# The $G$-Wishart Weighted Proposal Algorithm: Efficient Posterior Computation for Gaussian Graphical Models

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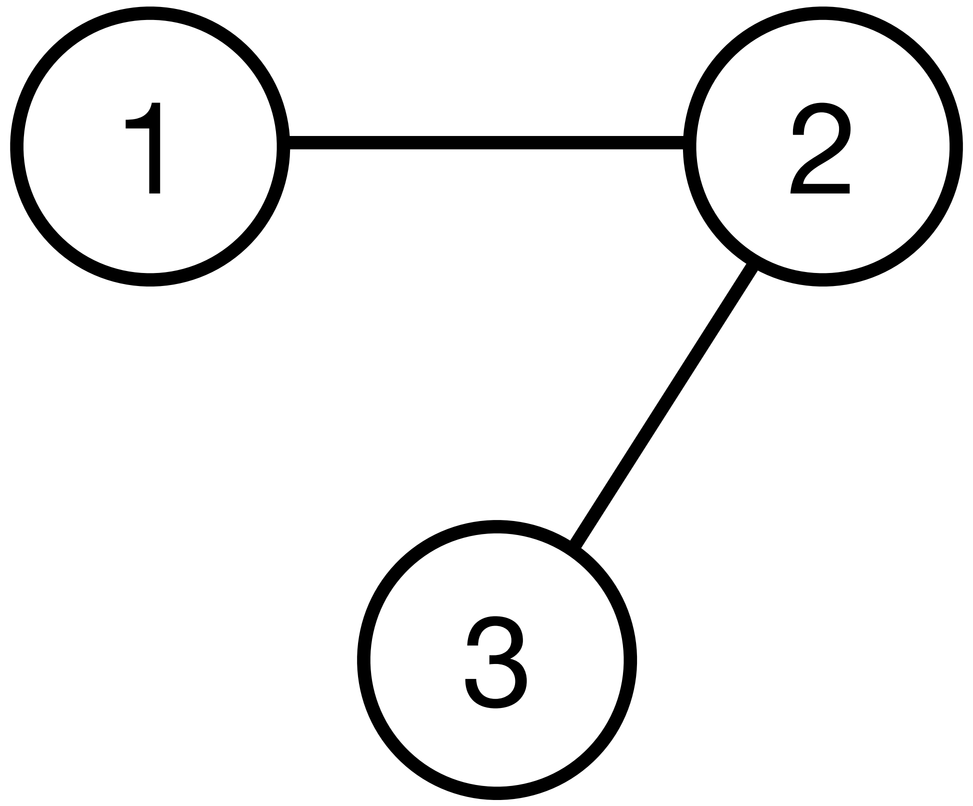
# Motivation

- Inference in graphical models is hard: $2^{p(p-1)/2}$ possible graphs on $p$ nodes
- Variety of approaches
  - Estimating the precision through penalized likelihood: Graphical lasso (Friedman et al., 2007), nodewise regression (Zhou et al., 2011), precision factor model (Chandra et al., 2022)
  - Continuous spike-and-slab prior (Wang, 2015; Li et al., 2020)
  - Subset of graph space: Decomposable graphs (Giudici and Green, 1999)
  - Full graph space with the $G$-Wishart prior (Giudici, 1996), e.g., BDgraph (Mohammadi and Wit, 2019) and the double conditional Bayes factor sampler (Hinne et al., 2014)
- The $G$-Wishart weighted proposal algorithm (WWA): Speed up through advances in MCMC
  - Informed proposal (Zanella, 2019)
  - Delayed Metropolis-Hastings acceptance (Christen and Fox, 2005)

# Gaussian graphical models

- $Y_i \mid K, G \sim \mathcal{N}(0, K^{-1})$ independently for $i = 1, \ldots, n$
  - $Y_i \in \mathbb{R}^p$
- Graph $G$ specifies conditional independencies.
  - $G = \{(1,2), (2,3)\}$
  - $Y_{i1} \perp Y_{i3} \mid Y_{i2}$ if and only if $K_{13} = 0$
  - $(i,j) \notin G \Rightarrow K_{ij} = 0$




