

EFFICIENT FITTING OF MULTI-PLANET KEPLERIAN MODELS TO RADIAL VELOCITY AND ASTROMETRY DATA

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ABSTRACT

We describe a technique for solving for the orbital elements of multiple planets from radial velocity (RV) and/or astrometric data taken with 1 m/s and μ s precision, appropriate for efforts to detect Earth-massed planets in their stars' habitable zones, such as NASA's proposed Space Interferometry Mission. We include details of calculating analytic derivatives for use in the Levenberg-Marquardt (LM) algorithm for the problems of fitting RV and astrometric data separately and jointly.

We also explicate the general method of separating the linear and nonlinear components of a model fit in the context of an LM fit, show how explicit derivatives can be calculated in such a model, and demonstrate the speed up and convergence improvements of such a scheme in the case of a five-planet fit to published radial velocity data for 55 Cnc.

Subject headings: astrometry — planetary systems — methods: data analysis — methods: numerical — techniques: radial velocities

1. INTRODUCTION

1.1. *Fitting Keplerian Curves*

The discovery of over 27 multiple-planet systems in recent years (Wright et al. 2009) has required algorithms for disentangling the radial-velocity signature of such complex systems. Because the parameters describing a radial velocity (RV) or astrometric curve are nonlinear, there is no way to fit for them analytically, and they must be found through an algorithmic search. Fitting for the Keplerian parameters of a single orbital companion is usually straightforward given a good period guess, and if necessary a “brute force” mapping of the χ^2 space is usually not computationally prohibitive. Fitting multiple planets involves searching a correspondingly higher-dimensional space and can require substantial computing time.

There is an art to searching such χ^2 spaces efficiently, and in this context there are many “tricks” for finding the global minimum. For instance, a Lomb-Scargle periodogram (Scargle 1982) is often used to identify promising periods for prospective planets, and all of the tallest peaks can be used as starting guesses for the fitting algorithm. In hierarchical systems, the dominant planet can be fit for alone, its signal subtracted from the data, and additional planets can be searched for among the residuals. This process can then be repeated until all of the planets have been identified, and then a full, multi-planet fit on the original data starting at the values found for the individual planets. (e.g. Fischer et al. 2008).

In many multi-planet systems, planet-planet interactions can significantly alter the radial velocity (RV) or astrometric signature of the system. In such cases where interactions are important, a full dynamical (Newtonian)

fit involving an n -body code must be used to properly fit the data and to ensure the short- and long-term stability of the solution. Even in these cases, a multi-planet Keplerian (kinematic) fit, which simply adds the reflex signatures of single planets and ignores planet-planet interactions, is still useful for efficiently identifying planets and providing good initial guesses to the n -body codes.

The Levenberg-Marquardt method (LM; Levenberg 1944; Marquardt 1963) is an efficient algorithm for finding a local minimum in a nonlinear χ^2 space (given good guesses), and is well-suited for the application of RV and astrometric fitting (Press et al. 1992). As a concrete example, we refer in this work to a useful IDL² implementation of this technique, MPFIT by Craig Markwardt³ (Markwardt 2009). Like most implementations of the algorithm, MPFIT requires a user-defined function that accepts, as an argument, trial values for the parameters being solved for, evaluates the model at those values, and returns the corresponding residuals to the data. MPFIT then uses this information to step through parameter space and locate the minimum in χ^2 using a combination of Newton's method and a steepest-descent method. Uncertainties in these parameters can then be calculated by mapping the χ^2 space near this minimum (e.g. Wright et al. 2007) or through error “bootstrapping” (e.g. Butler et al. 2006).

The user-defined function in MPFIT also optionally returns the values of the derivatives of these residuals with respect to the parameters being fit, computed “analytically” or “explicitly”. Absent these derivatives, MPFIT will calculate numerical derivatives with small

² IDL is a commercial programming language and environment by ITT Visual Information Solutions. <http://www.itervis.com/idl/>

³ Available at <http://purl.com/net/mpfit>. MPFIT is a port of MINIPACK-1 from FORTRAN, and is also available in C and Python.

