Estimating Stochastic Shortest Paths

Michael W. Ramsey

Abstract

We consider a stochastic version of the shortest path problem where edge weights have a known distribution and we derive efficient methods for computing the induced shortest path distribution. Stochastic edge weights often arise whenever weights result from a noisy measurement or collection process. To model this case we introduce noise to the edge weights of a standard weigthed graph. This produces a stochastic graph with simple edge and path length distributions. Using these distributions we present a new algorithm called Approximate Stochastic Paths (Asp) [1]. Preliminiary tests using the NetworkX Python library [2] suggest that Asp is faster and more accurate than the popular Monte Carlo simulation-based approach [3].

1 Introduction

In applied problems, graph traversal costs often result from noisy measurement or collection processes, or result from an inherently stochastic cost. For example, a traveler on her daily commute may experiences different travel costs due to varying taffic levels, weather conditions, or incident levels such as work zones, accidents, and vehicle breakdowns. In this case, a road network model with stochastic edge weights provides a more realistic representation of a road network than a deterministic one.

This paper focuses solely on deriving and computing the distribution of shortest paths for the graph. We assume that some modeling or data generation process has already occured and produced this graph with independent edge weights. These edge weights should therefore be interpreted in the most general sense. For example, edge weights might result from a machine learning process that incorporates a variety of factors.

This paper is organized as follows. Section 2 establishes prequisite definitions and results to formally define our problem. Next, in section 3 we present two methods for solving the problem. Section 4 discusses approximation methods for non-negative weights. Section 5 presents the Asp algorithm and provides test results. Section 6 discusses miscellaneous items.

2 Problem Definition

Consider a weighted graph G defined by triple $G = (V, E, C)$ where $V = 1, 2, ..., n$ is a set of nodes, E is the edges subset of $V \times V$, and C is the $n \times n$ matrix of edge weights or costs $c_{(i,j)} \in \mathbb{R}$. We discuss the non-negative case in the next section. Denote edges as $(i, j) \in E$ for $i, j \in V$.

2.1 Stochastic Graphs

We define the stochastic weighted graph induced by G as $G^* = (V, E, C^*)$ where C^* is the $n \times n$ matrix of edge cost random variables defined by:

$$C^*_{(i,j)} = X_{(i,j)} c_{(i,j)} + c_{(i,j)} \tag{1}$$

where $c_{(i,j)} \in C$ and $X_{(i,j)} \sim N(0, \sigma^2)$ i.i.d. Thus we perturb the edge weights by a multiple of the original edge weight. The variance σ^2 of the Gaussian noise parameterizes the magnitude.

Note that by linearity of expected value and a basic property of variance we immediately obtain the distribution for edge costs:

$$C^*_{(i,j)} \sim N(c_{(i,j)}, c^2_{(i,j)} \sigma^2). \tag{2}$$

2.2 Path Distributions

Next we define a path $\pi_{i,j}$ as an ordered sequence of nodes $(v_k)_{k=1}^m$ with $v_1 = i$ and $v_m = j$ as source and destination nodes respectively and $(v_k, v_{k+1}) \in E, \forall k$. A path is called simple if $v_k \neq v_l, \forall k, l$. That is, there are no loops or cycles in the path.

Let $i, j \in V$ and $\Pi_{i,j} = \{\pi_{i,j} \mid \pi_{i,j} \text{ is simple}\}$. Then, for $\pi \in \Pi_{i,j}$ we define a path π's length or total cost random variable:

$$Z_\pi = \sum_{v_k \in \pi} C^*_{(v_k, v_{k+1})}. \tag{3}$$

Again, by linearity of expectation and by the same basic property of variance used above we can derive the

mean and variance for π's length distribution:

$$\begin{aligned}\mathbb{E}(Z_\pi) &= \hat{Z}_\pi \\ &= \sum_{v_k \in \pi} \mathbb{E}(C^*_{(v_k, v_{k+1})}) \\ &= \sum_{v_k \in \pi} c_{(v_k, v_{k+1})} \\ \mathrm{Var}(Z_\pi) &= \sum_{v_k \in \pi} \mathrm{Var}(C^*_{(v_k, v_{k+1})}) \\ &= \sum_{v_k \in \pi} c^2_{(v_k, v_{k+1})} \sigma^2.\end{aligned}$$

