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Yu Nie 1
H. Michael Zhang 1
Will Recker 2

1 Department of Civil and Environmental Engineering
University of California, Davis

2 Department of Civil and Environmental Engineering and Institute of Transportation Studies, University of California, Irvine
wrecker@uci.edu

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Institute of Transportation Studies
University of California, Irvine
Irvine, CA 92697-3600, U.S.A.
http://www.its.uci.edu
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Yu Nie
Graduate Student Researcher
Department of Civil and Environmental Engineering
University of California, Davis
CA 95616, U.S.A.
Tel: 530-754-6429
Email: ynie@ucdavis.edu

H. Michael Zhang
Associate Professor
Department of Civil and Environmental Engineering
University of California, Davis
CA 95616, U.S.A.

Will W. Recker
Professor
Department of Civil and Environmental Engineering
University of California, Irvine
CA 92697, U.S.A.

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ABSTRACT

Recently, path flow estimator (PFE) has been used for the estimation of origin-destination (O-D) matrices. This paper develops a formulation that incorporates the decoupled path flow estimator in a generalized least squares (GLS) framework. The approach seeks to solve a GLS problem that minimizes the sum of errors in traffic counts and O-D matrices based on equilibrium assignment mapping, which is derived from a K-shortest path ranking procedure exogenously. Solving the GLS-PFE model inevitably involves non-invertible linear systems and nonnegative constraints. A solution algorithm is thus designed to iteratively identify active constraints and solve linear systems by computing the pseudo-inverse. A simplified version of this algorithm is further developed to improve its computational efficiency. The solution properties and computational efficiency of the two methods are tested and compared with small to mid-size networks. It is concluded that the simplified algorithm is efficient in solving the large-scale decoupled GLS-PFE model for O-D estimation.
INTRODUCTION

One of the essential elements of transportation planning and/or operations is to "allocate" travelers onto a transportation network according to either a static or dynamic assignment mapping. A fundamental input to traffic assignment is the origin-destination (O-D) matrix that depicts traffic demands between each origin and destination pair. Unfortunately, the "true" O-D matrices are rarely, if ever, directly obtainable in practice, which gives rise to many studies for its estimation from limited observations of traffic conditions on the network.

Traditionally, O-D matrices are derived from household or roadside surveys. However, survey-based approaches have two main shortcomings: they are costly and labor intensive, and they often fail to capture temporal changes in O-D demand patterns. Consequently, research efforts of O-D estimation have been focusing on inferring O-D matrices from traffic counts on road segments, which is a faster, cheaper and more convenient method than household or roadside surveys.

The fundamental framework of estimating an O-D matrix having \( o \) O-D pairs and \( m \) observed link traffic counts, can be expressed by a linear system:

\[
\sum \sum p_{rs}^a q_{rs} = \bar{x}_a \quad \forall r \in R, s \in S, a \in A
\]

where \( R, S \) and \( A \) denotes a set of origins, destinations and links, respectively. \( q_{rs} \) denotes the estimated traffic demand between O-D pair \( rs \), \( p_{rs}^a \) denotes the proportion of trips between O-D pair \( rs \) using link \( a \), and \( \bar{x}_a \) represents the average measured traffic volume on link \( a \).

Using matrix notation, system (1) can be written as:

\[
Pq = \bar{x}
\]

where \( P \) is a \( m \times o \) matrix, \( q \) is a \( o \times 1 \) vector and \( \bar{x} \) is a \( m \times 1 \) vector.

According to ways in which the coefficient matrix \( P \) is determined, O-D estimation can be categorized into two major approaches: proportional-assignment methods and equilibrium-assignment methods. If the traffic congestion effect of a network is of minor importance, i.e., travel time is actually independent of changes in the traffic flow on a given link, \( P \) is assumed to be exogenously determined and obtained by means of some proportional assignment procedures, which can for example be a simple all-or-nothing (AON) assignment or a more advanced stochastic assignment. However, when congestion becomes significant, the Wardrop's first principle [1],
which states the well-known user-equilibrium (UE) condition in a congested transportation network, should be taken into consideration. Consequently, $P$ is no longer a simple proportion matrix that depicts the proportion of each O-D trips using each link. Instead, $P$ becomes an equilibrium assignment mapping, which maps the O-D demand matrix to a flow pattern satisfying the UE state described by Wardrop's first principle. In a certain sense, the equilibrium-based O-D matrix estimation can be thought of as an inverse of the UE traffic assignment.

It now becomes evident that the problem of O-D matrix estimation is to solve the linear system (2) for $q$

given a certain matrix $P$. Conventional solution approaches solve system (2) by minimizing a generalized distance function, namely a least squares or maximum entropy (minimum information) function, between estimated and observed traffic counts when $P$ is specified either in a proportional or equilibrium-assignment form. In order to find a more realistic solution, a historical O-D matrix that is obtained from previous surveys would be used as the "target" of the estimated OD matrix, which suggests that the objective function of the minimization program will also take the distance between the estimated and the target O-D matrices into account.

Note that this distance function between the two O-D matrices is in general weighted appropriately according to the relative belief of the traffic counts and the target matrix. The earlier research efforts using proportionality-assignment O-D estimation approaches were credited to Willumsen [2], for introducing the maximum entropy form, Van Zuylen [3] for using the concept of minimizing information, and Cacchita [4] for casting the problem in a generalized least squares framework. Many researchers, such as Bell [5], Bremignier-Göthe et al. [6], Lo et al. [7], conducted tests or proposed improvements along the line of proportional-based estimation. On the other hand, Nguyen [8], Fisk and Boyce [9] led the way in equilibrium-based O-D matrix estimation. Yang [10] has shown that a bi-level optimization technique can be used to model the problem by integrating an upper level, where the distance function is minimized, with a lower level where the user-equilibrium flow pattern, thereby the coefficient matrix $P$, is sought through a standard traffic assignment routine. Instead of estimating the O-D matrix directly, Sherali et al. [11] proposed to infer optimal path flows by formulating a linear programming problem, which is referred to here as the linear path flow estimator (LPFE). The optimal path flows in Sherali's approach will be estimated so as to approach the user-equilibrium flow pattern, regenerate link traffic counts and converge with a target O-D matrix as closely as possible. Bell et al. [12, 13] extended Sherali's path flow estimator to the log-linear path flow estimator by using stochastic user-equilibrium assignment. In order to avoid enumerating paths or applying a column generation procedure, which is required by LPFE but computationally inefficient, Nie and Lee [14] suggested
decoupling Sherali's linear model through seeking equilibrium paths independently by a K-shortest path ranking procedure.