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steps in the fitted parameters and calculating the resulting change in the residuals. The user must choose step sizes that are not too large — thereby missing fine structure in the χ^2 space — or too small — increasing compute time and potentially losing numerical precision. Adding explicit-derivative capability to MPFIT, or any implementation of the LM algorithm, obviates the need for explicitly providing step-sizes, and can greatly improve performance in terms of the number of steps taken and the CPU time consumed per step.

The LM algorithm is useful for finding the best-fitting parameters of a nonlinear model to a set of data from a “frequentist” perspective. A Bayesian approach can provide for more robust estimates of parameter uncertainties, especially when those uncertainties are large. One Bayesian method of exploring complex or high-dimensional spaces is the Markov chain Monte Carlo method (MCMC; Metropolis et al. 1953; Hastings 1970), which has been productively employed in the context of orbital fitting (e.g. Ford 2004; Driscoll & Fischer 2005; Balan & Lahav 2008).

Future space missions, such as NASA’s Space Interferometry Mission (SIM Lite), will obtain μas astrometry of nearby stars, referenced to an inertial astrometric grid. These measurements will be sufficiently precise to detect Earth-mass planets with orbital periods shorter than the mission lifetime. Since multiple-planet systems are common,⁴ interpreting these data in conjunction with precise radial velocity data will require algorithms that can efficiently and robustly search the large nonlinear parameter space of multiple-planet systems.

In this paper, we describe the method of efficiently fitting multi-Keplerian models to such high precision RV and astrometric data separating the parameters into linear and nonlinear components in the context of a LM algorithm, and provide the explicit derivatives used in such a fit. With modifications, the principles here can also be applied to MCMC methods, as well (Catanzarite, Zhai, & Shao 2009; Bakos et al. 2009, e.g.).

1.2. Plan

We begin with an elementary exposition to familiarize the reader with our notation (detailed in Table 2) and provide context for the later discussion. In §2, we explicate the method of exploiting linear parameters in the Kepler problem using the example of an RV time series. The calculation of explicit derivatives in §2.4 is general to any application of the LM algorithm where the model contains both linear and nonlinear parameters. We apply this method to the problem of astrometric data in §3 and specifically to the problem of combined astrometric and RV data in §3.3. We discuss nonlinear terms relevant to μas astrometric work and how to accommodate them in §4. In §5 we quantify the improvement in speed and convergence from exploiting linear parameters and from the use of explicit derivatives in the LM algorithm.

2. AN EXAMPLE: RADIAL VELOCITIES

2.1. Costs and Benefits of Exploiting Linear Parameters

When fitting RV data, there are $5n + 1$ Keplerian parameters to be fit, where n is the number of planets:⁵ P , the period of the planet’s orbit; K , the semi-amplitude of the radial velocity signal; e , the eccentricity of the orbit; ω , the argument of periastron; t_p , a date of periastron passage; and γ , the apparent radial velocity of the center of mass of the system⁶

Exploiting linear parameters, as described below, reduces the search space to $3n$ dimensions (corresponding to P , e , and t_p for each planet) and combines the other orbital elements into a set of linear parameters, which can be solved analytically (and therefore quickly and exactly) at each step in the search. The exact, analytic solution of these linear parameters greatly increases the speed and stability of search algorithms, but at a cost: the nonlinear parameters cannot be varied independently of the linear parameters.

Further reduction in the number of nonlinear parameters per planet is certainly possible. By exploiting an epicyclic or harmonic series expansion one can reduce the problem to only one nonlinear parameter per planet, P_j . Cumming et al. (2003) and Ford (2008) analyze the RV problem in the case of a circular orbits, and discuss the relationship between periodograms and Bayesian approaches to orbit fitting. Konacki & Maciejewski (1999) pursued a method analogous to ours in their approach to RV curve fitting, and Konacki, Maciejewski, & Wolszczan (2002) did the same for astrometry. Such approximations offer a different set of costs and benefits to the one presented here. For instance, when K and e are both large, it may require a large number of terms to adequately describe a set of RV data. We may pursue such an approach in a future version of our code.

