On residual and guided proposals for diffusion bridge simulation

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Abstract: Recently Whitaker et al. (2017b) considered Bayesian estimation of diffusion driven mixed effects models using data-augmentation. The missing data, diffusion bridges connecting discrete time observations, are drawn using a “residual bridge construct”. In this paper we compare this construct (which we call residual proposal) with the guided proposals introduced in Schauer et al. (2017). It is shown that both approaches are related, but use a different approximation to the intractable stochastic differential equation of the true diffusion bridge. It reveals that the computational complexity of both approaches is similar. Some examples are included to compare the ability of both proposals to capture local nonlinearities in the dynamics of the true bridge.

Keywords: Diffusion process, guided proposals, multidimensional diffusion bridge; linear process; modified diffusion bridge; residual bridge construct.

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1. Introduction

Simulation of diffusion bridges has received considerable attention over the past two decades. An important application lies in Bayesian estimation of parameters when discrete time observation are obtained from a diffusion process. The main difficulty here is the intractability of the likelihood. If instead of discrete time observations continuous time trajectories of the diffusion process were to be observed, then the problem would be simplified due to tractability of the likelihood. This has inspired many authors to adopt a data-augmentation strategy, where the latent diffusion paths in between two discrete time observations are introduced as (infinite-dimensional) latent variables (see for instance Roberts and Stramer (2001), Golightly and Wilkinson (2005), Golightly and Wilkinson
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(2008) and van der Meulen and Schauer (2017)). A non-exhaustive list of references on diffusion bridge simulation is Eraker (2001), Elerian et al. (2001), Durham and Gallant (2002), Clark (1990), Bladt et al. (2016), Beskos et al. (2008), Hairer et al. (2009), Bayer and Schoenmakers (2013), Lin et al. (2010)), Beskos et al. (2006), Dellyon and Hu (2006), Lindström (2012), Schauer et al. (2017) and Whitaker et al. (2017a). A somewhat more detailed overview is given in the introductory section of Whitaker et al. (2017a).

As direct and exact simulation of diffusion bridges in complete generality is infeasible, most approaches consist of simulating a process that resembles the true diffusion bridge (a proxy) and correcting for the discrepancy by either weighting, accept/reject methods or the Metropolis-Hastings algorithm. In the following, any stochastic process which is used as a proxy for the diffusion bridge is called a proposal.

Here we are particularly interested in the connections between the “guided proposals” and “residual proposals” introduced in Schauer et al. (2017) and Whitaker et al. (2017a) respectively (the terminology “residual proposals” being ours). This is motivated by the recent paper of Whitaker et al. (2017b) where the authors apply residual proposals for Bayesian estimation of diffusion driven mixed effects models.

They note that finding a guided proposal that is both accurate and computationally efficient may be difficult in practice (at the bottom of page 441 of their paper.) We show in fact that a variation of the residual proposals used in Whitaker et al. (2017b) can be obtained as special cases of guided proposals. Moreover, we explain that the choices to be made for constructing either residual or guided proposals are similar, as is their computational cost. For that reason we don’t see a strong argument to dismiss guided proposals. On the contrary, we present some examples where guided proposals appear to perform better than residual proposals. That is not to say that residual proposals cannot give a substantial improvement to the modified diffusion bridge of Durham and Gallant (2002) which ignores nonlinearities in the drift.

The structure of this paper is as follows. In section 2 we introduce notation and concepts used throughout. In sections 3 and 4 we recap the approaches introduced in Whitaker et al. (2017a) and Schauer et al. (2017) respectively. Moreover, in section 3 we derive the likelihood of residual proposals with respect to the true diffusion bridge without resorting to discretisation. For guided proposals we give some new insights for an efficient implementation in subsection 4.1. In section 5 we expose the relations and similarities of these two approaches and illustrate these with a couple of numerical examples.

2. Diffusion bridges

In the following we assume the dynamics of the diffusion process $X = (X_t, t \geq 0)$ are governed by the stochastic differential equation (sde)

$$dX_t = b(t, X_t) \, dt + \sigma(t, X_t) \, dW_t, \quad X_0 = u.$$
Here $b: [0, \infty) \times \mathbb{R}^d \to \mathbb{R}^d$ and $\sigma: [0, \infty) \times \mathbb{R}^d \to \mathbb{R}^{d \times d'}$ are referred to as the drift and dispersion coefficient respectively and $W$ is a $d'$-dimensional vector of uncorrelated Wiener processes. If we condition the process on hitting the point $v$ at time $T$, the conditioned process is denoted by $X^\ast$.