The LPFE model, either coupled or decoupled, has difficulty in driving its estimates to the real O-D matrix (not target matrix) as close as possible when the target matrix subjects to considerable errors, even if the equilibrium flow pattern can be precisely regenerated. This shortcoming is mainly due to the limitation of a linear programming structure. This paper attempts to fix the problem by incorporating the decoupled path flow estimator [9] with the well-known generalized least squares (GLS) technique. Although GLS-based O-D estimation has been extensively studied, our decoupled GLS-PFE model sheds light on two problems deserving further investigation. First, one may have to invert a matrix whose strict inversion does not exist when solving the GLS-based PFE model. This is typically caused by the fact that path-link matrix $P$ is not full rank, which can be physically explained as some paths can be decomposed into other two or more paths. In this research, a pseudo-inverse of a non-invertible matrix, computed based on singular value decomposition, is adopted to find a least squares solution (or minimum distance solution) for the corresponding linear system. Second, non-negative constraints for path flows cannot be ignored, as many previous researchers did, because a good many of constraints will get activated during estimation when paths are used as estimated variables. Based on Lawson and Hanson's method [15] for a standard nonnegative least squares (NNLS) problem, we present an algorithm for the constrained PFE model (ACPFE), which iterates between figuring out the set of active constraints and solving the least squares problem consecutively. ACPFE is further simplified in order to improve the computational efficiency while maintaining sufficient estimation accuracy.

The remaining of this paper is structured as follows: The next section reviews the ordinary least squares (OLS) model for proportional-based O-D matrix estimation. Section 3 develops the GLS path flow estimator that integrates the equilibrium assignment mapping and covariance matrices of measurement errors of link traffic counts and the target O-D matrix. The discussions of solving non-invertible linear systems and dealing with nonnegative constraints are also covered in Section 3. Solution algorithms are presented in Section 4, and Section 5 reports numerical results. In the last section, we draw some conclusions and give directions for further research.

**OLS PROPORTIONAL-ASSIGNMENT MODEL FOR O-D ESTIMATION**

We first assume that $P$ is given as the link-use proportion matrix. The O-D estimation problem can be formulated as a classic ordinary least squares problem:
\[
\min \frac{1}{2}(\bar{x} - Pq)'(\bar{x} - Pq)
\]

(3)

Given \( P \in \mathbb{R}^{n \times n} \) and \( \bar{x} \in \mathbb{R}^n \). As shown by Trefethen [16], a classic approach for solving problem (3) is to solve the following normal equation:

\[
P^*Pq = P^*\bar{x}
\]

(4)

where \( P^* \) denotes the transpose of \( P \). System (4) can be solved by constructing a Cholesky factorization \( P^*P = R^*R \), where \( R \) is upper-triangular.

Note Problem (3) has two apparent shortcomings. First, the estimated O-D traffic demands may become negative, which is not acceptable in reality. Second, we mentioned in Section 1 that a more realistic estimation could be obtained by considering a target O-D matrix obtained from earlier surveys. To address these two issues, we introduce explicit nonnegative constraints and add the “distance” between the estimated and target O-D matrix into the objective function:

\[
\min \quad z(q) = \frac{1}{2}(\bar{x} - Pq)'(\bar{x} - Pq) + \frac{1}{2}(q - q_t)'(q - q_t)
\]

subject to:

\[
q \geq 0
\]

(6)

where \( q_t \) denotes the target O-D matrix. Let \( \mu \) represents the Lagrange multipliers associated with constraints (6). We can formulate the Lagrangean function of the problem as follows:

\[
\tilde{L}(q, \mu) = z(q) - \mu'q
\]

(7)

Since the original problem (5)+(6) is a convex optimization program with linear constraints, it has a unique optimal solution. The necessary and sufficient conditions for its optimality can be stated explicitly according to Karush-Kuhn-Tucker (KKT) conditions:

\[
\frac{\partial \tilde{L}}{\partial q} = 0
\]

(8)

\[
\frac{\partial \tilde{L}}{\partial \mu} = 0
\]

(9)

From (8), it is easy to obtain the following relation:
\[(q - q_0) = (\tilde{x} - Pq)^T P \mu' = 0\]  \hfill (10)

After taking transformation on both sides and collecting terms, we reach

\[(P^T P + I)q = P^T \tilde{x} + q_0 + \mu\]  \hfill (11)

Note Equation (11) is structurally similar to the normal equation (4). To obtain a clear physical interpretation for (11), we proceed to derive an explicit expression for \(q\) using the well-known Matrix Inversion Lemma:

\[(P^T P + I)^{-1} = I - P^T (PP^T + I)^{-1} P\]  \hfill (12)

Applying relation (12) in (11) and let \(PP^T + I = D\), we get:

\[q = q_0 - P^T D^{-1} P q_0 + (I - P^T D^{-1} P) P^T \tilde{x} + (I - P^T D^{-1} P) \mu\]  \hfill (13)

Furthermore, note that the following relation holds:

\[(I - P^T D^{-1} P) P^T \tilde{x} = P^T D^{-1} \tilde{x}\]  \hfill (14)

Now, putting (14) into Equation (13), we obtain

\[q = q_0 + P^T D^{-1} (\tilde{x} - P q_0) + (I - P^T D^{-1} P) \mu\]  \hfill (15)

The second and third terms on the right-hand side of Equation (15) can be interpreted as two adjustments to the prior estimation (or survey results): the first is related to the difference between the observed traffic counts and those inferred on the basis of the prior estimates, and the second is adjusted according to the Lagrange multipliers due to the nonnegative requirement on O-D demands.

**DECOUPLED GLS PATH FLOW ESTIMATOR**

The basic OLS model introduced in Section 2 is based on two assumptions: the measurement errors of observed traffic counts and the target O-D matrix are uncorrelated and have same values, and the traffic assignment mapping matrix \(P\) is known a priori. These assumptions are relaxed in this section.