The linear parameters in our treatment are not coefficients in a series expansion; rather, we recast the problem, separating linear parameters, which can be solved for exactly with linear algebra, from nonlinear parameters, which must be solved for algorithmically (using LM). As described in §2.2, the linear parameters are algebraic combinations of K , ω , γ , and an optional trend parameter, while P , t_p , and e are nonlinear parameters.

Two complications are introduced by exploiting linear parameters. First, because the linear parameters are computed analytically, and not algorithmically, their errors and covariances with the nonlinear parameters are not computed automatically in the procedure outlined here. (They also cannot be held fixed in the fit, although the issue of fixing the trend parameter can be finessed — see §2.6). The second complication is that computation of the explicit derivatives for the LM algorithm is not straightforward: in the context of the algorithm, the Keplerian model is not a simple function of the $3n$ nonlinear parameters being fit, but also depends on the data. For example, increasing the nonlinear parameter e slightly not only changes the model because it is more eccentric, but also because at this new value of e the linear parameters have different values. These complications can

⁵ Occasionally, an additional “trend” parameter is used to fit out long-term RV trends caused by massive, long-period companions. The other two elements, i , the inclination, and Ω , the position angle of the ascending node, can only be determined astrometrically.

⁶ In practice, γ is degenerate with an arbitrary instrument-dependent RV offset.

⁴ At least 1/4 of known planetary systems show evidence of multiple companions (Wright et al. 2007)

be avoided if one uses the linear basis of the orbits presented here in an ordinary, nonlinear $5n + 1$ parameter fit, but the convergence and speed-up benefits will not be as great.

The sections below describe a general method of calculating an n -planet Keplerian radial velocity model given values for the $3n$ nonlinear parameters, and of calculating the derivatives of that model with respect to those parameters. These equations can be used in a user-defined function for input to an LM minimization code, or a brute-force χ^2 map.

2.2. Linear Parameters in the Radial Velocity Problem

We wish to find the parameters of the n -planet model

$$u(t) = \sum_{j=1}^n [K_j (\cos(\omega_j + f_j(t)) + e_j \cos \omega_j)] + \gamma + d \cdot (t - t_0) \quad (1)$$

which best fits the set of observed radial velocities \vec{v} , measured at times \vec{t} , with uncertainties $\vec{\sigma}$ in a least-squares sense. Here, K_j and ω_j are the usual Keplerian parameters for planet j , γ is the time-independent velocity offset, d is the trend parameter, $f_j(t)$ is the true anomaly of planet j at time t , and t_0 is a conveniently chosen epoch of the observations. The true anomaly is defined implicitly in terms of the other three Keplerian parameters (P_j , $t_{p,j}$, and e_j) through the relations

$$\tan \frac{f_j(t)}{2} = \sqrt{\frac{1+e_j}{1-e_j}} \tan \frac{E_j(t)}{2} \quad (2)$$

$$E_j(t) - e_j \sin E_j(t) = \frac{2\pi(t - t_{p,j})}{P_j} = M_j(t) \quad (3)$$

In Eq. 3 (known as Kepler's Equation) E_j is called the *eccentric anomaly* of planet j , and M is known as the *mean anomaly*.⁷

We identify the linear parameters by rewriting Eq. 1 as

$$u(t) = \sum_{j=1}^n [h_j \cos f_j(t) + c_j \sin f_j(t)] + v_0 + d \cdot (t - t_0) \quad (4)$$

where

$$h_j = K_j \cos \omega_j \quad (5)$$

$$c_j = -K_j \sin \omega_j \quad (6)$$

and

$$v_0 = \gamma + \sum_{j=1}^n K_j e_j \cos \omega_j \quad (7)$$

These linear parameters can be converted back to Keplerian orbital elements through the relations

$$K_j = \sqrt{h_j^2 + c_j^2} \quad (8)$$

$$\tan \omega_j = \frac{-c_j}{h_j} \quad (9)$$

⁷ Instead of t_p , many authors (especially dynamicists) prefer to parameterize orbits in terms of the *mean longitude at epoch*, defined as $M(t_0) + \Omega + \omega$.