The process $X^\ast$ is the solution of the SDE

$$dX^\ast_t = b(t, X^\ast_t)\, dt + a(t, X^\ast_t) \nabla_x \log p(t, x, T, v) \, dt + \sigma(t, X^\ast_t) \, dW_t, \quad X^\ast_0 = u,$$

where $a(t, x) = \sigma(t, x) \sigma(t, x)'$ is diffusion coefficient, $r(t, x) = \nabla_x \log p(t, x, T, v)$ and $p$ denotes the transition densities of the diffusion $X$. Hence, the sde for the bridge process $X^\ast$ has an additional pulling term in the drift to ensure it hits $v$ at time $T$. Note that as $p$ is intractable, it is impossible to obtain diffusion bridges by discretising the sde for $X^\ast$.

However, in case $b \equiv 0$ and $\sigma$ is constant (so that $X$ is a scaled Wiener process), transition densities are tractable and the diffusion bridge has dynamics

$$dX^\ast_t = \frac{v - X^\ast_t}{T - t} \, dt + \sigma \, dW_t, \quad X^\ast_0 = u.$$

This has motivated Delyon and Hu (2006) to consider proposals $\bar{X}$ driven by the sde

$$d\bar{X}_t = \lambda b(t, \bar{X}_t) \, dt + \frac{v - \bar{X}_t}{T - t} \, dt + \sigma(t, \bar{X}_t) \, dW_t, \quad \bar{X}_0 = u,$$

where either $\lambda = 0$ or $\lambda = 1$ is chosen. Realisations of $\bar{X}$ can then be used in a Metropolis-Hastings acceptance ratio, or by importance sampling as a proxy for $X^\ast$. Key to the feasibility of this approach is the derivation of the likelihood ratio $\frac{d\mathbb{P}^\ast}{d\mathbb{P}}(\bar{X})$, where $\mathbb{P}^\ast$ and $\mathbb{P}$ denote the laws of $X^\ast$ and $\bar{X}$ on $C[0, T]$ respectively and $\bar{X} = (\bar{X}_t, t \in [0, T])$. For further details we refer to Papaspiliopoulos et al. (2013) and van der Meulen and Schauer (2017).

The choice $\lambda = 0$ appears to be most popular in the literature, especially when applied with a particular correction to Euler discretisation proposed by Durham and Gallant (2002) yielding the “modified diffusion bridge”. Clearly, this approach completely ignores the drift and can only be efficient when the drift is approximately constant on $[0, T]$. Its simplicity is however attractive as there is no tuning parameter.

3. Residual proposals

The key idea in Whitaker et al. (2017a) is to define a proposal $X^\triangle$ that does take the drift of the diffusion into account by using the decomposition

$$X^\triangle_t = x(t) + C_t,$$

where $x(t)$ is defined as the solution to

$$dx(t) = b(t, x(t)) \, dt, \quad x(0) = u$$

(3.1)
and the residual process \( C \) is given by
\[
dC_t = \frac{v - x(T) - C_t}{T - t} \, dt + \sigma(t, x(t) + C_t) \, dW_t, \quad C_0 = 0. \tag{3.2}
\]
In this approach, first the process \( x(t) \) is determined, either in closed form or by a numerical procedure. Subsequently, the sde for \( C \) is solved using Euler discretisation. It is easily seen that \( X^\triangle \) satisfies the sde
\[
dX_t^\triangle = b(t, x(t)) \, dt + \frac{v - X^\triangle_t - (x(T) - x(t))}{T - t} \, dt + \sigma(t, X^\triangle_t) \, dW_t, \quad X^\triangle_0 = u. \tag{3.3}
\]
Compared to the sde for \( X^\bullet \) given in (2.1), it appears that
1. \( b(t, X^\bullet_t) \) is approximated by \( b(t, x(t)) \),
2. the pulling term is replaced with
\[
\frac{v - X^\triangle_t}{T - t} - \frac{1}{T - t} \int_t^T b(s, x(s)) \, ds
\]
where we recognise the first term as the pulling term appearing in the proposals introduced by Delyon and Hu (2006).

