GPS Solutions

Online Resource 1

Supplementary Information

ZTD constraint information and station-height response

Article title

Over-injection of time-correlated tropospheric constraints biases PPP height: a Gauss–Markov remedy

Authors

Jing Wu; Zhizhao Liu

Corresponding author

Zhizhao Liu

Department of Land Surveying and Geo-Informatics, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, China

Email: george.liu@polyu.edu.hk

Content

Derivations of the effective sample size, correlation-adjusted scalar constraint information, and the propagation of zenith total delay (ZTD) constraint errors into station height in a reduced precise point positioning (PPP) model.

Contents

S1 Effective sample size and equivalent constraint information 2

S2 Height response to a scalar ZTD constraint 4

References 6

Equation numbers prefixed by S refer to this resource. References to Eqs. (15)–(20) refer to the main manuscript.

S1 Effective sample size and equivalent constraint information

This section derives the effective sample size and the information fractions used in Eqs. (15)–(17) of the main text. The effective sample size is defined by matching the variance of an arithmetic mean to that of a mean of independent observations (Bayley and Hammersley 1946). Its conversion into a constraint weight is therefore made for a scalar representation of the arc mean.

S1.1 Variance of the arc-mean error

Consider N equally spaced constraint errors with sampling interval Δt. Let ε_i denote the centered stochastic error at epoch i. To isolate the effect of temporal correlation, adopt the working covariance model

$$\begin{aligned} \mathbb{E}[\varepsilon_i] = 0, \qquad \rho(0) = 1, \\ \mathrm{Cov}(\varepsilon_i, \varepsilon_k) = \sigma_c^2 \rho(|i-k|\Delta t)\,. \end{aligned} \tag{S1}$$

Here $\sigma_c^2 > 0$ is the common marginal variance used in the model, and ρ is the autocorrelation function of the injected error sequence. This model assumes second-order stationarity over the arc. The covariance matrix is assumed to be valid and the variance of the arc mean to be positive. The variance calculations below describe actual uncertainty when this working covariance matches the error covariance; otherwise, they describe the adopted formal uncertainty.

For the arithmetic mean

$$\bar{\varepsilon} = \frac{1}{N}\sum_{i=1}^{N} \varepsilon_i, \tag{S2}$$

the covariance sum gives

$$\begin{aligned} \mathrm{Var}(\bar{\varepsilon}) &= \frac{1}{N^2}\sum_{i=1}^{N}\sum_{k=1}^{N} \mathrm{Cov}(\varepsilon_i, \varepsilon_k) \\ &= \frac{\sigma_c^2}{N^2}\left[N + 2\sum_{j=1}^{N-1}(N-j)\rho(j\Delta t)\right] \\ &= \frac{\sigma_c^2}{N}\left[1 + 2\sum_{j=1}^{N-1}\left(1-\frac{j}{N}\right)\rho(j\Delta t)\right]. \end{aligned} \tag{S3}$$

The factor $N - j$ counts the pairs separated by lag j, and the factor 2 accounts for the two symmetric off-diagonal parts of the covariance matrix. Defining N_{eff} by $\mathrm{Var}(\bar{\varepsilon}) = \sigma_c^2/N_{\mathrm{eff}}$ yields

$$N_{\mathrm{eff}} = \frac{N}{1 + 2\sum_{j=1}^{N-1}\left(1-\frac{j}{N}\right)\rho(j\Delta t)}, \tag{S4}$$

which is Eq. (15) of the main text. This is a finite-arc identity under the adopted covariance model; it does not require an infinite-series approximation.