Therefore, since the sum of normal random variables is again a normal random variable, π's length distribution:

$$Z_\pi \sim N(\sum_{v_k \in \pi} c_{(v_k, v_{k+1})}, \sum_{v_k \in \pi} c^2_{(v_k, v_{k+1})} \sigma^2). \quad (4)$$

2.3 Stochastic Shortest Path

Now that we have each path's length distribution, we can define the stochastic shortest path and the expected shortest path random variables:

$$\pi^*_{i,j} = \min_{\pi \in \Pi_{i,j}} Z_\pi \quad (5)$$

$$\hat{\pi}^*_{i,j} = \min_{\pi \in \Pi_{i,j}} \hat{Z}_\pi. \quad (6)$$

Note that $\hat{\pi}^*_{i,j}$ can be computed directly from Dykstra's Algorithm (see [4]) and that $\hat{\pi}^*_{i,j}$ is the mode of $\pi^*_{i,j}$.

We can now give our problem definition:

> Given any weighted graph G and $i, j \in V$, find $p^*(\pi_{i,j}) := P(\pi_{i,j} = \pi^*_{i,j}), \forall \pi \in \Pi_{i,j}$.

Solving this provides the probability that $\pi_{i,j}$ is the shortest path between nodes i, j for a random draw of edge weights from G^* for any path $\pi_{i,j}$.

3 Stochastic Path Distribution

We present two approaches to computing the stochastic shortest path distribution p^*. The first solves for the distribution directly and requires numeric integration. The second estimates the distribution by sampling and calculating frequencies. The former tends to be more accurate, the latter faster.

3.1 Analytic Solution

Given any weighted graph G, let $\pi \in \Pi_{i,j}$ for some $i, j \in V$ and $\Gamma_\pi = \Pi_{i,j} - \{\pi\}$. We can recast $P(\pi = \pi^*)$ as $P(Z_\pi < Y)$ where $Y = \min_{\gamma \in \Gamma_\pi} Z_\gamma$. By conditioning on $Z_\pi = s$ for some $s \in \mathbb{R}$ we obtain:

$$\begin{aligned}P(Z_\pi = s, Z_\pi < Y) &= P(Z_\pi = s) P(Y > s \mid Z_\pi = s) \\ &= P(Z_\pi = s) \prod_{\gamma \in \Gamma_\pi} P(Z_\gamma > s) \\ &= P(Z_\pi = s) \prod_{\gamma \in \Gamma_\pi} (1 - P(Z_\gamma \leq s)) \\ &= f_{Z_\pi}(s) \prod_{\gamma \in \Gamma_\pi} (1 - F(Z_\gamma(s))) \\ &= f_{Z_\pi}(s) \prod_{\gamma \in \Gamma_\pi} SF(Z_\gamma(s)) \quad (7)\end{aligned}$$

where f is the density for Z_π and F and SF are the cumulative distribution function and the survival function for Z_γ. Again, we limit our scope in this paper to the case where all the stochastic costs are independent. As a reminder, Z_π and Z_γ are distributed according to (4).

To determine $P(Z_\pi < Y)$ we simply need to integrate (8) over s:

$$\begin{aligned}P(Z_\pi < Y) &= \int_{-\infty}^{\infty} P(Z_\pi = s, Z_\pi < Y) ds \\ &= \int_{-\infty}^{\infty} f_{Z_\pi}(s) \prod_{\gamma \in \Gamma_\pi} SF(Z_\gamma(s)) ds \quad (8)\end{aligned}$$

Therefore, given any simple path between any two nodes in a graph with noisy edge weights, (8) gives the probability it is the shortest path.

3.2 Random Sample Solution

Alternatively, by sampling each Z_π directly using (4), we can calculate the frequency that $Z_\pi \leq \min_{\gamma \in \Gamma_\pi} Z_\gamma$ and use this to estimate $p^*(\pi_{i,j})$, $\forall \pi \in \Pi_{i,j}$.