(where ω_j is chosen so that $\sin \omega_j$ has the sign of the numerator) and

$$\gamma = v_0 - \sum_{j=1}^n K_j e_j \cos \omega_j \quad (10)$$

The masses of the orbiting planets can be inferred from their corresponding semi-amplitudes K_j , defined for a single-planet system with planet mass m and stellar mass m_* as

$$K^3 = \frac{2\pi G}{P(1-e^2)^{\frac{3}{2}}} \left(\frac{m^3 \sin^3 i}{(m_* + m)^2} \right) \quad (11)$$

where G is Newton's gravitational constant. The fraction in parentheses is known as the *mass function* of the system.

The problem can now be divided into two parts: an algorithmic search through parameter space for the best-fit nonlinear parameters P_j , e_j , and $t_{p,j}$ with a computer routine such as an LM or an MCMC code, and at each step in that search an analytic solution for the linear parameters that fit best there.

2.3. Solving for the Linear Parameters

Given a set of values for the nonlinear parameters, we can fit for the linear parameters in Eq. 4 through χ^2 minimization. We denote the row vector of linear parameters

$$\vec{\beta} = \{h_1, c_1, h_2, c_2, \dots, h_n, c_n, v_0, d\} \quad (12)$$

We define χ^2 the usual way:

$$\chi^2 = \sum_{k=1}^N \frac{(v_k - u(t_k))^2}{\sigma_k^2} \quad (13)$$

and minimize it with respect to each of the linear parameters in $\vec{\beta}$ simultaneously:

$$\frac{\partial \chi^2}{\partial \beta_l} = -2 \sum_{k=1}^N \frac{v_k - u(t_k)}{\sigma_k^2} \frac{\partial u}{\partial \beta_l} \Big|_{t=t_k} = 0 \quad (14)$$

We can express this more compactly by invoking matrix algebra. For the problem of Keplerian orbits, we define the matrix \mathbf{F} as

$$\mathbf{F} = \begin{bmatrix} \cos f_{1,1} & \cos f_{1,2} & \dots \\ \sin f_{1,1} & \sin f_{1,2} & \dots \\ \cos f_{2,1} & \cos f_{2,2} & \dots \\ \sin f_{2,1} & \sin f_{2,2} & \dots \\ \vdots & \vdots & \\ \cos f_{n,1} & \cos f_{n,2} & \dots \\ \sin f_{n,1} & \sin f_{n,2} & \dots \\ 1 & 1 & \dots \\ t_1 - t_0 & t_2 - t_0 & \dots \end{bmatrix} \quad (15)$$

where $f_{j,k} \equiv f_j(t_k)$. This allows us to write the model velocities at times \vec{t} (Eq. 1) as

$$\vec{u} = \vec{\beta} \mathbf{F} \quad (16)$$

We also define the diagonal weight matrix \mathbf{W} such that

$$W_{kl} = \delta_{kl} / \sigma_k^2 \quad (17)$$

where we have used the Kronecker delta symbol. We can then write the system of equations in Eq. 14 as

$$\frac{\partial \chi^2}{\partial \vec{\beta}} = -2(\vec{v} - \vec{\beta} \mathbf{F}) \mathbf{W} \mathbf{F}^T = \vec{0} \quad (18)$$

Solving for $\vec{\beta}$ we have

$$\vec{\beta} = \vec{v} \mathbf{W} \mathbf{F}^T \epsilon \quad (19)$$

where we have denoted the error matrix (also called the variance-covariance matrix)

$$\epsilon = (\mathbf{F} \mathbf{W} \mathbf{F}^T)^{-1} \quad (20)$$

Eq. 19 represents the general solution to the linear least-squares problem for an appropriately defined \mathbf{F} . In the context of Keplerian fits, given a set of nonlinear parameters P , e , and t_p for each planet, the remaining Keplerian orbital elements can be found from $\vec{\beta}$ using Eqs. 8–10.