**Introduce The Equilibrium Assignment Mapping**

Since the effects of peak-time congestion are unavoidable in urban transportation network, using a proportional assignment mapping for O-D matrix estimation will produce inconsistency in system (2). A conventional way of introducing the equilibrium assignment mapping into the O-D estimation is to combine the
user-equilibrium (UE) traffic assignment procedure and the estimation process as an integrated model. This means the assignment and estimation will be performed simultaneously. Consequently, the computational overhead is substantially high even for mid-size networks since the formulation is no longer cast in the form of simple convex optimization. Moreover, obtaining a converged solution becomes more difficult. It is thus desirable to maintain the simple convex structure of the original problem while taking the equilibrium assignment into consideration.

Nie and Lee [9] proposed an algorithm to solve the LPFE model by Sheffi et al. [12] for O-D estimation, where the equilibrium path flow pattern is determined by an exogenous K-shortest path ranking procedure. The K-shortest path ranking problem is a generalization of the shortest path tree problem, in which not one but a set of shortest paths will be produced according to user-specified criteria. If the UE condition is held exactly in a given network, in general, there exist more than one path connecting each O-D pair with the smallest and identical travel cost. Intuitively, performing a sequence of K-shortest paths search could pick up all of these UE paths. Once these paths are available, they will serve to form the coefficient matrix $P$ whose columns are equal to the paths in the UE flow pattern. Since $P$ has been accommodated within the UE condition, the inconsistency from proportional assignment assumption is prevented while the computation is kept relatively simple. Consequently, this strategy "decouples" the equilibrium-based O-D estimation problem by determining the equilibrium assignment mapping matrix $P$ from the observed link traffic counts independently.

We can apply this "decoupled" idea in a least squares framework instead of solving a linear programming problem as done in [9]. Note that an important difference from a PFE model is that we do not estimate the O-D demand $q$ directly. Instead, path flows are inferred and each O-D demand is derived by summing up flows of its associated equilibrium paths.

Let $f^{ra}_{nk}$ denotes the flow on the $k$th equilibrium path between origin $r$ and destination $a$, and $e^{ra}_{nk}$ denotes the path-link incidence matrix, where $e^{ra}_{nk}$ equals to 1 if link $a$ belongs to path $k$, and 0 otherwise. We have the following expression:

$$
\sum_{n} \sum_{k} \sum_{r} f^{ra}_{nk} e^{ra}_{nk} = \mathbf{x} \quad \forall a \in A, k \in K, r \in R, s \in S
$$

or

$$
\mathbf{M} = \mathbf{x}
$$

(16)
where $\Lambda$ plays a similar role as $P$ in (2). However, $\Lambda$ is regarded to represent an equilibrium assignment mapping since its columns are so generated as to conform with the UE condition. It will be shown how to obtain $\Lambda$ from a K-shortest path ranking procedure in the next section. At this point, let us assume $\Lambda$ is known. The ordinary least squares path flow estimator for O-D matrix estimation can be formulated as follows:

Model [OLS-PFE]

\[
\min_z \; z'f = \frac{1}{2} (\bar{\lambda} - \Delta f)'(\bar{\lambda} - \Delta f) + \frac{1}{2} (M\Delta - q_\Delta)'(M\Delta - q_\Delta)
\]

subject to:

\[
\Gamma \geq 0
\]

where $M$ is an $o \times n$ ($o$ is the total number of paths) matrix which converts equilibrium path flows to O-D demands. Note constraint (18) guarantees

\[
q = M\Delta \geq 0
\]

Some may argue that restricting $q$ to be nonnegative would be a plausible way than using (18) since negative path flows might not necessarily generate negative O-D demands. However, using $M\Delta \geq 0$ as constraints makes the problem much harder to solve, as we will see later on. Furthermore, the estimated path flow pattern itself is an important output of a PFE model because it has to conform to the UE state when the optimality is reached. Thus, a path flow pattern having negative path flows, on which the final O-D estimation is directly based, is not acceptable.

According to the first-order optimality condition, we get the following normal-type equation:

\[
(\lambda' \Lambda + M'W)g = \lambda'\Delta + M'q_\Delta + \lambda
\]

where $\lambda$ is the Lagrange multiplier associated with the constraint (18).

Consider Correlated and Homoskedastic Errors

We proceed to consider the case where the observed link counts and the target matrix subject to correlated and homoskedastic random errors by extending the OLS-PFE model to a generalized least squares (GLS) PFE. It should be noted, however, that observation errors of traffic counts are assumed to be small enough to keep all paths contained in the UE state unchanged. This assumption is to guarantee that the K-shortest path ranking algorithm can produce a "real" UE assignment mapping.
A GLS-PFE model can be obtained by introducing the variance-covariance matrices of \( \mathbf{x} \) and \( \mathbf{q}_e \). Let \( \mathbf{S} \) and \( \mathbf{T} \) represent the variance-covariance matrices for target matrix and traffic count respectively, [OLS-PFE] can be reformulated as:

\[
\begin{align*}
\min_{\mathbf{f}} \; & f = \frac{1}{2} (\mathbf{x} - \mathbf{A})^\top \mathbf{S}^{-1} (\mathbf{x} - \mathbf{A}) + \frac{1}{2} (\mathbf{Mf} - \mathbf{q}_e)^\top \mathbf{S}^{-1} (\mathbf{Mf} - \mathbf{q}_e) \\
\text{subject to} \; & f \geq 0
\end{align*}
\]

(20)

where both \( \mathbf{S} \) and \( \mathbf{T} \) are positive definite symmetric matrices. The normal equation of model (20) can be derived from its first-order optimality condition as:

\[
(\mathbf{A}^\top \mathbf{S}^{-1} \mathbf{A} + \mathbf{M}^\top \mathbf{S}^{-1} \mathbf{M}) \mathbf{f} = \mathbf{A}^\top \mathbf{S}^{-1} \mathbf{x} + \mathbf{M}^\top \mathbf{S}^{-1} \mathbf{q}_e + \lambda
\]

(21)

We refer to Equation (21) as the fundamental equation for solving the uncoupled GLS-PFE model. In case the matrix \( \mathbf{V} = \Delta^\top \mathbf{S}^{-1} \mathbf{A} + \mathbf{M}^\top \mathbf{S}^{-1} \mathbf{M} \) is invertible and all constraints are inactive, the solution for the fundamental equation can be straightforwardly expressed as follows:

\[
\mathbf{i} = \mathbf{V}^{-1} \mathbf{b}
\]

(22)

where \( \mathbf{b} = \Delta^\top \mathbf{S}^{-1} \mathbf{x} + \mathbf{M}^\top \mathbf{S}^{-1} \mathbf{q}_e \).