Let z_π be a random draw from Z_π and $z_{\pi,k}$ be the kth random draw from Z_π, out of $N \in \mathbb{N}$ many. Then $(z_{\pi,k})_{\pi \in \Pi_{i,j}}$ is a random draw from all the Z_π, that is, a draw from $(Z_\pi)_{\pi \in \Pi_{i,j}}$. Define $m_k = \min_{\gamma \in \Gamma_\pi} z_{\gamma,k}$. Then the relative frequency that $Z_\pi \leq \min_{\gamma \in \Gamma_\pi} Z_\gamma$ is computed as:

$$\omega_N(\pi = \pi^*) = \frac{\sum_{k=1}^N \mathbf{1}_{\mathbb{R}^+}(m_k - z_{\pi,k})}{N} \quad (9)$$

where $\mathbf{1}_{\mathbb{R}^+} \colon X \to \{0, 1\}$ is the indicator function defined by:

$$\mathbf{1}_{\mathbb{R}^+}(x) := \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{if } x \leq 0. \end{cases}$$

Therefore, by the Law of Large Numbers, as $N \to \infty$:

$$\omega_N(\pi = \pi^*) \longrightarrow P(\pi = \pi^*) \tag{10}$$

where $P(\pi = \pi^*) := \mathbb{E}(1_{\mathbb{R}^+}(m_k - z_{\pi,k}))$.

4 Non-Negative Weights

Often, in applied settings, negative edge weights do not have a meaningful interpretation. Consider time or distance costs. In this case we apply the truncated normal distribution. However, to reproduce our results above we need to know the effect of scaling, shifting, and summing truncated normal random variables.

4.1 Truncated Normal Distribution

The Truncated Normal Distribution [5] is defined in two steps: (1) select parameters μ and σ^2 for a parent normal random variable $\phi \sim N(\mu, \sigma^2)$ with CDF Φ and (2) select a truncation range (a, b). The truncated normal PDF $\psi(\mu, \sigma^2, a, b; x)$ is defined as:

$$\psi(\mu, \sigma, a, b; x) = \frac{\frac{1}{\sigma}\phi(\frac{x-\mu}{\sigma})}{\Phi(\frac{b-\mu}{\sigma}) - \Phi(\frac{a-\mu}{\sigma})}$$

for $a \leq x \leq b$ and 0 elsewhere. If X has PDF $\psi(x; \mu, \sigma^2, a, b)$ we say $X \sim TN(\mu, \sigma^2)$ over (a, b).

Note that the parameters μ and σ^2 are the mean and variance of the parent normal distribution, not of the truncated normal PDF itself. These are more complicated. Let $X \sim TN(\mu, \sigma^2)$ over (a, b), $\alpha = (a - \mu)/\sigma$, and $\beta = (b - \mu)/\sigma$. Then:

$$\mathbb{E}(X) = \mu - \sigma\Delta_0$$
$$\mathrm{Var}(X) = \sigma^2\left[1 - \Delta_1 - \Delta_0^2\right]$$

where $\Delta_k = \frac{\beta^k\phi(\beta) - \alpha^k\phi(\alpha)}{\Phi(\beta) - \Phi(\alpha)}$.

By integrating ϕ appropriately, the truncated normal CDF:

$$\Psi(\mu, \sigma, a, b; x) = \begin{cases} 0 & \text{if } x \leq a, \\ \frac{\Phi(\frac{x-\mu}{\sigma}) - \Phi(\frac{a-\mu}{\sigma})}{\Phi(\frac{b-\mu}{\sigma}) - \Phi(\frac{a-\mu}{\sigma})} & \text{if } a < x < b, \\ 1 & \text{if } x \geq b. \end{cases}$$

4.2 Transformations

Suppose $X \sim TN(\mu, \sigma^2)$ over (a, b) and $c, d \in \mathbb{R}$. If $Y = cX + d$ then analogously to the Normal distribution:

$$Y \sim TN(c\mu + d, d^2\sigma^2) \tag{11}$$
$$\text{over } (ca + d, cb + d).$$

In general, summing truncated normal random variables does not necessarily produce another truncated normal random variable. Fortunately though, the sum of truncated normal variables can be approximated by a truncated normal in the case where the summands are truncated symmetrically about their means (see [5] again).

Let $X_k \sim TN(\mu_k, \sigma_k^2)$ over (a_k, b_k) for $k = 1, 2, \ldots n$ such that $\frac{b_k + a_k}{2} = \mu_k$. Then we can approximate the distribution of $Y = \sum_{k=1}^n X_k$ by

$$Y \approx TN(\sum_{k=1}^n \mu_k, \sum_{k=1}^n \sigma_k^2) \tag{12}$$
$$\text{over } (\sum_{k=1}^n a_k, \sum_{k=1}^n b_k).$$

4.3 Stochastic Path Distribution

We can use (11) and (12) to retrace the steps in Section 2 for the truncated normal distribution.