Define \( \kappa(s, x) = (T - s)^{-1} (v - x) \) (considering \( T \) and \( v \) to be fixed). Denote by \( \varphi(x; \mu, a) \) the value of the normal density with mean vector \( \mu \) and covariance matrix \( a \), evaluated at \( x \). Denote the law of \( X^\triangle \) on \( C_r, 0, T \) by \( P^\triangle \). The following theorem reveals that \( P^\bullet \) is absolutely continuous with respect of \( P^\triangle \). This is crucial, as otherwise of course the process \( X^\triangle \) cannot be used as a proposal.

**Theorem 3.1.** Assume the \( C^{1,2} \)-function \( \sigma \) with values in \( \mathbb{R}^{d \times d} \) is bounded and has bounded derivatives and is invertible with a bounded inverse. Assume the function \( b \) is locally Lipschitz with respect to \( x \) and is locally bounded. Finally, assume the sde for \( X \) admits a strong solution. Then
\[
\frac{dP^\bullet}{dP^\triangle}(X^\triangle) = \frac{\varphi(v; u, a(0, u)T)}{\varphi(0, u; T, v)} \sqrt{\frac{|a(0, u)|}{|a(T, v)|}} \Psi_1(X^\triangle) \Psi_2(X^\triangle),
\]
with
\[
\Psi_1(X^\triangle) = \int_0^t b(s, X_s^\triangle) a^{-1}(s, X_s^\triangle) \, dX_s^\triangle - \frac{1}{2} \int_0^t b(s, X_s^\triangle) a^{-1}(s, X_s^\triangle) b(s, X_s^\triangle) \, ds
- \frac{1}{2} \int_0^t \kappa(s, X_s^\triangle) \circ da^{-1}(s, X_s^\triangle)(v - X_s^\triangle),
\]
where the \( \circ \)-integral is obtained as the limit of sums where the integrand is computed at the right limit of each time interval as opposed to the left limit used.
in the definition of the Itô integral; and

\[ \Psi_2(X^\triangle) = \exp \left( \frac{1}{2} \int_0^T f(s, X^\triangle_s)^2 a(s, X^\triangle_s)^{-1} f(s, X^\triangle_s) \, ds \right. \]

\[ \left. - \int_0^T f(s, X^\triangle_s)^2 a(s, X^\triangle_s)^{-1} \, dX^\triangle_s + \int_0^T f(s, X^\triangle_s)^2 a^{-1}(s, X^\triangle_s) \kappa(s, X^\triangle_s) \, ds \right) . \]

Here, \( f(s, x) = b(s, x(s)) - (T - s)^{-1}(x_T - x) \) with \( x(s) \) as defined in (3.1).

**Proof.** Absolute continuity of \( P^\ast \) with respect to \( \tilde{P} \) was proved in Delyon and Hu (2006) under the stated assumptions (which is assumption 4.2 in that paper). Here we consider the proposal with \( \lambda = 0 \) and the likelihood ratio being proportional to \( \Psi_1(X^\triangle) \). The normalising constant in the likelihood ratio was derived in Papaspiliopoulos et al. (2013). Now \( \tilde{P} \) is absolutely continuous with respect to \( P^\triangle \) with Radon-Nikodym derivative \( \frac{d\tilde{P}}{dP} \triangle \Psi_2(X^\triangle) \). The result now follows from \( \frac{dP^\ast}{dP} \triangle \frac{dP}{dP} \frac{dP}{dP^\triangle} \)(\( X^\triangle) = \Psi_2(X^\triangle) \).

The preceding theorem The unknown transition density only shows up as a multiplicative constant in the denominator and henceforth cancels in all calculations for performing MCMC for Bayesian estimation of diffusion processes with a data-augmentation strategy (Cf. van der Meulen and Schauer (2017)).