However, both the path-link incidence matrix \( \mathbf{A} \) and the path-OD matrix \( \mathbf{M} \) are in general neither full rank nor over-determined. To see this, first note that \( \mathbf{M} \) becomes non-full rank and underdetermined whenever an O-D pair has more than one path, which often happens in a transportation network with reasonable amount of congestion. Moreover, the number of paths available is often larger than that of observed link counts. Even if this is not the case, different paths still possibly correlate with one another so as to produce a non-full rank \( \mathbf{A} \). As a result, \( \mathbf{V} \) is non-invertible thereby Equation (22) cannot be adopted to solve the fundamental equation (21).

**Solve The Fundamental Equation With Non-Invertible \( \mathbf{V} \)**

It has been shown [15] that a pseudoinverse of a matrix \( \mathbf{V} \), denoted by \( \mathbf{V}^+ \), which always exists, provides a unique minimum distance solution \( \mathbf{V}^+ \mathbf{b} \) (i.e., a solution for a least squares problem) for the linear system \( \mathbf{Vf} = \mathbf{b} \). Penrose [15] proved that a matrix \( \mathbf{X} \equiv \mathbf{V}^+ \) if and only if the following conditions hold:

\[
\mathbf{VXV} = \mathbf{V}
\]
\[ XVX = X \]
\[ (VX)' = VX \]
\[ (XV)' = XV \] (23)

Therefore, in case of non-invertible \( V \), one has to resort to the pseudoinverse of \( V \) to obtain an approximate solution (minimum distance solution) for the fundamental equation. A classical approach of obtaining a pseudoinverse of \( V \) is to decompose \( V \) through singular value decomposition (SVD) as follows:

\[ V = W\Sigma U' \] (24)

where both \( W \) and \( U \) are \( n \times n \) unitary matrices, i.e., \( W^* = W^{-1} \) and \( U^* = U^{-1} \), and \( \Sigma \) is \( n \times n \) and diagonal with non-negative entries. When the rank of \( V \) is \( l < n \), we can rewrite \( \Sigma \) as:

\[ \Sigma = \begin{bmatrix} S & 0 \\ 0 & 0 \end{bmatrix} \]

where \( S \) is a \( l \times l \) diagonal matrix whose all entries are positive. It is easy to prove, using Penrose's conditions, that the pseudoinverse of \( \Sigma \) is:

\[ \Sigma^+ = \begin{bmatrix} S^{-1} & 0 \\ 0 & 0 \end{bmatrix} \]

Consequently, the pseudoinverse of \( V \) is given by:

\[ V^* = U\Sigma^+ W' \] (25)

To prove this is true, we need to show that Equation (25) satisfies all Penrose conditions:

\[ VV'V = W\Sigma U'(U\Sigma^+ W')W\Sigma U' = W\Sigma\Sigma\Sigma U' U = W\Sigma U' = V \]
\[ V'VV' = U\Sigma^+ W'(W\Sigma U')U\Sigma W' = U\Sigma^+ \Sigma \Sigma^+ U' U = U\Sigma^+ W' = V^* \]
\[ (VV')' = (W\Sigma U'U\Sigma^+ W')' = (W\Sigma\Sigma^+ W')' = W\Sigma^+ W' = VV^* \]
\[ (V'V)^* = (U\Sigma^+ W'W\Sigma U')^* = (U\Sigma^+ U')^* = U\Sigma^+ U' = V'V \]

Thus, a solution for Equation (21) is given in the form of the pseudoinverse as:

\[ f = V^*b = U\Sigma^+ W'b \] (26)
Computing the SVD of $V$, which is highly related to the eigenvalue decomposition of $VV^T$, has been available in some software packages like MATLAB as a standard subroutine. For conciseness, we will not introduce details of SVD computation in this paper. Readers who are interested can refer to [16] (Chapter 31, page 234-240).

Deal with Nonnegative Constraint

A good many researchers ignored the nonnegative constraints when applying GLS-based O-D estimation because they observed these constraints are rarely active. This might be true if a compact link use proportion (OD-link) matrix is adopted. However, the path flow estimator significantly increases the possibility of activating nonnegative constraints, as shown by these authors' experience, since it manipulates directly upon path-link and path-OD matrices. Moreover, the increase of problem size will likely activate more constraints. We thus have to seriously consider these nonnegative constraints.

Bell [1] has presented a simple algorithm for solving this constrained generalized least squares problem. The algorithm iterates between solving the fundamental equation and updating Lagrange multipliers by scaling negative estimated O-D entries with principal diagonal entries of $V^{-1}$. Yet, to the best of our knowledge, no implementation and/or computational experiments for Bell's algorithm is found in literature. Furthermore, this algorithm neither considers the case where $V^{-1}$ does not exist nor appears to work well for the GLS-PFE model.