2.4. Calculation of Explicit (Analytic) Derivatives for Use in the LM Algorithm

The derivative of the model velocities \vec{u} with respect to any nonlinear parameter can be found from Eq. 16:

$$\frac{d\vec{u}}{dx} = \frac{d\vec{\beta}}{dx} \mathbf{F} + \vec{\beta} \frac{d\mathbf{F}}{dx} \quad (21)$$

where x stands for any of the nonlinear parameters (here, P_j , e_j , or $t_{p,j}$).

From Eq. 19 we have

$$\frac{d\vec{\beta}}{dx} = \vec{v} \mathbf{W} \left(\frac{d\mathbf{F}^T}{dx} \epsilon + \mathbf{F}^T \frac{d\epsilon}{dx} \right) \quad (22)$$

From the definition of a matrix inverse we can express the last derivative as

$$\frac{d\epsilon}{dx} = -\epsilon \left(\frac{d}{dx} \epsilon^{-1} \right) \epsilon \quad (23)$$

Using Eq. 20 we then have

$$\frac{d\epsilon}{dx} = -\epsilon \frac{d}{dx} (\mathbf{F} \mathbf{W} \mathbf{F}^T) \epsilon \quad (24)$$

$$= -\epsilon \left(\left(\frac{d\mathbf{F}}{dx} \mathbf{W} \mathbf{F}^T \right) + \left(\frac{d\mathbf{F}}{dx} \mathbf{W} \mathbf{F}^T \right)^T \right) \epsilon \quad (25)$$

Eqs. 16–24 are not specific to the RV Kepler problem, but are a general method of calculating explicit derivatives in a model with both linear and nonlinear parameters, and so can be applied to any analogous problem. For instance, the problem of fitting an orbit using astrometric data also has linear parameters as we show in §3.

2.5. Explicit Derivatives for the Radial Velocity Model

For the case of a Keplerian RV model, from Eq. 15 we have

$$\frac{d\mathbf{F}}{dx} = \begin{bmatrix} -\sin f_{1,1} f'_{1,1} & -\sin f_{1,2} f'_{1,2} & \cdots \\ \cos f_{1,1} f'_{1,1} & \cos f_{1,2} f'_{1,2} & \cdots \\ -\sin f_{2,1} f'_{2,1} & -\sin f_{2,2} f'_{2,2} & \cdots \\ \cos f_{2,1} f'_{2,1} & \cos f_{2,2} f'_{2,2} & \cdots \\ \vdots & \vdots & \ddots \\ -\sin f_{n,1} f'_{n,1} & -\sin f_{n,2} f'_{n,2} & \cdots \\ \cos f_{n,1} f'_{n,1} & \cos f_{n,2} f'_{n,2} & \cdots \\ 0 & 0 & \cdots \\ 0 & 0 & \cdots \end{bmatrix} \quad (26)$$

where $f'_{j,k} \equiv df_{j,k}/dx$. Note that since $f'_{j,k}$ refers to the true anomaly of planet j , it vanishes when x refers to a

parameter of a different planet (e.g., $df_{j,k}/dP_l = 0$ when $j \neq l$). This means that the matrix $d\mathbf{F}/dx$ has only two nonzero rows. We can therefore suppress subscripts below for clarity.