### 3.1. Improved residual proposals using the LNA

Clearly, any deterministic trajectory \((x(t), t \in [0, T])\) can be used and the definition of residual proposals is not restricted to (3.1). One particular choice proposed by Whitaker et al. (2017a) is based on the linear noise approximation (abbreviated by LNA, see for instance van Kampen (1981)). It uses the decomposition

\[ X^\triangle_t = x(t) + \rho(t) + C_t, \]

where \( x(t) \) is defined in (3.1) and \( \rho(t) = E[Y_t \mid Y_T = v] \) with

\[ dY_t = V(t, x(t))Y_t \, dt + \sigma(x(t)) \, dW_t, \quad Y_0 = u. \]

Here \( V(t, y) \) is the matrix with elements \( V(t, y)_{i,j} = \frac{\partial b_i(t, y)}{\partial y_j} \) for \( y \in \mathbb{R}^d \).

### 4. Guided proposals

The basic idea in Schauer et al. (2017) is to replace the generally intractable transition density \( p \) that appears in (2.1) by the transition density of an auxiliary diffusion process \( \tilde{X} \) with tractable transition densities. Assume \( \tilde{X} \) satisfies the sde

\[ d\tilde{X}_t = \tilde{b}(t, \tilde{X}_t) \, dt + \tilde{\sigma}(t, \tilde{X}_t) \, dW_t \]
and denote the transition densities of $\tilde{X}$ by $\tilde{\rho}$. Define the process $X^\circ$ as the solution of the sde

$$dX^\circ_t = b^\circ(t, X^\circ_t)\,dt + \sigma(t, X^\circ_t)\,dW_t, \quad X^\circ_0 = u,$$

with

$$b^\circ(t, x) = b(t, x) + a(t, x)\nabla x \log \tilde{\rho}(t, x; T, v).$$

A process $X^\circ$ constructed in this way is referred to as a **guided proposal**.

Let $\tilde{a} = \tilde{\sigma}^\circ$. It is proved in Schauer et al. (2017) that if $\tilde{a}(T) = a(T, v)$ (and a couple of other somewhat technical conditions)

$$\frac{d\mathbb{P}^*}{d\mathbb{P}^\circ}(X^\circ) = \tilde{\rho}(0, u; T, v) \exp \left( \int_0^T \mathbb{G}(s, X^\circ_s) \,ds \right),$$

where $G$ depends on $b$, $a$, $\tilde{b}$ and $\tilde{a}$, but not on $p$. Note that the unknown transition density only appears as a multiplicative constant in the dominator.

Regarding the choice of $\tilde{X}$, the class of linear processes,

$$d\tilde{X}_t = \tilde{B}(t, \tilde{X})dt + \tilde{\beta}(t)dt + \tilde{\sigma}(t)dW_t,$$

is a flexible class with known transition densities and its induced guided proposals will be referred to as **linear guided proposals**. Not surprisingly, the efficiency of guided proposals depends on the choice of $\tilde{B}$, $\tilde{\beta}$ and $\tilde{\sigma}$. A particularly simple type of linear guided proposals is obtained upon choosing $d\tilde{X}_t = \tilde{\beta}(t)dt + \sigma(T, v)dW_t$. For this choice

$$b^\circ(t, x) = b(t, x) + a(t, x)a(T, v)^{-1}v - x - \int_0^T \tilde{\beta}(s)\,ds.$$

An alternative is to use the LNA, where $b(t, X_t)$ is approximated by $b(t, x(t)) + V(t, x(t))(X_t - x(t))$. Here, $V(t, y)$ is the matrix with elements $V(t, y)_{i,j} = \partial b_i(t, y) / \partial y_j$ for $y \in \mathbb{R}^d$. This gives linear guided proposals with

$$\tilde{\beta}(t) = b(t, x(t)) - V(t, x(t))x(t) \quad \text{and} \quad \tilde{B}(t) = V(t, x(t)).$$

An easy choice for $\tilde{\sigma}$ is $\tilde{\sigma}(t) = \sigma(T, v)$.