Lawson and Hanson [7] proposed an algorithm for a standard nonnegative least squares problem (NNLS), based on which they proved the following important theorem that describes the property of a NNLS solution:

**Theorem 1: Lawson and Hanson's Theorem**

The optimal solution $f^*$ for the problem NNLS

$$
\min \frac{1}{2} (Pf - x)^T(Pf - x) \text{ subject to } f \geq 0
$$

satisfies the following conditions simultaneously, given $\Phi$ and $\Omega$ denotes the index sets of active and inactive constraints respectively:

1. $f_i^* =
   \begin{cases} 
   > 0 & \text{if } i \in \Omega \\ 
   = 0 & \text{if } i \in \Phi 
   \end{cases}$
2. \( \lambda_i := \begin{cases} 0 & \text{if } i \in \Omega \\ > 0 & \text{if } i \in \Phi \end{cases} \) where \( \lambda = \mathbf{P}^T \mathbf{f}^s - \mathbf{P}^* \mathbf{x} \)

3. \( \mathbf{f}^s \) is a solution vector for the following least squares problem

\[
\min \frac{1}{2} (\mathbf{P}_i \mathbf{f} - \mathbf{x})^T (\mathbf{P}_i \mathbf{f} - \mathbf{x}) \text{ where } \mathbf{P}_i := \begin{cases} \text{column } i \text{ of } \mathbf{P} & \text{if } i \in \Omega \\ 0 & \text{if } i \in \Phi \end{cases}
\]

Note \( \lambda \) in the theorem denotes the Lagrange multipliers and Conditions 1 and 2 are corresponding to KKT conditions (8) and (9). We are going to show in the following that this theorem can be easily extended to our decoupled PFE model.

**Theorem 2**

The optimal solution \( \mathbf{f}^s \) for Model [OLS-PFE] satisfies the following conditions simultaneously, given \( \Phi \) and \( \Omega \) denotes the index sets of active and inactive constraints respectively:

1. \( \mathbf{f}_i^s := \begin{cases} > 0 & \text{if } i \in \Omega \\ = 0 & \text{if } i \in \Phi \end{cases} \)

2. \( \lambda_i := \begin{cases} > 0 & \text{if } i \in \Omega \\ = 0 & \text{if } i \in \Phi \end{cases} \) where

\[ \lambda = \mathbf{V} \mathbf{f}^s - \mathbf{b} \quad \mathbf{V} = \Delta \mathbf{M}^* \mathbf{M}, \quad \mathbf{b} = \Delta \mathbf{x} + \mathbf{M}^* \mathbf{q}_0 \] (27)

3. \( \mathbf{f}^s \) is a solution vector for the following least squares problem

\[
\min \frac{1}{2} (\Delta_{\alpha} \mathbf{f} - \mathbf{x})^T (\Delta_{\alpha} \mathbf{f} - \mathbf{x}) + \frac{1}{2} (\mathbf{M}_{\alpha} \mathbf{f} - \mathbf{q}_\alpha)^T (\mathbf{M}_{\alpha} \mathbf{f} - \mathbf{q}_\alpha)
\]

where

\[
\Delta_{\alpha} := \begin{cases} \text{column } i \text{ of } \Delta & \text{if } i \in \Omega \\ 0 & \text{if } i \in \Phi \end{cases} \quad \mathbf{M}_{\alpha} := \begin{cases} \text{column } i \text{ of } \mathbf{M} & \text{if } i \in \Omega \\ 0 & \text{if } i \in \Phi \end{cases}
\] (28)

**Proof:** We first show that [OLS-PFE] is equivalent to the following standard NLLS problem:

\[
\min \frac{1}{2} (\mathbf{H} \mathbf{f} - \mathbf{x})^T (\mathbf{H} \mathbf{f} - \mathbf{x}) \quad \text{subject to } \mathbf{f} \geq 0,
\] (29)

where \( \mathbf{H} := \begin{bmatrix} \Delta \\ \mathbf{M} \end{bmatrix} \) is a \((m + o) \times n\) matrix and \( \mathbf{x} = \begin{bmatrix} \mathbf{x} \\ \mathbf{q}_\alpha \end{bmatrix} \) is a \((m + o) \times 1\) matrix. To see this, note...
\[(H - \pi)\text{'} (H - \pi) - \left( \begin{bmatrix} \Delta & \bar{f} \\ M & q_a \end{bmatrix} \right) \left( \begin{bmatrix} \Delta & \bar{f} \\ M & q_a \end{bmatrix} \right) \text{'} \]

\[= f' (\Delta' \bar{f} + \Delta' M f - \Delta' \bar{f} + \Delta' M f) + (\bar{x}' \bar{x} + q_a' q_a)\]

\[= (f' M' M f - \Delta' \bar{f} - \Delta' M f + \Delta' \bar{f} + \Delta' M f) + (\bar{x}' \bar{x} + q_a' q_a)\]

\[= (\bar{x}' - \Delta f)' (\bar{x}' - \Delta f) + (M f - q_a)' (M f - q_a)\]

Condition 1 and 3 can be established directly from Theorem 1 and the equivalence between [OLS-PFE] and the program (29).

To prove that Condition 2 holds, Theorem 1 shows that Lagrange multipliers of the program (29) can be denoted by:

\[\lambda = H' H f - H' \pi - \left( \begin{bmatrix} \Delta & \bar{f} \\ M & q_a \end{bmatrix} \right) \left( \begin{bmatrix} \Delta & \bar{f} \\ M & q_a \end{bmatrix} \right) \text{'} (\Delta' \Delta + M' M) f - (\Delta' \bar{x} + M q_a)\]

This completes our proof.

It is easy to see that Theorem 2 can be directly applied for Model [GLS-PFE]. Note Theorem 1 cannot be easily extended to Theorem 2 smoothly if we take \( M f \geq 0 \) as constraints. This explains why constraints \( f \geq 0 \) have to be used in our PFE model.

Theorem 2 implies that a constrained PFE model can be transformed into an unconstrained PFE model, which is much easier to solve, once the set of active constraints is identified a priori. This sheds lights on designing efficient algorithms for Model [GLS-PFE], which we will address in details in the next section.

**SOLUTION ALGORITHMS**

We in this section present solution algorithms for the decoupled GLS path flow estimator. These include a K-shortest path ranking algorithm to determine matrices \( \Delta \) and \( M \) independently, and an iterative procedure to derive nonnegative equilibrium path flows based on the least squares method.