S1.2 Information inflation and the scalar constraint weight

Under the white-noise assumption, the variance of the same mean is σ_c^2/N. Consequently,

$$F = \frac{N}{N_{\mathrm{eff}}} = \frac{\mathrm{Var}(\bar{\varepsilon})}{\sigma_c^2/N} = 1 + 2\sum_{j=1}^{N-1}\left(1-\frac{j}{N}\right)\rho(j\Delta t). \tag{S5}$$

Thus Eq. (16) of the main text is also the variance inflation factor for the arc mean, relative to the white-noise model with the same marginal variance. An interpretation as information over-injection requires $F > 1$, or a positive weighted sum of the nonzero-lag correlations. Independence gives $F = 1$ and $N_{\text{eff}} = N$, whereas perfectly correlated errors give $F = N$ and $N_{\text{eff}} = 1$. Some negatively correlated sequences can instead have $F < 1$.

Compressing the arc to its arithmetic mean and assigning the reciprocal of its variance as the scalar precision gives

$$q_{\text{WN}} = \frac{N}{\sigma_c^2}, \qquad q_{\text{eff}} = \frac{1}{\text{Var}(\bar{\varepsilon})} = \frac{N_{\text{eff}}}{\sigma_c^2} = \frac{q_{\text{WN}}}{F}. \tag{S6}$$

These quantities compare weights at a common variance scale. If the actual marginal error variance is s^2 rather than σ_c^2, while the correlation function is unchanged, the actual precision of the mean is N_{eff}/s^2. In that case, F isolates the effect of correlation; it does not include any error in the marginal variance assigned to the constraint.

The precision in Eq. (S6) is specific to the arithmetic mean. To distinguish it from the information in the complete observation vector, let $\mathbf{R}$ denote the covariance matrix in Eq. (S1) and $\mathbf{1}$ the vector of N ones. Then

$$q_{\text{eff}} = \frac{N^2}{\mathbf{1}^T\mathbf{R}\mathbf{1}}. \tag{S7}$$

For a Gaussian observation model of a single common scalar, the information obtained by generalized least squares is instead

$$q_{\text{GLS}} = \mathbf{1}^T\mathbf{R}^{-1}\mathbf{1}, \tag{S8}$$

provided $\mathbf{R}$ is positive definite. These expressions are generally different because generalized least squares can assign unequal weights to the observations. They coincide when the covariance matrix has constant row sums. Accordingly, q_{eff} is used here as an equivalent weight for the arc-mean diagnostic, rather than as a general expression for the information in a complete time-varying PPP filter.

S1.3 Fraction of information supplied by the constraint

Let $I_0 > 0$ be the information supplied by the original data for the same scalar quantity, with other estimated parameters allowed to adjust. The following addition of information assumes that the external constraint is treated as independent of the original data. Its information fraction under the white-noise model is

$$\gamma_{\text{WN}} = \frac{q_{\text{WN}}}{I_0 + q_{\text{WN}}}. \tag{S9}$$

Replacing only the external weight by q_{WN}/F, while keeping I_0 fixed, gives

$$\begin{aligned} \gamma_{\text{eff}} &= \frac{q_{\text{WN}}/F}{I_0 + q_{\text{WN}}/F} = \frac{1}{1 + FI_0/q_{\text{WN}}} \\ &= \frac{\gamma_{\text{WN}}}{\gamma_{\text{WN}} + F(1 - \gamma_{\text{WN}})}, \end{aligned} \tag{S10}$$

which proves Eq. (17) of the main text. For $F > 1$, the corrected information fraction is smaller than γ_{WN}. This identity concerns the same scalar model before and after the weight change; its application to an arc-scale PPP diagnostic requires I_0 and both constraint weights to refer to the same quantity and temporal scale.

S1.4 Covariance representation at the injection interval

The autocorrelation in Eq. (S4) must describe the errors at the actual injection epochs. Evaluating a correlation model at multiples of $\Delta t = 300\,\text{s}$ assumes that the model is applicable at those epochs.