Define the truncated stochastic weighted graph induced by G as $G^*_{a,b} = (V, E, C^*)$ where C^* is the $n \times n$ matrix of edge cost distributions defined by:

$$C^*_{(i,j)} = X_{(i,j)}c_{(i,j)} + c_{(i,j)} \tag{13}$$

where $c_{(i,j)} \in C$ and $X_{(i,j)} \sim TN(0, \sigma^2)$ over $(-1, 1)$ i.i.d. Thus we perturb the edge weights by a percent of the original edge weight, but since $-1 \leq X_{(i,j)} \leq 1$, then $C^*_{(i,j)} \geq 0$.

Applying (11) to (13) we immediatly obtain:

$$C^*_{(i,j)} \sim TN(c_{(i,j)}, c^2_{(i,j)}\sigma^2)$$
$$\text{over } (0, 2c_{(i,j)}).$$

Following our steps in Section 2, Let $\Pi_{i,j}$ and Z_π be defined as before. Next we can apply (13) to Z_π to get:

$$Z_\pi \approx TN(\sum_{v_k \in \pi} c_{(v_k, v_{k+1})}, \sum_{v_k \in \pi} c^2_{(v_k, v_{k+1})}\sigma^2) \tag{14}$$
$$\text{over } (0, \sum_{v_k \in \pi} 2c_{(v_k, v_{k+1})}).$$

The results of Section 3 then follow analogously substituting (14) for (4).

4.4 Contribution

In addition to generating the performance improvements provided by Asp, detailed in the next section, the above results provide several benefits.

- Numerically solving the integral in (8) provides an accurate, well studied benchmark for validating code and algorithms.

- Detailing path distributions, as in (4), allows for more sophisticated modeling of path selection decision making. For example, depending on the utility function under consideration, path selection can use (4) to pick the path with the least risk (variance) rather than lowest expected cost.

5 Computing Distributions

Next, we detail a new algorithm, called Approximate Stochastic Paths (Asp) [1], that combines the above results with a standard k-shortest paths algorithm. Preliminiary tests using the NetworkX Python library suggest that Asp is faster and more accurate than the common simulation-based approach (see [3]). We present the results of our test below.

5.1 The Asp Algorithm

Asp estimates $p^*(\pi_{i,j})$ for any nodes i, j in a weighted graph G in two main steps. The first step, denoted SHORT, uses the top k shortest paths (kSP) between nodes i, j using NetworkX's version of Yen's algorithm (see [2], [6]) on the deterministic edge weights $c_{(v_k,v_{k+1})}$, $v_k \in \pi$, from G. The second step, denoted FREQ, estimates $\omega_N(\pi = \pi^*)$ using equation (9). Aspvcan automatically estimats k using a user provided tolerance.

Yen's algorithm computes the k shortest simple paths for a graph with non-negative edge cost. The algorithm employs any shortest path algorithm to find the best path, then proceeds to find $k-1$ deviations of the best path. The NetworkX implementation uses a bi-directional Dijkstra's algorithm and returns a Python generator allowing iterative queries for the next shortest path.

Asp uses the Python generator's efficiency to retrieve shortest paths in batches of size k and stops when the probability that the last path retrieved would ever be shorter than the first retrieved, is below a user provided threshold *tol*. More formally, the stopping condition is $P(Z_\pi < Z_\gamma) < tol$ where γ and π are the first and last path retrieved respectively. This works because $P(Z_\pi < Z_\gamma)$ is an upper bound on $P(Z_\pi < Y)$ where $Y = \min_{\gamma \in \Gamma_\pi} Z_\gamma$ and it is likely to be a good upper bound, because Z_γ has the lowest expected length.