We can calculate the nonzero derivatives as

$$\frac{df}{dx} = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial E} \frac{dE}{dx} \quad (27)$$

where, from Kepler's Equation (Eq. 3), we have

$$\frac{dE}{dP} = \frac{-2\pi(t - t_p)/P^2}{1 - e \cos E} \quad (28)$$

$$\frac{dE}{dt_p} = \frac{-2\pi/P}{1 - e \cos E} \quad (29)$$

$$\frac{dE}{de} = \frac{\sin E}{1 - e \cos E} \quad (30)$$

and from Eq. 2 we have

$$\frac{\partial f}{\partial E} = \sqrt{\frac{1+e}{1-e}} \frac{1 + \cos f}{1 + \cos E} \quad (31)$$

From Eq. 2 we can also write

$$\frac{\partial f}{\partial e} = \frac{2 \tan(E/2) \cos^2(f/2)}{(1-e)\sqrt{1-e^2}} \quad (32)$$

but it is more computationally convenient to note that this happens to simplify to

$$\frac{\partial f}{\partial e} = \frac{\partial f}{\partial E} \frac{\sin E}{1 - e^2} \quad (33)$$

Finally,

$$\frac{\partial f}{\partial P} = \frac{\partial f}{\partial t_p} = 0 \quad (34)$$

Eqs. 22–34 can be used to calculate the terms in Eq. 21, yielding the explicit derivatives used by LM method fitting routines, such as MPFIT.

2.6. Variations on the n -Planet RV Model

In the context of the Kepler problem, the above equations include a parameter for a linear trend in the data. In practice, fitting for such a trend will only occasionally be necessary. When not needed the d parameter in $\vec{\beta}$ and the bottom rows of the \mathbf{F} and $d\mathbf{F}/dx$ matrices can simply be left out of the calculations. Similarly, the trend parameter can effectively be held fixed at a nonzero value by simply subtracting the desired value from the data before fitting.

These matrices can also be easily extended to handle the case of combining data from multiple telescopes between which there exist RV offsets. This is accomplished by extending the data vectors \vec{v} , \vec{t} , and $\vec{\sigma}$ to include data from all telescopes, and extending the vector $\vec{\beta}$ to include a separate offset parameter for each telescope after the first. The corresponding rows of \mathbf{F} must then be filled with 1's in those columns corresponding to data from the appropriate telescope, and 0's elsewhere. Naturally, in $d\mathbf{F}/dx$ the elements of these rows are all 0.

3. APPLICATIONS TO ASTROMETRY

3.1. Astrometry Alone

The above method can also be extended to the problem of fitting for the Keplerian elements of an orbit from astrometric data. Here we present a simplified model of μ as astrometric data of the sort that might be provided by a space observatory such as NASA's Space Interferometry Mission (SIM Lite). We anticipate modifying our algorithms for a more realistic model of interferometric data and its noise sources (Sozzetti 2005; Eriksson & Lindgren 2007; Catanzarite, Law, & Shao 2008) in the near future.

The linear basis for astrometric coordinates are the Thiele-Innes constants (e.g. Binnendijk 1960), and are well documented as useful tools for astrometric curve-fitting (e.g. Casertano et al. 2008). The astrometric perturbations caused by an orbiting companion can be described in terms of six astrometric orbital elements: in addition to e and t_p , we have a , the semi-major axis of the star's apparent orbit on the sky in units of arc; Ω , the longitude of the ascending (approaching) node (measured as a position angle on the sky); i , the inclination of the orbit on the sky (such that $i = 0$ corresponds to a face-on, clockwise orbit); and ω_* , the longitude of periastron of the *star's* orbit.⁸