This assumption also concerns any error dependence introduced by interpolation. For a product-error component obtained solely by linear interpolation of hourly errors, covariance propagation gives

$$\mathbf{R}_{\text{inj}} = \mathbf{L}\mathbf{R}_{\text{hour}}\mathbf{L}^T, \tag{S11}$$

where $\mathbf{L}$ is the interpolation matrix. If the total constraint error also includes an interpolation approximation error, its covariance and any cross-covariances must be included. The propagated covariance need not have constant diagonal elements or depend only on the lag. Without the stationary, equal-variance approximation, the mean variance is obtained directly as $\mathbf{1}^T\mathbf{R}_{\text{inj}}\mathbf{1}/N^2$, using the covariance of the complete injected error.

A non-decaying covariance component represents a random component shared across epochs. A fixed deterministic bias does not contribute to a centered covariance and is treated separately as a displacement of the constraint value. These distinctions specify the covariance assumptions needed to use the effective sample size as an arc-scale information diagnostic.

S2 Height response to a scalar ZTD constraint

This section derives Eqs. (18)–(19) of the main text and states the conditions needed to use their result as the diagnostic approximation in its Eq. (20). All exact identities below refer to a fixed linear model and a fixed constraint weight.

S2.1 Quadratic model and constraint perturbation

Let $\hat{\mathbf{x}}_0$ be the solution without the external ZTD constraint. The original observations and any retained prior or dynamical information define a symmetric positive-definite normal matrix $\mathbf{N}_0$, scaled so that its inverse is the formal covariance $\mathbf{Q}_0 = \mathbf{N}_0^{-1}$. Up to an additive constant, the original quadratic objective can be written as

$$J_0(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \hat{\mathbf{x}}_0)^T\mathbf{N}_0(\mathbf{x} - \hat{\mathbf{x}}_0). \tag{S12}$$

The linear term vanishes because $\hat{\mathbf{x}}_0$ satisfies the original normal equations.

Let Z and U be the scalar ZTD and height coordinates in the reduced parameter vector. The unit coordinate vectors $\mathbf{e}_Z$ and $\mathbf{e}_U$ select these entries:

$$Z = \mathbf{e}_Z^T\mathbf{x}, \qquad U = \mathbf{e}_U^T\mathbf{x}. \tag{S13}$$

For example, if $\mathbf{x} = (Z, U, a_1, \ldots)^T$, then $\mathbf{e}_Z = (1, 0, 0, \ldots)^T$ and $\mathbf{e}_U = (0, 1, 0, \ldots)^T$.

An independent external scalar constraint with value Z_c and assigned precision $q \geq 0$ adds $q(\mathbf{e}_Z^T\mathbf{x} - Z_c)^2/2$ to Eq. (S12). Its solution $\hat{\mathbf{x}}_c(Z_c)$ therefore satisfies

$$\underbrace{(\mathbf{N}_0 + q\mathbf{e}_Z\mathbf{e}_Z^T)}_{\mathbf{N}_c}\hat{\mathbf{x}}_c(Z_c) = \mathbf{N}_0\hat{\mathbf{x}}_0 + q\mathbf{e}_Z Z_c. \tag{S14}$$

The rank-one term is the constraint contribution to the normal matrix. Comparing the value Z_c with a reference constraint value $Z_c - \delta$, with all other inputs unchanged, gives

$$\Delta\mathbf{x}_\delta \equiv \hat{\mathbf{x}}_c(Z_c) - \hat{\mathbf{x}}_c(Z_c - \delta) = \mathbf{N}_c^{-1}q\mathbf{e}_Z\delta. \tag{S15}$$

If δ is the error relative to an error-free constraint value, this is the parameter perturbation attributable to that error.