**An Algorithm to Generate Equilibrium Mapping**

We have mentioned in the last section that the critical idea behind the uncoupled method is to use an exogenous K-shortest path ranking procedure to generate the UI assignment mapping. The K-shortest path ranking, a classic network programming problem of determining not only the shortest path, but also the second, the
third..., to the \( k \)th (for a given integer \( k > 1 \)) shortest path, was found [9] to be appropriate for recognizing paths that reproduces the user-equilibrium flow pattern, so as to determine matrices \( \Delta \) and \( M \) in (20). The K-shortest path ranking algorithm presented in [9] is based on Eppestein's approach [17], which picks shortest paths from a graph representing all possible deviations from a standard shortest path tree. However, Eppestein's method was originally designed for the unconstrained shortest path ranking and allows cycles of the repeated nodes in the generated paths. Nie and Lee [9] incorporated a heuristics procedure into Eppestein's algorithm, which guarantees the generated paths to be cyclic-free and cost-identical. We in this paper focus on procedures of generating matrices \( \Delta \) and \( M \). Reader may refer to [4, 9] for details of the K-shortest path ranking algorithm.

The complete algorithmic steps to obtain \( \Delta \) and \( M \) is summarized as follows:

**Step 0:** Initialization. Set the current O-D pair \( k = 0 \) and path number \( l = 0 \).

**Step 1:** Let \( k = k + 1 \), if \( k > a \), stop, the total number of paths \( m = l \). \( r \) and \( s \) denotes the origin and destination corresponding to O-D pair \( k \).

**Step 2:** Calculating the shortest path tree \( T_r^* \) rooted at \( r \).

**Step 3:** Build the pseudo path tree that contains all cost-identical (in terms of the tolerant error specified by users) shortest paths.

**Step 4:** Get paths and update matrices \( \Delta \) and \( M \).

**Step 4.1:** Using a backward tracking procedure to obtain a cyclic-free path \( p^m \). If no path can be found, go to **Step 1**; otherwise set \( l = l + 1 \).

**Step 4.2:** Set \( \Delta(r, l) = p^m \) and \( M(r, l) = 1 \). Go to **Step 4.1**.

**Algorithms for Estimating Nonnegative Equilibrium Path Flows**

Once equilibrium assignment maps, that is, matrices \( \Delta \) and \( M \), are available, we can estimate the corresponding path flows as well as O-D traffic demands by solving the constrained PFE model. Theorem 1 shows that the optimal solution of this constrained GLS problem heavily depends on the set of active constraints. Since specifying a priori these constraints is impossible, one has to apply iterative methods in which solving the unconstrained GLS problem and identifying active constraint are carried out iteratively.

In the following, we first present an algorithm for solving the constrained PFE model based on Lawson and Hanson’s iterative method for a standard NNLS problem:
Algorithm for constrained PFE (ACPFE)

Step 0: Initialization. Set $\Omega = \phi$, $\Phi = \{1, 2, ..., n\}$ and $f = 0$.

Step 1: Compute the Lagrange multipliers $\lambda$ according to (27). If $\Phi = \phi$ or $\lambda_i \geq 0$ for all $i \in \Phi$, stop.

Step 2: Move the index $t = \arg \min \{ \lambda_i, i \in \Phi \}$ from $\Phi$ to $\Omega$.

Step 3: Set $\Delta$ and $M$ according to (28).

Step 4: Compute $f' = V^*b$ using SVD decomposition (25), then set $f_i' = 0$ if $i \in \Phi$. where $V = \Delta^{-1}X + M^{-1}S^{-1}M$ and $b = \Delta^{-1}X + M^{-1}S^{-1}q_s$.

Step 5: If $f_i' > 0$ for all $i \in \Omega$, set $f = f'$ and go to Step 1, otherwise, go to Step 6.

Step 6: Set $f = f + \alpha(f' - f)$, where $\alpha = \min\{\frac{f_i}{f_i'}, f_i' \leq 0, i \in \Phi\}$

Step 7: Move all indices from $\Omega$ to $\Phi$ for which $f_i = 0$, go to Step 3.

The convergence of ACPFE has been proven in [7]. However, the algorithm is not efficient enough even for mid-size problems since the number of its major iteration, in which an unconstrained GLS problem has to be solved, is bounded from below by the number of non-active constraints. Experience has shown that the number of non-active constraints can be substantially large in a real-size estimation problem, which makes the computational overhead of the algorithm prohibitively high. In order to overcome this computational difficulty, a heuristic algorithm is designed to decrease the number of iterations in ACPFE while making the solution satisfy the conditions given in Theorem 2. We describe this simplified ACPFE (SACPFE) as follows:

Step 0: Initialization. Set $\Phi = \phi$, $\Omega = \{1, 2, ..., n\}$ and $f = 0$.

Step 1: Set $\Delta$ and $M$ according to (28).

Step 2: Compute $f = V^*b$ using SVD decomposition (25).

Step 3: If $f_i \geq 0$ for all $i = 1, 2, ..., n$, stop; otherwise, move all indices from $\Omega$ to $\Phi$ for which $f_i < 0$, go to Step 1.

Note that this algorithm will terminate after a limited number of iterations. This is due to that all $f_i$ associated with active constraints will be actually set to zero compulsorily when $\Delta$ and $M$ is changed accordingly.
by (28), which means a constraint, if it is activated in some iteration, will never become inactive later. The simplified ACPF can dramatically decrease the number of iterations required by the original method, as our numerical experiments would show later on. However, the algorithm may jeopardize the solution accuracy in misestimating the set of active constraints. Intuitively, activating some constraints can cause other active constraints to be inactive, which cannot be detected precisely by SACPF. Nevertheless, it turns out that the simplified algorithm can produce an approximate optimal path solution that is comparable to ACPF in reproducing UE link flow pattern and driving estimated O-D traffic matrix to approach a real one. From a practical point of view, the considerable gain in computational efficiency is well-worth the modest degradation in solution accuracy.

We will end this section by mentioning that the algorithms presented here demand all link counts being available, which is definitely an unreasonable requirement in reality. This demand could be relaxed by either applying flow conservation principle and prior information (as suggested by Skelat et al. [11]), or introducing an outer loop that consecutively updates link flows as well as link travel times according to estimated path flow pattern. Options of these improvements will be investigated subsequently in a separate work.

**NUMERICAL RESULTS**

In this section, we give numerical results to demonstrate how algorithms presented in the last section work using small- to mid-size examples. The cyclic-free Eppstein's K-shortest path ranking algorithm was implemented on PC using VC++ 6.0 while the GLS path flow estimator algorithm was implemented on PC using MATLAB 6.0. We choose C++ to implement K-shortest path ranking because MATLAB is not efficient enough for this type of problem where a huge number of iterations are unavoidable.