$Y_i \in \mathbb{R}^3$

$Y_{i1} \perp Y_{i3} \mid Y_{i2}$

# Prior specification

- Hierarchical prior $p(K, G) = p(K \mid G)\, p(G)$
- $G$-Wishart distribution as prior on the precision matrix (Giudici, 1996)
  - Wishart distribution truncated to matrices with $K_{ij} = 0$ for $(i, j) \notin G$
  - $p(K \mid G) = \mathscr{W}_G(K \mid \delta, D) = \dfrac{1}{I_G(\delta, D)} \, |K|^{\delta/2-1} \exp\left\{ -\frac{1}{2}\mathrm{tr}(K^\top D) \right\}$
- $K \mid G, Y \sim \mathscr{W}_G(\delta^\star, D^\star)$ where $\delta^\star = \delta + n$ and $D^\star = D + Y^\top Y$

# Goal

- The objective is inference on the graph $G$.

$$p(G \mid Y) \propto p(G) \int p(K \mid G)\, p(Y \mid K)\, dK = \frac{p(G)\, I_G(\delta^\star, D^\star)}{(2\pi)^{np/2}\, I_G(\delta, D)}$$

- The normalizing constant $I_G(\delta, D)$ is intractable.

- Posterior computation is challenging and of interest.
  - Roverato, 2002; Dellaportas et al., 2003; Atay-Kayis and Massam, 2005; Moghaddam et al., 2009; Lenkoski and Dobra, 2011; Wang and Li, 2012; Cheng and Lenkoski, 2012; Lenkoski, 2013; Hinne et al., 2014; Mohammadi and Wit, 2015, 2019; Mohammadi et al., 2021

# WWA's speedups

**Problem:** Expensive to resample the full precision matrix $K$

**Solution:** Gibbs update based on the Cholesky decomposition

**Problem:** Exploring the large discrete space of graphs

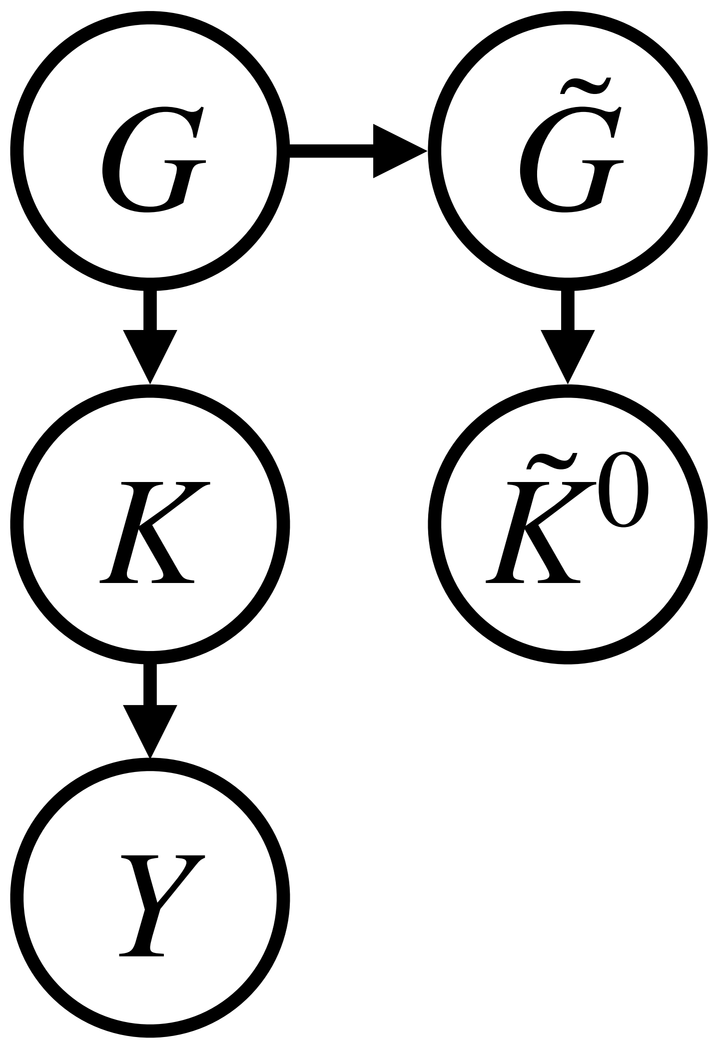
**Solution:** Informed proposal (Zanella, 2019) using a posterior approximation (Mohammadi et al., 2021) resulting in more efficient exploration

**Problem:** Most computational effort on proposed graphs that are rejected

**Solution:** Reject fast and cheaply using delayed Metropolis-Hastings acceptance (Christen and Fox, 2005)

# Review: Exchange algorithm

- The exchange algorithm (Murray et al, 2006) avoids evaluating $I_G(\delta, D)$ (Wang and Li, 2012).