The Sherman–Morrison identity gives

$$\mathbf{N}_c^{-1} = \mathbf{Q}_0 - \frac{q\mathbf{Q}_0\mathbf{e}_Z\mathbf{e}_Z^T\mathbf{Q}_0}{1 + q\mathbf{e}_Z^T\mathbf{Q}_0\mathbf{e}_Z}. \tag{S16}$$

Writing $V_Z = \mathbf{e}_Z^T \mathbf{Q}_0 \mathbf{e}_Z > 0$ and multiplying by $q\mathbf{e}_Z\delta$ gives Eq. (18) of the main text:

$$\begin{aligned}\Delta\mathbf{x}_\delta &= \left[q\mathbf{Q}_0\mathbf{e}_Z - \frac{q^2 V_Z \mathbf{Q}_0\mathbf{e}_Z}{1+qV_Z}\right]\delta \\ &= \frac{q\mathbf{Q}_0\mathbf{e}_Z}{1+qV_Z}\,\delta,\end{aligned} \tag{S17}$$

S2.2 ZTD–height coupling and the information fraction

Define $C_{UZ} = \mathbf{e}_U^T \mathbf{Q}_0 \mathbf{e}_Z$. Projection onto the two selected coordinates gives

$$\Delta Z_\delta = \frac{qV_Z}{1+qV_Z}\,\delta, \qquad \Delta U_\delta = \frac{qC_{UZ}}{1+qV_Z}\,\delta. \tag{S18}$$

Thus

$$\Delta U_\delta = \kappa\gamma\delta, \qquad \kappa = \frac{C_{UZ}}{V_Z}, \qquad \gamma = \frac{qV_Z}{1+qV_Z}, \tag{S19}$$

which proves Eq. (19) of the main text.

To interpret κ, prescribe a ZTD displacement z and allow the remaining parameters to adjust so that the original objective increases as little as possible:

$$\min_{\Delta\mathbf{x}} \frac{1}{2}\Delta\mathbf{x}^T\mathbf{N}_0\Delta\mathbf{x}, \qquad \mathbf{e}_Z^T\Delta\mathbf{x} = z. \tag{S20}$$

The Lagrangian stationarity condition is $\mathbf{N}_0\Delta\mathbf{x} = \lambda\mathbf{e}_Z$. The constraint then gives $\lambda = z/V_Z$, so

$$\Delta\mathbf{x}(z) = \frac{\mathbf{Q}_0\mathbf{e}_Z}{V_Z}\,z, \qquad \Delta U(z) = \frac{C_{UZ}}{V_Z}\,z = \kappa z. \tag{S21}$$

Hence κ is the height response per unit ZTD displacement along the minimum-cost adjustment of the original model. It incorporates the other estimated parameters through the full covariance matrix. It is a response slope, rather than a correlation coefficient, and its sign sets the direction of the coupled height response.

Substituting Eq. (S21) into the original quadratic form gives the minimized cost

$$J_{0,\mathrm{prof}}(z) = \frac{z^2}{2V_Z} = \frac{1}{2}I_0 z^2, \qquad I_0 = \frac{1}{V_Z}. \tag{S22}$$

Thus I_0 is the effective scalar ZTD information after allowing the other parameters to adjust. It generally differs from the ZTD diagonal entry of $\mathbf{N}_0$, which describes curvature with the other parameters fixed. Equation (S19) can consequently be written as

$$\gamma = \frac{q}{I_0+q}, \qquad \Delta Z_\delta = \gamma\delta, \qquad \Delta U_\delta = \kappa\Delta Z_\delta. \tag{S23}$$

This establishes the information-share interpretation and connects the height response to Section S1. Using $q = q_{\mathrm{WN}}$ or $q = q_{\mathrm{eff}}$ gives the corresponding information fractions, provided both sections describe the same scalar ZTD quantity.

For fixed $\mathbf{Q}_0$ and δ,

$$\frac{\partial\gamma}{\partial q} = \frac{V_Z}{(1+qV_Z)^2} > 0, \qquad \lim_{q\to 0}\gamma = 0, \qquad \lim_{q\to\infty}\gamma = 1. \tag{S24}$$

Increasing the assigned weight therefore increases the magnitude of the height response when $\kappa\delta \neq 0$, with limiting magnitude $|\kappa\delta|$. Excessive weight amplifies the response to an existing constraint error; the weight alone does not create that error.