Algorithm: Asp - Truncated Normal Version
Data: $G = (V, E, C)$, i, j, σ, k, *tol*.
Result: $\{(\omega_N(\pi = \pi^*), (v_k, v_{k+1})) \mid v_k \in \pi \subset \Pi_{i,j}\}$.

begin
  $g = \text{kSP}(G, i, j)$
  SHORT(G, g, k, *tol*, σ)
    $\Pi = \emptyset$
    begin
      $p = 1$
      while $p >$ *tol* **do**
        $\Pi = \Pi \cup g(k)$
        $\gamma = \text{First}(\Pi)$
        $\pi = \text{Last}(\Pi)$
        $\bar{\mu} = \sum_\pi c_{(v_k,v_{k+1})} - \sum_\gamma c_{(v_k,v_{k+1})}$
        $\bar{\sigma}^2 = \sum_\pi c^2_{(v_k,v_{k+1})}\sigma^2 + \sum_\gamma c^2_{(v_k,v_{k+1})}\sigma^2$
        $Z_\gamma - Z_\pi = TN(\bar{\mu}, \bar{\sigma}^2)$
        $p = SF_{Z_\gamma - Z_\pi}(0)$
    return Π
  FREQ(G, Π, σ, N)
    begin
      $\Omega = \emptyset$
      for $\pi \in \Pi$ **do**
        $\bar{\mu}_\pi = \sum_\pi c_{(v_k,v_{k+1})}$
        $\bar{\sigma}^2_\pi = \sum_\pi c^2_{(v_k,v_{k+1})}\sigma^2$
        $Z_\pi = TN(\bar{\mu}, \bar{\sigma}^2)$
      for $\pi \in \Pi$ **do**
        $((z_{\pi,k})_{\pi\in\Pi}) = \text{DRAW}(N, (Z_\pi)_{\pi\in\Pi})$
        $\Gamma_\pi = \Pi - \{\pi\}$
        $m_k = \min_{\gamma\in\Gamma_\pi} z_{\gamma,k}$.
        $\omega_\pi = \frac{\sum_{k=1}^N \mathbf{1}_{\mathbb{R}^+}(m_k - z_{\pi,k})}{N}$
        $\Omega = \Omega \cup (\omega_\pi)$
      return Ω
  return FREQ(G, SHORT(g, k, *tol*, σ), σ, N)

This bound can be computed quickly as:

$$\begin{aligned} P(Z_\pi < Z_\gamma) &= P(Z_\pi - Z_\gamma < 0) \\ &= 1 - P(Z_\gamma - Z_\pi \leq 0) \\ &= 1 - CDF_{Z_\gamma - Z_\pi}(0) \\ &= SF_{Z_\gamma - Z_\pi}(0) \end{aligned}$$

where

$$Z_\gamma - Z_\pi \approx TN(\mu_\gamma - \mu_\pi, \sigma_\gamma^2 + \sigma_\pi^2)$$
$$\text{over } (-2\mu_k, 2\mu_k).$$

5.2 Simulating p^*

The popularity of estimating p^* via simulation comes from its relative simplicity: for some number of iterations $i = 1 \ldots n$, the algorithm computes f_N by running Dykstra's algorithm on G_i^*, where G_i^* is newly generated from G in each iteration.

5.3 Experimental Results

As a preliminary test of Asp, we compare its performace to Monte Carlo simulation on a series of small synthetic graphs where we control the number and length of paths between two points. Each test graph consists of a set number m of disjoint paths with random length and weights drawn uniformly from $(10, 15)$ and $(0, 10)$ respectively. For this study, we used $m = 2 \ldots 10$.

To evaluate Asp's accuracy in the absence of groundtruth, we exploit the fact that the simulation estimate of p^* should improve as the number of iterations increases. If Asp is more accurate than the simulation estimates, then as we increase the number of iterations, the simulation estimate should approach Asp's estimate. Therefore, this experiment records the difference between Asp's estimates and the simulated estimates, along with their respective computation times.

In this experiment we performed three trials and averaged the results for each test graph. Each trial consisted of running Asp and the simulation algorithm on each test graph. We ran the simuation for each of 10^2, 10^3, and 10^4 iterations. For each trial we recorded the average difference between Asp's estimates and the simulated estimates, along with their respective computation times. We also set $\sigma = .2$ because simulation took too many iterations and too much time to achieve reasonable probability estimates.

The experimental results, shown in Figure 1 and Figure 2, indicate that Asp is both faster and its estimate is more accurate than the simulations. As the number of simulation runs increases, the simulation estimate deviates proportionatly less from the Asp estimate. Given that the similation estimate should be getting better as the iteration runs increase, we conclude Asp is more accurate. Spot checking the results and one-off comparisons to numerical integration estimates based on (8) also supports this conclusion. Further, the computation times of Asp remains relatively constant as the number of paths increases, whereas simulation times increase significantly.