- Augmented state space $(K, G, \tilde{K}^0, \tilde{G})$:
  - Propose $\tilde{G}$ from $G$ by changing one edge.
  - "Prior" precision $\tilde{K}^0 \mid \tilde{G} \sim \mathscr{W}_{\tilde{G}}(\delta, D)$
  - Metropolis-Hastings acceptance ratio:

$$\frac{p(\tilde{K}, \tilde{G}, K^0, G)}{p(K, G, \tilde{K}^0, \tilde{G})} = \frac{p(\tilde{K} \mid \tilde{G})\, p(\tilde{G})\, p(Y \mid \tilde{K})\, p(K^0 \mid G)\, q(G \mid \tilde{G})}{p(K \mid G)\, p(G)\, p(Y \mid K)\, p(\tilde{K}^0 \mid \tilde{G})\, q(\tilde{G} \mid G)}$$

Exchange

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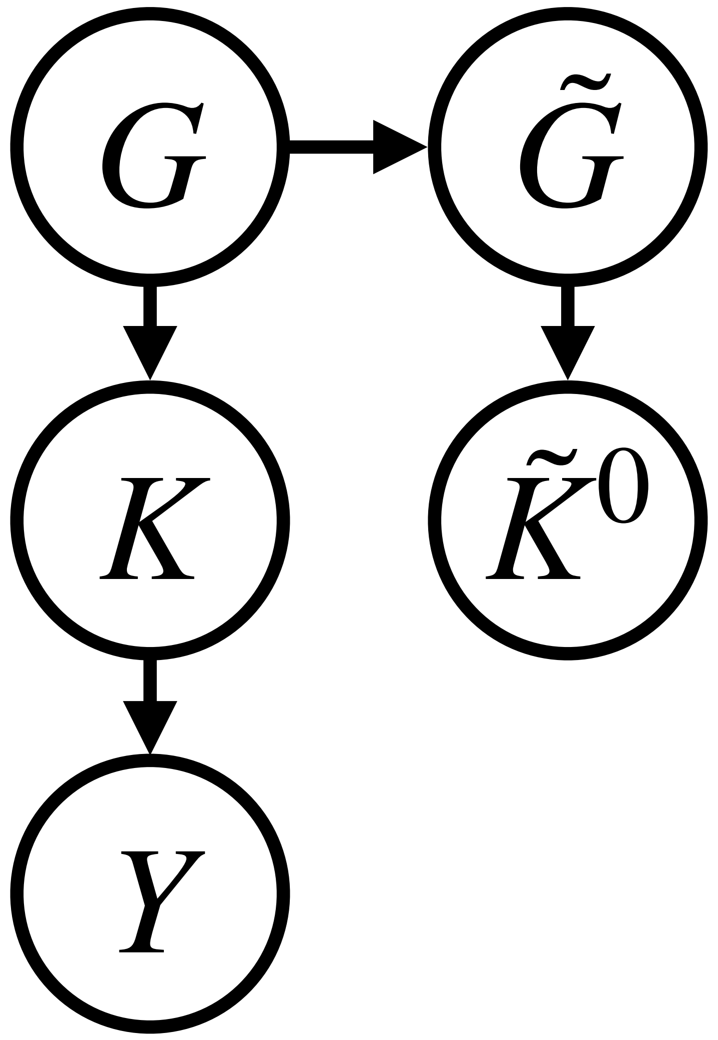


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$$\frac{p(\tilde{K}, \tilde{G}, K^0, G)}{p(K, G, \tilde{K}^0, \tilde{G})} = \frac{\boxed{p(\tilde{K} \mid \tilde{G})}\, p(\tilde{G})\, p(Y \mid \tilde{K})\, \boxed{p(K^0 \mid G)}\, q(G \mid \tilde{G})}{\boxed{p(K \mid G)}\, p(G)\, p(Y \mid K)\, \boxed{p(\tilde{K}^0 \mid \tilde{G})}\, q(\tilde{G} \mid G)}$$

Exchange

$I_G(\delta, D)$ and $I_{\tilde{G}}(\delta, D)$ cancel out.