In all simulation experiments, "observed" traffic counts are generated from a standard traffic assignment procedure that allocates real O-D traffic demands onto a given network such that a UE flow pattern is produced. For simplicity, we assume that the traffic counts generated from TAP subject to error whose covariance matrix \( \mathbf{T} = \mathbf{I} \), where \( \mathbf{I} \) is an identity matrix. Link travel time, based on which the K-shortest path ranking algorithm recasts the equilibrium paths, is assumed to be only dependent on the traffic flow on that link, that is, link interactions are ignored. In this paper, link travel time is computed from the standard BPR (Bureau of Public Road) function, which takes the following form:
where \( t_0 \) denotes the free flow travel time, \( C \) is the link capacity and \( x \) denotes the traffic volume/counts.

In order to obtain a target O-D demand matrix, an artificial deviation is applied upon the real O-D matrix that is used for producing "observed" link counts. There are three types of target matrix being tested for each example: an error-free (EF) target matrix that is exactly equivalent to the real matrix, a weak-prior-information (WPI) matrix whose O-D entries take the same values of demands crossing the same origin-total demands from the origin divided by its associated number of O-D pair), and a strong-prior-information (SPI) matrix whose all O-D entries are changed in small proportions (less than 30%).

To specify the variance-covariance matrix of \( \mathbf{q} \), we introduce a weighting parameter \( \gamma \) that depicts the relative belief in the traffic counts compared to the target matrix, following Bensmenger-Gothe et al [4]. The covariance matrix \( \mathbf{S} \) is set as a diagonal matrix with principal diagonal elements equivalent to the inverse of \( \gamma \). \( \gamma \) can take values between 0 and 1, which means the target matrix is as most regarded as accurate as the observed link counts, when the covariance matrix of target demands \( \mathbf{S} = I \). This is a reasonable assumption because the model will make no improvement upon the target matrix from using link counts that are even inaccurate than the given target itself.

In our experiments, we use the following heuristic to calculate \( \gamma \):

\[
\gamma = \min (1, \frac{\sigma}{|\mathbf{q} - \mathbf{q}_0|})
\]

where \( \mathbf{q}_0 \) denotes the real O-D matrix.

Note Equation (31) cannot be applied for practical situations since it requires information of the "real" O-D, which is very thing one sets up to estimate, and unavailable in reality.

**Yang’s 9-node Network**

The first test example, which contains 9 nodes, 14 links and 4 O-D pairs, is taken from Yang [18]. Figure 1 depicts the network topology and real O-D matrix. The “observed” link traffic counts as well as travel times, which are produced by a UE traffic assignment subroutine, are reported in Table 1.

Eight equilibrium paths (see Table 2) are picked up from the K-shortest path ranking algorithm, with the tolerance error of 0.001% (which means all cycle-free paths whose costs is less than or equal to 1.00000 times of the shortest path cost will be regarded as identical to the shortest one).
Three different target matrices, as described before, are adopted and given in Table 3. Table 3 also provides the estimated O-D matrix, root mean square error between the estimated and the real matrix (RMSE_{\text{e}}), and RMSE between the estimated link traffic flows and the observed link counts (RMSE_{\text{l}}), based on algorithms ACPE and SACPE for the three different targets. The equilibrium path solution as well as Lagrange multipliers is reported in Table 4.

When an error-free (EF) target matrix is applied (\( \gamma = 1 \)), both RMSE_{\text{e}} and RMSE_{\text{l}} are observed to be nearly zero, which implicts in this case the real O-D matrix is exactly obtained from our decoupled path flow estimator while the user-equilibrium link flow pattern is reproduced perfectly. As shown in Table 3 and 4, the algorithm ACPE took seven iterations to identify the second constraint, whose associated Lagrange multipliers is 0, as being active. On the other hand, SACPE only consumed one iteration to terminate with a different path flow pattern whose active constraint is the fourth one with the associated Lagrange multipliers of zero.

For weak-prior-information (WPI) target matrix, whose RMSE from the real matrix is about 23.78, the relative belief parameter \( \gamma \) is calculated according to (30) as \( 1/23.78^2 \approx 0.002 \). Both ACPE and its simplified version generated an estimation that is much closer to the real O-D matrix than the given target (RMSE_{\text{e}} = 0.22), indicating that the target matrix can be improved substantially by applying traffic counts. At the same time, the observed link counts are regnerated precisely from estimation, with RMSE_{\text{l}} of 0.22.

A similar observation was made when the strong-prior-information (SPI) target matrix was adopted: RMSE_{\text{e}} of the O-D matrix estimated (0.09) is much less than that of SPI target (19.20), while the user-equilibrium flow pattern is reproduced with a satisfying accuracy (RMSE_{\text{l}}=0.12).

We further highlight the following facts for algorithms ACPE and SACPE. Firstly, the two algorithms generated nearly the same link flow pattern and the estimation of O-D matrix for three target matrices, even though they came up with different path flow patterns. This is a positive indication that the SACPE can offer satisfying solutions for the proposed decoupled PFE model. Secondly, this example shows that ACPE needs much more iterations to converge than the proposed simplified method, a phenomenon coincident with theoretical expectations. Because of the small size of the network, CPU time consumed by both algorithms is relatively small to have no significant difference in this example, as shown in Table 4. However, the computational merit of the simplified algorithm would emerge when the network size becomes reasonably large. Moreover, more than half of the CPU time has been spent on finding equilibrium paths and form matrices \( \Delta \) and \( \mathbf{M} \) in both algorithms. One may thus doubt the
overall efficiency of the presented model since the K-shortest path ranking seems to be a computationally expensive module. However, as we will see later on, this is again due to the small size of the example. The proportion of CPU time taken by K-shortest path ranking will drop steeply as network size increases.

