High-Dimensional Gaussian Sampling

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Problem Definition

Sampling from a d-dimensional Gaussian distribution $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, where d may be large.

$$\pi(\boldsymbol{\theta}) = \frac{1}{(2\pi)^{d/2}\det(\boldsymbol{\Sigma})^{1/2}} \exp\left(-\frac{1}{2}(\boldsymbol{\theta}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{\theta}-\boldsymbol{\mu})\right).$$

Covariance matrix $\boldsymbol{\Sigma}$ positive definite. Precision matrix $\mathbf{Q} = \boldsymbol{\Sigma}^{-1}$ exists and also positive definite.

Vanilla Cholesky Sampler

Algorithm 1 Cholesky sampler

1: Set $\mathbf{C} = \mathrm{chol}(\mathbf{Q})$. ▷ $\mathbf{Q} = \mathbf{C}\mathbf{C}^\top$
2: Draw $\mathbf{z} \sim \mathcal{N}(\mathbf{0}_d, \mathbf{I}_d)$.
3: Solve $\mathbf{C}^\top \mathbf{w} = \mathbf{z}$ w.r.t. $\mathbf{w}$.
4: **return** $\theta = \mu + \mathbf{w}$.

Problem: computational cost $\Theta(d^3)$ and storage requirement $\Theta(d^2)$.

Better Solutions

- Square Root approximation: Approximate $\mathbf{Q}^{1/2}$.
- Conjugate Gradient: Solve a linear system w.r.t. $\mathbf{Q}$.
- Matrix Splitting: A generation of Gibbs Sampler.
- Data Augmentation: Introduce auxiliary variable.

Improvement: computational cost $\mathcal{O}(d^2)$ and storage requirement $\Theta(d)$.

Guidelines to Choosing the Sampler