**Problem:** Expensive to resample the full precision matrix $K$

**Solution:** Gibbs update based on the Cholesky decomposition

- Augmenting the state space by sampling $K \mid G \sim \mathscr{W}_G(\delta^\star, D^\star)$ is the main computational bottleneck.
- If $\tilde{G}$ is accepted, update $K$ such that it is distributed as $\mathscr{W}_{\tilde{G}}(\delta^\star, D^\star)$.
- Sampling one element of a Cholesky decomposition suffices.
  - Distribution of the Cholesky decomposition of a permuted $K$ differs in only one element for $G$ and $\tilde{G}$.
  - WWA samples this element from its Gaussian full conditional.

**Problem:** Exploring the large discrete space of graphs

**Solution:** Informed proposal

- Informed proposal puts more mass on regions with higher posterior probability (Zanella, 2019):

$$Q(\tilde{G} \mid G) \propto g\left\{\frac{p(\tilde{G} \mid Y)}{p(G \mid Y)}\right\} q(\tilde{G} \mid G)$$

  - Embarrassingly parallel scan over all $\tilde{G}$ that differ from $G$ by one edge.
  - WWA uses balancing function $g(t) = t/(1+t)$.

- WWA uses a modified version because $p(G \mid Y)$ is intractable:

$$Q(\tilde{G} \mid K, G) \propto g\left\{\frac{p(K, \tilde{G} \mid Y)}{p(K, G \mid Y)}\right\} q(\tilde{G} \mid G)$$

  - The ratio involves a ratio of intractable normalization constants $I_G(\delta, D)$.
  - Fast approximation of this ratio (Mohammadi et al., 2021)

**Problem:** Most computational effort on proposed graphs that are rejected

**Solution:** Reject fast and cheaply

- Delayed Metropolis-Hasting acceptance exploits a fast approximate acceptance probability (Christen and Fox, 2005).

- Approximation of ratio of $I_G(\delta, D)$ (Mohammadi et al., 2021) provides approximate acceptance without:
  - Exchange algorithm
  - The computational bottleneck of sampling $\tilde{K}^0 \mid \tilde{G} \sim \mathscr{W}_{\tilde{G}}(\delta, D)$

- The exchange algorithm only if $\tilde{G}$ is "promoted" to be considered for delayed acceptance