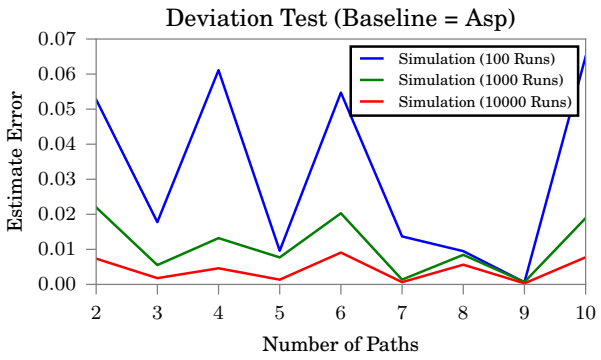

Figure 1: Deviation of simulation estimates from Asp's estimate for each of 10^2, 10^3, and 10^4 iterations.

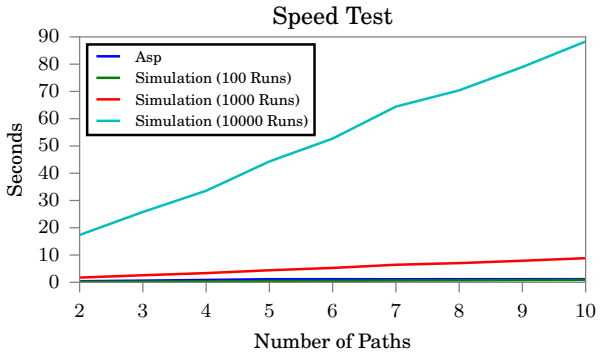

Figure 2: Computing times of Asp and simulation estimates for each of 10^2, 10^3, and 10^4 iterations.

6 Discussion

6.1 Caveats

It is important to stress the limitations of this experiement and note that futher research is required. Experimental results could vary depending on σ, Asp paramenter choices, software implementations, or graph properties. We did run one variation of the study

using kSP as input into the simulation to help prune the computation, but found little performance improvement.

6.2 Edge Traversal Probability

Extending estimates for p^* to edge traversal probabilities arises naturally in the simulation algorithm since edge traversal counts can be easily obtained from path traversals. Such accounting does not come easily with Asp. However, the probability of an edge being traversed can be computed from the probabilities of the paths containing it.

For example, suppose there is a distribution over the nodes giving the probability $P((i,j) = (s,e))$ each pair of nodes would be selected as endpoints (s,e). Then, given any edge (u,v), the probability (u,v) is traversed could be defined as:

$$P((u,v) \text{ traversed }) = \sum_{(u,v)\in\pi_{i,j}} p^*_{\pi_{i,j}} P((i,j) = (s,e))$$

6.3 Other Distributions

Reproducing our resutls only requires knowing the effect of scaling, shifting, and summing a random variable for any distribution. Therefore, both our derivations and Asp should be extendable to a wide range of edge cost noise models.

6.4 Other Decision Models

This paper focuses on the the global shortest path using a single decision criteria - edge weights. There are many situations where path selection is based on local information, only the next path, or multiple criteria, such as total edge cost and the number to nodes traversed. Possible extentions include investigating multiobjective models and short-sighted decision making (see [7], [8]).

7 Conclusion

We considered a special case of the Stochastic Shortest Path problem in which edge costs have a known distribution and we derive the induced shortest path distribution. We induced a stochastic weighted graph from a standard weighted graph by introducing white noise to the edge weights. Using this graph we derived computational methods for the stochastic shortest paths distribution p^* and presented a new algorithm based on these methods, called Approximate Stochastic Paths (Asp).

Our experimental results indicate that Asp is both faster and its estimate is more accurate than the more common Monte Carlo simulation approach. As the number of simulation runs increases, the simulation estimate deviates proportionatly less from the Asp estimate. Given that the simulation estimate should be getting better as the iteration runs increase, we conclude Asp is more accurate. Spot checking the results and one-off comparisons to numerical integration estimates based on (9) also supports this conclusion. Further, the computation times of Asp remains relatively constant as the number of paths increases, whereas simulation times increase significantly.

In addition to generating these performance improvements, our results provide several benefits. First, Numerically solving the integral in (9) provides a accurate, well studied benchmark for validating code and algorithms. Second, detailing path distributions, as in (5), allows for more sophisticated modeling of path selection decision making. For example, depending on the utility function under consideration, path selection can use (5) to pick the path with the least risk (or variance) rather than lowest expected cost.

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