusion

Summary

Get the source of this theme and the demo presentation from

`github.com/matze/mtheme`

Questions?

Backup slides

Sometimes, it is useful to add slides at the end of your presentation to refer to during audience questions.

The best way to do this is to include the `appendixnumberbeamer` package in your preamble and call `\appendix` before your backup slides.

metropolis will automatically turn off slide numbering and progress bars for slides in the appendix.

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