# Overview of WWA

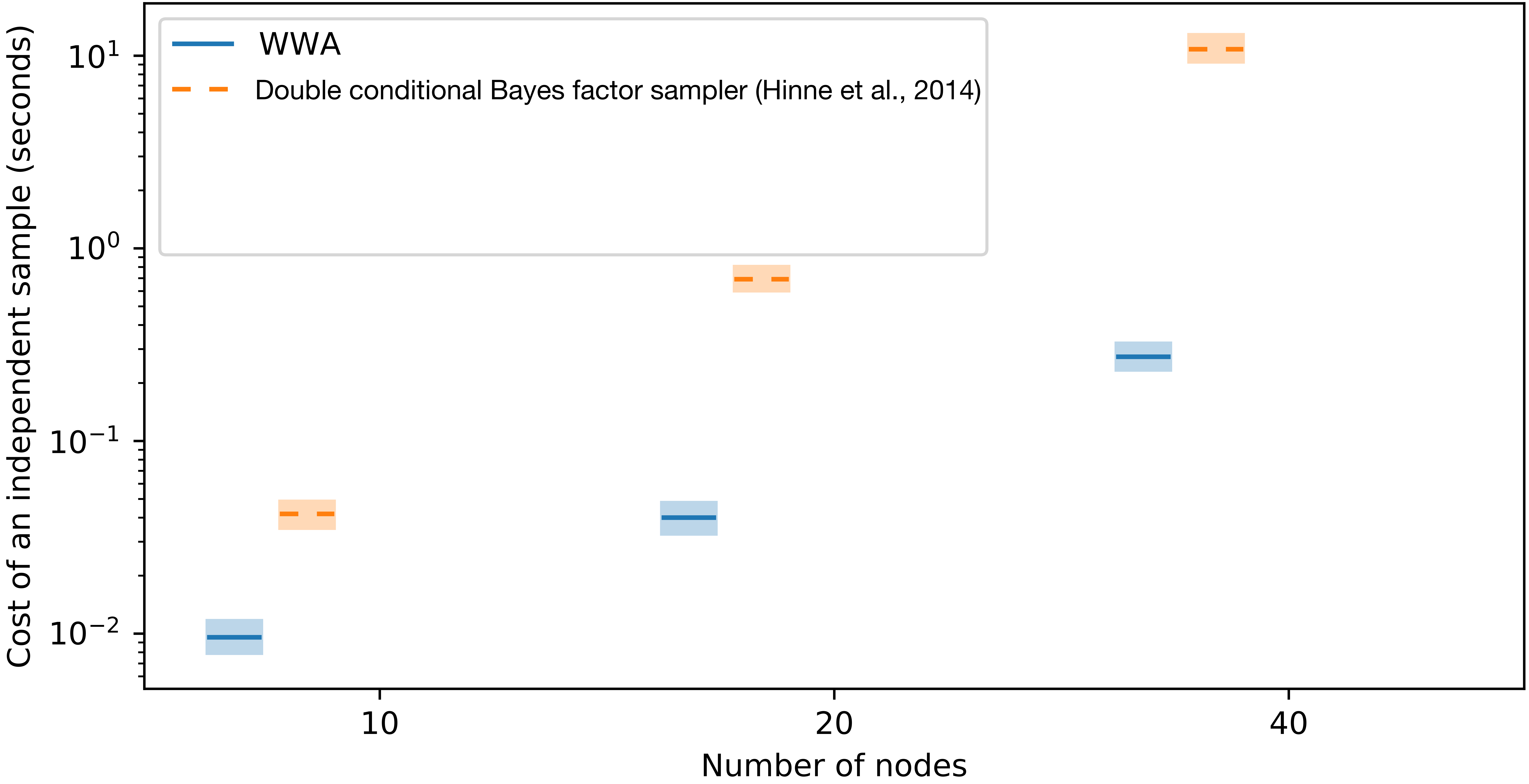
- MCMC step with $p(K, G \mid Y)$ as stationary distribution:
  - Propose $\tilde{G}$ from the informed proposal $Q(\tilde{G} \mid K, G)$.
  - Obtain $\tilde{K} \sim \mathscr{W}_{\tilde{G}}(\delta^\star, D^\star)$ by a Gibbs update and compute $Q(G \mid \tilde{K}, \tilde{G})$.
  - “Promote” $\tilde{G}$ using an approximate acceptance probability.
  - If promoted, sample $\tilde{K}^0 \mid \tilde{G} \sim \mathscr{W}_{\tilde{G}}(\delta, D)$ and set $(K, G) = (\tilde{K}, \tilde{G})$ with probability deriving from the exchange algorithm and delayed acceptance.
- Computation of $Q(\tilde{G} \mid K, G)$ is embarrassingly parallel.
- The computational bottleneck $\mathscr{W}_{\tilde{G}}(\delta, D)$ only occurs if $\tilde{G}$ is promoted.

# Empirical results

- Quantify MCMC efficiency:
  - Computational cost of a single MCMC iteration
  - MCMC mixing, e.g., effective sample size

$$\text{cost of an independent sample} = \frac{\text{number of MCMC steps}}{\text{effective sample size}} \times \text{cost per step}$$