A 100-Node Hypothetical Network

This example presents computational experiments with two algorithms using a larger network, which is obtained from a random grid-network generator. A 10 by 10 hypothetical network is generated in such a way that its nodes are arranged in a square planar grid with a grid arc (whose link performance function is also randomly determined) connecting each pair of adjacent grid nodes in each direction. A node at a corner has two successors while a node at an edge has three. All other nodes have four successors. Twelve nodes are chosen as zone centroids, that is, a 12 by 11 matrix will be randomly produced to be the real O-D trip matrix.

The K-shortest path ranking procedure found 312 paths contained in the UE flow pattern, given a tolerant error of 0.01%. Estimated results for three target matrices are given in Table 5.

When an error-free O-D matrix is used as the target, the presented algorithms regenerate the observed link counts precisely and obtain an estimation that is exactly equivalent to both target and real O-D matrices (RMSEa = RMSEb = 0). Again, the optimal path solutions from the two algorithms are quite different. ACPFE recognized 138 active constraints when optimality is reached while the simplified algorithm got only 90. However, it seems that the two distinctive path flow patterns produced quite similar link flows as well as the estimated O-D matrices, which once again shows that the SACPFE maintains the accuracy of O-D estimator while dramatically improving the computational performance of ACPFE.

Figures 2 and 3 visualize the WPI target and estimated O-D matrices for ACPFE and SACPFE respectively. X axis of the plot represents the real O-D traffic demands while Y axis stands for the target demands (denoted by crosses) or estimated demands (denoted by circle). It is obvious that a perfect estimation, that is, estimated demands equals to real demands exactly, should follow a straight line with a slope of 1, which we refer to as the perfect estimation line hereafter. An immediate observation from these two figures is that ACPFE and SACPFE have produced nearly identical O-D matrix estimates. Furthermore, it can be seen that the estimated demands from both algorithms have an apparent tendency to approach the perfect estimation line compared with the target demands pattern. This can be also verified numerically by noting that RMSEA of the estimated matrix (67.03) is much smaller than that of the WPI target (200.68).
We obtained the SPI target matrix in this example by uniformly scaling down all real O-D demands by 25 percent. This produced a SPI target with RMSĒ equivalent to 128.88. The estimated O-D matrices obtained from ACPFE and SACPFE significantly reduced the RMSĒ of SPI target to about 34.69. The improvement of estimated O-D matrices upon the SPI target is shown in Figures 4 and 5, which explicitly demonstrate, how the proposed algorithms drive the SPI target toward the perfect estimation line with link counts information.

In this example, the simplified method outperforms ACPFE significantly for three tested scenarios in terms of the computational overhead. Taking the WPI target case as an example, SACPFE spent only 4 iterations and 10.45 seconds CPU time to converge while ACPFE took about 173 iterations and 253.73 seconds CPU time. Note SACPFE cannot obtain as accurate optimal path solution as ACPFE does since it is likely to fail to recognize all active constraints. However, estimates of SACPFE for O-D matrices and link counts turn out to be sufficiently precise.

Moreover, CPU time consumed by K-shortest path ranking in this example becomes relatively trivial compared with those spent in the estimation; it takes around 18% of total CPU time for SACPFE, and only 0.8% for ACPFE, to find all equilibrium paths. Therefore, K-shortest path ranking will not become a computation bottleneck for the overall decoupled GLS-based PFE model.

CONCLUSIONS

This paper combines the decoupled path flow estimator with the generalized least squares techniques for equilibrium-based O-D trip matrix estimation. The presented formulation incorporates measurement errors of link flows and target matrix naturally through the GLS structure, and maintains the major advantage of the decoupled SACPFE model, that is, simplifying the work of determining the equilibrium assignment mapping by exogenously identifying the optimal paths conforming to a user-equilibrium state.

The solution of the GLS-PFE model differs from previous GLS-based models in two aspects: the former often requires the solution of a non-invertible linear system and imposes nonnegative constraints. The algorithm presented in this paper is based on Lawson and Hanson’s method, was presented to solve the GLS-PFE model. The algorithm continuously solves the restricted GLS problem through singular value decomposition and determines the set of active constraints. ACPFE suffers from slow convergence due to its one-at-a-time update strategy for the...
active constraint set. We thus simplified ACPFE by applying an all-at-a-time update strategy, which simply marks all constraints that are violated in an estimation to be active.

Our limited numerical experiments lead to the following findings:

1. When solved by either ACPFE or its simplified version, GLS-PFE model can substantially improve the given target O-D matrix (i.e., producing an estimate that is much closer to the real O-D matrix than the target) after using link traffic counts, while producing a path flow pattern which concurs with a UE state.

2. SACPFE would generate optimal path solutions and active constraint sets that are quite different from those of ACPFE. However, these different path solutions correspond to quite similar estimates for the O-D matrix and link traffic counts. Given its computational advantage, it is recommended that SACPFE be considered in solving the large-scale constrained O-D matrix estimation problem.

3. The computational cost used for finding equilibrium paths is fairly modest when the problem size is reasonably large.

One of the most important further work, as we mentioned earlier in this paper, is to relax the assumption that all link traffic counts are available. It is also interesting to investigate the statistical characteristics of the GLS-based path flow estimator when many constraints are activated, and to study the effects of the relative belief parameter γ on estimation results.

REFERENCES


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FIGURE 2  WTP Target vs. Estimated O-D Matrix for Hypothetical Network
FIGURE 3  SIP Target vs. Estimated O-D Matrix for Hypothetical Network
Table 1 Input Data For Yang's Network

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### Table 3 Estimated Results for Yang’s Network

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<th>CPU Time</th>
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* -- The number in parentheses is the CPU time consumed by K-shortest path searching.
### Table 4: Equilibrium Path Solutions and Lagrange Multipliers for Yang’s Network

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<tr>
<td>SACPFE</td>
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Zone Centroid

Real OD Trip Matrix:

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<tr>
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Figure 1 Topology and Real O-D Trip Matrix of Yau's Network
Figure 2.1 Comparison based on Algorithm ACPFE

Figure 2.2 Comparison based on Algorithm SACPFE

Figure 2 WIP Target vs. Estimated O-D Matrix for Hypothetical Network
Figure 3.1 Comparison based on Algorithm ACPFE

Figure 3.2 Comparison based on Algorithm SACPFE

Figure 3. SIP Target vs. Estimated O-D Matrix for Hypothetical Network