**Remark 4.1.** Whitaker et al. (2017a) compare various proposals, among which the guided proposal with $\tilde{\beta}$ and $\tilde{B}$ as in (4.5) and $\tilde{\sigma}(t) = \sigma(t, x(t))$. However, as correctly remarked in their paper, such proposals do not satisfy the key requirement $\tilde{a}(T, v) = a(T, v)$. Therefore, the measure $\mathbb{P}^*$ will be singular with respect to the law of such proposals. As a fix to this they also considered proposals where the deterministic process is continually restarted and simulated on $[t, T]$, where $0 < t < T$. This comes naturally with a huge increase in computing time. We would rather propose to either take $\tilde{\sigma}(t) = \sigma(T, v)$ or

$$\tilde{\sigma}(t) = \begin{cases} \sigma(t, x(t)) & \text{for } t \in [0, t_0] \\ \sigma(T, v) - \sigma_0(t - t_0) + \sigma_0 & \text{for } t \in (t_0, T] \end{cases},$$
where $\sigma_0 = \sigma(t_0, x(t_0))$. The latter choice naturally raises the question on how to choose $t_0$ but for sure satisfies the requirement for absolute continuity of $P^*$ with respect to the law of the proposal.

4.1. Implementation

For guided proposals, the computational cost consists of discretising the sde (4.1) and evaluating the likelihood ratio in (4.2). For linear guided proposals, there is a convenient expression for $r$ i.e. $r(s, x) = \bar{H}(s)(v(s) - x)$, where $\bar{H}(t) = K^{-1}(t)$ with

$$K(t) = \int_t^T \Phi(t, s)\tilde{\alpha}(s)\Phi(t, s)' \, ds$$

$$v(t) = \Phi(t, T)v - \int_t^T \Phi(t, s)\tilde{\beta}(s) \, ds$$

and $d\Phi(t) = \bar{B}(t)\Phi(t) \, dt$, $\Phi(0) = I$.

We propose computing $K$ and $v$ recursively backwards using the differential equations

$$\frac{d}{dt} K(t) = \bar{B}(t)K(t) + K(t)\bar{B}(t)' - \tilde{\alpha}(t), \quad K(T) = 0 \quad (4.6)$$

and

$$\frac{d}{dt} v(t) = \bar{B}(t)v(t) + \tilde{\beta}(t), \quad v(T) = v.$$ 

These equations can be discretised using for example an explicit backwards Runge-Kutta scheme. Next, $\bar{r}(s, x)$ can be obtained from solving $K(s)\tilde{r}(s, x) = v(s) - x$ for which the Cholesky decomposition can be used.

In case $\bar{B}$ and $\tilde{\alpha}$ are not time-dependent (that is, constant), then $K$ (and of course $v$) can also be computed in closed form. Let $\Lambda$ be the solution to the continuous Lyapunov equation

$$\bar{B}\Lambda + \Lambda\bar{B}' + \tilde{\alpha} = 0.$$ 

Then, as verified by direct computation

$$K(t) = e^{-(T-t)}\bar{B}\Lambda e^{-(T-t)}\bar{B}' - \Lambda$$

and, with $\mu$ solving $\bar{B}\mu + \beta = 0$,

$$v(t) = e^{-(T-t)}\bar{B}(v - \mu) + \mu,$$

LAPACK includes the function trsyl to solve the continuous Lyapunov equation in an efficient manner, and correspondingly many high level computing environments provide this functionality. Nevertheless, computing $K$ from the closed form expression is computationally more demanding than discretising (4.6), at the cost of allowing for discretisation error. However, when using a 3rd order Runge-Kutta scheme (say), this error is small compared to the discretisation error induced by the Euler-Maruyama scheme for $X^\circ$. 
5. Connections

The idea of using \( x(t) \), the solution of the dynamical system given in (3.1), can also be used with linear guided proposals. Indeed, in section 4.4 of van der Meulen and Schauer (2017) it was proposed to take guided proposals with

\[
\beta(t) = b(x(t)), \quad \hat{B} = 0 \quad \text{and} \quad \hat{\sigma} = \sigma(T, v). \tag{5.1}
\]

It follows immediately from (4.4) that the resulting guided proposal satisfies the sde

\[
dX_t^\circ = b(t, X_t^\circ) \, dt + a(t, X_t^\circ) a(T, v)^{-1} v - x(T) - x(t) \frac{dt}{T - t} + \sigma(t, X_t^\circ) \, dW_t, \quad X_0^\circ = u.
\]

This is to be compared to the sde for the residual proposal given in (3.3). From this we infer the following:

- The computational effort for computing either guided or residual proposals is of the same order. The inverse of \( a(T, v) \) needs to be computed only once and besides that the only extra calculation required by guided proposals is premultiplication by \( a(t, X_t^\circ) \).
- If \( \sigma \) is constant and the residual process defined in (3.2) is redefined to satisfy the sde

\[
dC_t = (b(t, x(t) + C_t) - b(t, x(t))) \, dt + \frac{v - x(T) - C_t}{T - t} \, dt + \sigma(t, x(t) + C_t) \, dW_t, \quad C_0 = 0,
\]

then these adjusted residual proposals are in fact linear guided proposals with \( \beta, \hat{B} \) and \( \hat{\sigma} \) specified in (5.1). Note that the difference with the definition of residual proposals is the addition of the first term on the right-hand-side in the preceding display.
- If the residual process defined in (3.2) is redefined to satisfy the sde

\[
dC_t = (b(t, x(t) + C_t) - b(t, x(t))) \, dt + a(t, x(t) + C_t) a(T, v)^{-1} v - x(T) - C_t \frac{dt}{T - t} + \sigma(t, x(t) + C_t) \, dW_t, \quad C_0 = 0,
\]

then these adjusted residual proposals are simply linear guided proposals with \( \beta, \hat{B} \) and \( \hat{\sigma} \) specified in (5.1) (also when \( \sigma \) is nonconstant).

We conclude with a couple of examples in which we investigate the behaviour of guided and residual proposals.
Example 5.1. Suppose $\sigma$ is constant and $b(t,x) = -\alpha x$. Suppose we condition the process to hit 1 at time $T$, when $X_0 = 0$. The dynamical system’s solution is given by $x(t) = u e^{-\alpha t}$ and the sde for the (true) bridge can be computed in closed form

$$dX^*_t = -\alpha X^*_t \, dt + 2\alpha e^{\alpha(T-t)} \frac{v - X^*_t}{e^{2\alpha(T-t)} - 1} \, dt + \sigma \, dW_t, \quad X_0 = u.$$ 

We took $u = 0.1$, $v = 1$, $T = 3$, $\sigma = 0.1$, $\alpha = 2$ and simulated a realisation of both the guided and residual proposal using the same Wiener increments (Euler discretisation with time step $10^{-4}$ was used). We then repeated this 4 more times and also simulated 5 realisations of true bridges; the result is in figure 1. Clearly, both proposals deviate from true bridges, though the guided proposals resemble true bridges better than residual proposals.

Example 5.2. Assume again that $\sigma$ is constant, $X_0 = 0$ and $b(t,x) = -\sin(2\pi x)$. In this case $x(t) \equiv 0$ and then residual proposals have dynamics

$$dX^\triangle_t = \frac{v - X_t^\triangle}{T - t} \, dt + \sigma \, dW_t, \quad X_0^\triangle = 0$$

whereas guided proposals with (5.1) take the form

$$dX_t^\circ = b(t,X_t^\circ) \, dt + \frac{v - X_t^\circ}{T - t} \, dt + \sigma \, dW_t, \quad X_0^\circ = 0.$$
Both of these proposals have been proposed earlier by Delyon and Hu (2006). As the drift has multiple wells and the process starts in one of those, residual proposals will completely miss the nonlinear dynamics of the true bridge. The guided proposals in this example may do slightly better in resembling true bridges, but will in most cases also perform unsatisfactory. Nevertheless, the class of guided proposals is way more flexible and not restricted to the choice in (5.1). For a very similar drift as considered in this example, this was illustrated in section 1.3 of Schauer et al. (2017).

Example 5.3. Suppose \( b(x) = -\frac{1}{2}x - \sin(2\pi x) \), \( \sigma = 0.15 \), \( u = 5 \), \( v = 2 \) and \( T = 5 \). In this case the solution of the (deterministic) dynamical system is not available in closed form. However, it can easily be obtained using the 4-th order Runge-Kutta scheme. In the top left panel of figure 2 the obtained solution is displayed. Note that \( b(x) = 0 \) for \( x \approx 1.9 \) which is close to \( v \). Hence bridges follow approximately the solution of the dynamical system, which makes proposals based on this solution suitable. In this case we can also simulate true bridges using the method by Bladt and Sørensen (2014) which is implemented in the \texttt{sde}-library in \texttt{R}. In figure 2, 25 realisations of the bridges and both proposals are shown (Euler discretisation with time step \( 10^{-4} \) was used). In this case it is guided proposals appear to perform somewhat better than residual proposals.
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