# Data simulated from cycle graphs



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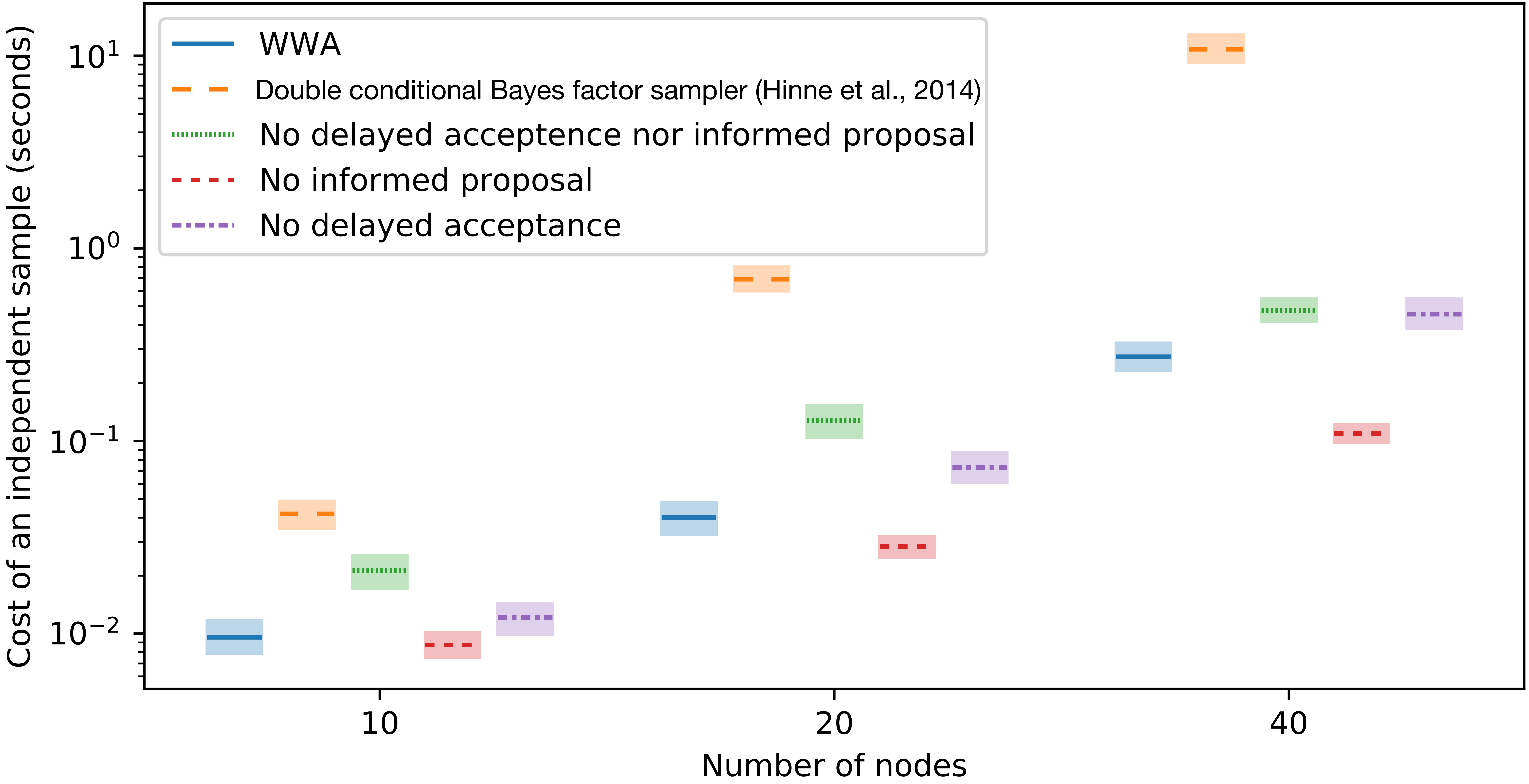
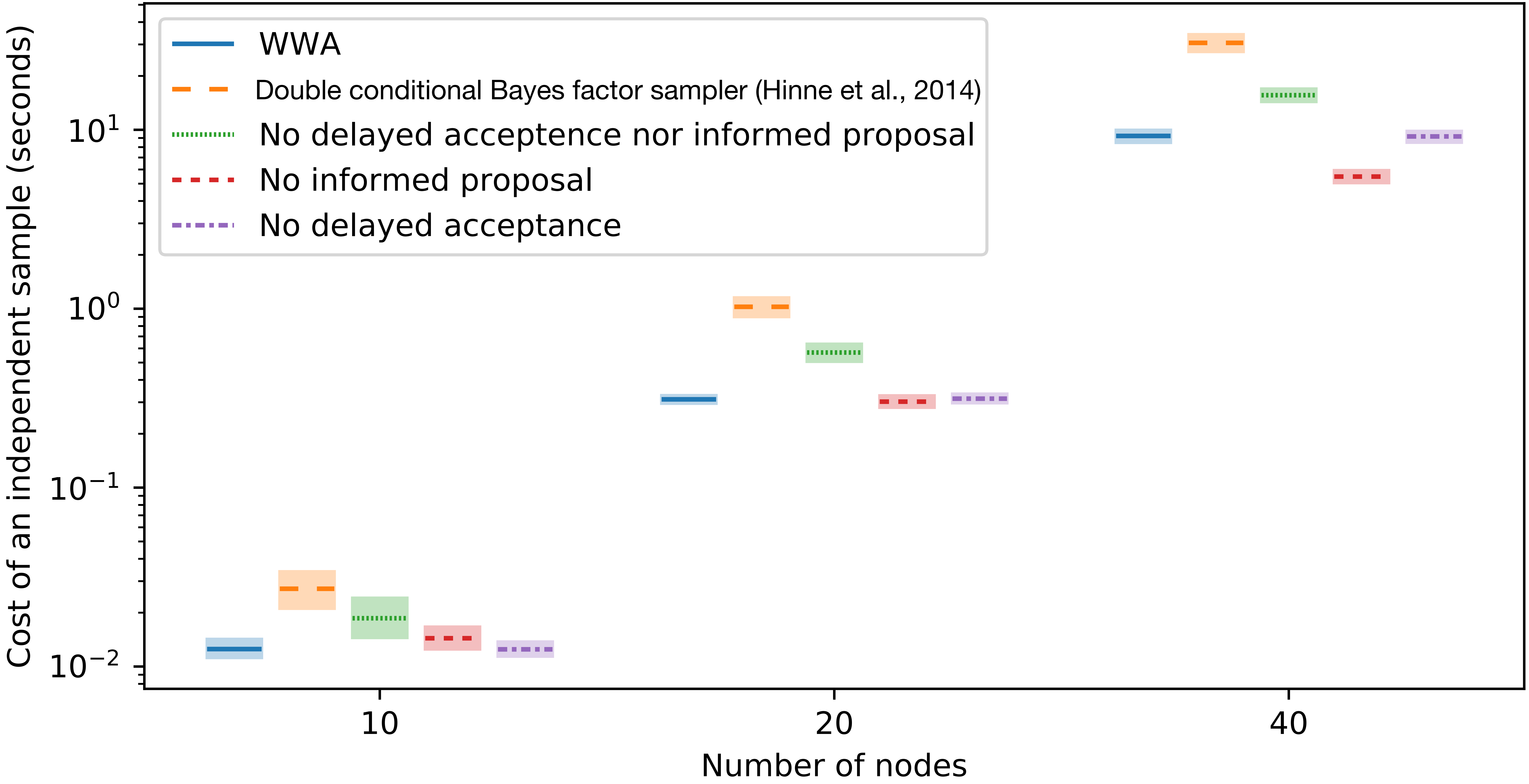