S2.3 Constraint-error response and the constrained-minus-unconstrained shift

The perturbation in Eq. (S17) compares two constrained solutions. To obtain the change relative to the solution without the external constraint, subtract $\mathbf{N}_c\hat{\mathbf{x}}_0$ from Eq. (S14). With $\hat{Z}_0 = \mathbf{e}_Z^T\hat{\mathbf{x}}_0$, this yields

$$\begin{aligned} \hat{\mathbf{x}}_c(Z_c) - \hat{\mathbf{x}}_0 &= \frac{q\mathbf{Q}_0\mathbf{e}_Z}{1 + qV_Z}(Z_c - \hat{Z}_0), \\ \Delta U &= \kappa\gamma(Z_c - \hat{Z}_0). \end{aligned} \tag{S25}$$

Let Z^* be the true value of the same scalar ZTD quantity, and define

$$\delta = Z_c - Z^*, \qquad \varepsilon_{Z,0} = \hat{Z}_0 - Z^*. \tag{S26}$$

Then the exact reduced-model relation is

$$\Delta U = \kappa\gamma(\delta - \varepsilon_{Z,0}). \tag{S27}$$

In contrast, the difference between using $Z^* + \delta$ and using Z^* as the constraint remains $\Delta U_\delta = \kappa\gamma\delta$. A zero constraint error therefore does not generally imply a zero constrained-minus-unconstrained height shift. If a reference product replaces Z^* in the data analysis, the same algebra applies to differences from that common reference, but those differences need not equal the true estimation errors.

In the full PPP filter, the response can depend on the complete temporal pattern of the constraint errors and on the state dynamics. For station-day i, a scalar diagnostic representation is

$$\Delta U_i = K_i\delta_i + \eta_i, \qquad K_i = \kappa_i\gamma_i, \qquad \eta_i = -K_i\varepsilon_{Z,0,i} + r_i, \tag{S28}$$

where r_i represents departures from the reduced scalar relation. It is zero within the exact reduced model. The approximation in Eq. (20) of the main text requires the remaining contribution to be sufficiently small for the intended diagnostic. In particular, errors with the same arc mean can produce different responses when their temporal patterns differ. For kinematic processing, the scalar height summary must also be defined consistently with the chosen arc-scale diagnostic.

For a group in which K_i is treated as a constant K, the population slope of a regression with an intercept is

$$\beta = \frac{\mathrm{Cov}(\delta, \Delta U)}{\mathrm{Var}(\delta)} = K + \frac{\mathrm{Cov}(\delta, \eta)}{\mathrm{Var}(\delta)}, \tag{S29}$$

assuming $\mathrm{Var}(\delta) > 0$. Interpreting the fitted slope as K thus requires a sufficiently small covariance between the constraint error and the remaining contribution; a zero mean of that contribution is not sufficient.

When the gains vary between station-days, define the predicted responses as $\widetilde{\Delta U_i} = K_i\delta_i$. For example, an unweighted least-squares fit with an intercept gives the predicted slope

$$\beta_{\mathrm{pred}} = \frac{\sum_i(\delta_i - \bar{\delta})K_i\delta_i}{\sum_i(\delta_i - \bar{\delta})^2}, \tag{S30}$$

where $\bar{\delta}$ is the mean across the station-days in that comparison group. The observed and predicted responses must be subjected to the same regression weights and intercept treatment. A single arithmetic average of K_i is not generally the corresponding predicted slope. Computing K_i without fitting the height shifts avoids calibrating the prediction to its evaluation data, but does not by itself guarantee the covariance condition in Eq. (S29).

References

Bayley GV, Hammersley JM (1946) The "effective" number of independent observations in an auto-correlated time series. Supplement to the Journal of the Royal Statistical Society 8(2):184–197. https://doi.org/10.2307/2983560