# Data simulated from uniformly sampled graphs



# Conceptual comparison of MCMC

| ***Feature*** | **(Exact) exchange algorithm** | **Gibbs update for *K*** | **Embarrassingly parallel** |
|---|---|---|---|
| *Benefit* | Stationary distribution equals the posterior | Reduced computational cost | Exploit available compute power |
| Wang and Li (2012) | ✗ | ✗ | ✗ |
| Cheng and Lenkoski (2012) | ✗ | ✓ | ✗ |
| Hinne et al. (2014) | ✓ | ✗ | ✗ |
| Mohammadi and Wit (2015) | ✓ | ✗ | ✓ |
| WWA | ✓ | ✓ | ✓ |

# Conclusion

- WWA provides a major speedup in MCMC with the $G$-Wishart prior.
  - Avoid resampling of the precision matrix via a Gibbs update
  - Informed proposal (Zanella, 2019) on the graph space
  - Reject fast and cheaply via delayed acceptance (Christen and Fox, 2005)
- Single edge update limits performance.
- WWA enables inference on the whole graph space in more scenarios:
  - Sparse seemingly unrelated regression (work in progress)
  - Learning of graph substructures (van den Boom et al., 2022)

# Related article

van den Boom, W., Beskos, A., and De Iorio, M. (2022). The G-Wishart weighted proposal algorithm: Efficient posterior computation for Gaussian graphical models. *Journal of Computational and Graphical Statistics*, advance online publication.

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