The Thiele-Innes constants are defined in terms four of the astrometric elements of the star's orbit about the secondary:

$$A = a(\cos \Omega \cos \omega_* - \sin \Omega \sin \omega_* \cos i) \quad (35)$$

$$B = a(\sin \Omega \cos \omega_* + \cos \Omega \sin \omega_* \cos i) \quad (36)$$

$$F = a(-\cos \Omega \sin \omega_* - \sin \Omega \cos \omega_* \cos i) \quad (37)$$

$$G = a(-\sin \Omega \sin \omega_* + \cos \Omega \cos \omega_* \cos i) \quad (38)$$

$$C = a \sin \omega_* \sin i \quad (39)$$

$$H = a \cos \omega_* \sin i \quad (40)$$

These constants can be quickly computed using rotation matrices:

$$\begin{bmatrix} A & B & C \\ F & G & H \\ a \sin i \sin \Omega & -a \sin i \cos \Omega & a \cos i \end{bmatrix} = a R_z(\omega_*) R_x(i) R_z(\Omega) \quad (41)$$

where R is the 3-D rotation matrix

$$R_z(\Omega) = \begin{bmatrix} \cos \Omega & \sin \Omega & 0 \\ -\sin \Omega & \cos \Omega & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (42)$$

and ω_* is the argument of periastron of the orbit of the *star*.

We can transform the Thiele-Innes constants back to Keplerian orbital elements of the planet with the relations:

$$\tan(\omega_* + \Omega) = \frac{B - F}{A + G} \quad (43)$$

$$\tan(\omega_* - \Omega) = \frac{-(B + F)}{A - G} \quad (44)$$

$$\tan^2\left(\frac{i}{2}\right) = \frac{(A - G) \cos(\omega_* + \Omega)}{(A + G) \cos(\omega_* - \Omega)} \quad (45)$$

⁸ The orbital parameters of the star and those of the unseen companion are all identical except a , which differs by a factor of m/m_* , and ω , which differs by π .

$$a = \frac{(A \cos \omega_* - F \sin \omega_*) \cos \Omega - (A \sin \omega_* + F \cos \omega_*) \sin \Omega \sec i}{\cos \Omega} \quad (46)$$

and

$$\omega = \omega_* + \pi \quad (47)$$

where the quadrants of $\omega_* - \Omega$ and $\omega_* + \Omega$ are determined by the signs of the numerators in Eqs. 43 & 44. These relations leave a $\pm\pi$ ambiguity in ω_* , ω , and Ω that can only be resolved by radial velocities, without which convention dictates that we choose the solution with $\Omega < \pi$.

The Thiele-Innes constants C and H are closely related to the c and h constants of Eqs. 5 & 6. The set of six constants have the identity

$$a^2 = A^2 + B^2 + C^2 = F^2 + G^2 + H^2 \quad (48)$$

In astrometry there are five parameters that describe a star's motion in the absence of orbiting companions: $\Delta\alpha_0 \cos \delta$ and $\Delta\delta_0$, the difference between the true and nominal position of the system at t_0 ; μ_α and μ_δ , the proper motions in the RA and Dec directions; and ϖ , the parallax of the system. Our model for the astrometric displacement of a star due to parallax, proper motion, and a system of unseen planets in terms of the Thiele-Innes constants at times $\bar{\tau}$ is:

$$\Delta\delta_k = \sum_{j=1}^n [A_j X_{j,k} + F_j Y_{j,k}] + \Delta\delta_0 + \varpi \Pi_{\delta,k} + \mu_\delta (\tau_k - t_0) \quad (49)$$

$$\Delta\alpha_k \cos \delta = \sum_{j=1}^n [B_j X_{j,k} + G_j Y_{j,k}] + \Delta\alpha_0 \cos \delta + \varpi \Pi_{\alpha,k} + \mu_\alpha (\tau_k - t_0) \quad (50)$$

where X and Y are the so-called elliptical rectangular coordinates, defined as

$$X_{j,k} = \cos E_j(\tau_k) - e_j \quad (51)$$

$$Y_{j,k} = \sqrt{1 - e_j^2} \sin E_j(\tau_k) \quad (52)$$

where E is the eccentric anomaly and the quantities $\Pi_{\alpha,k}$ and $\Pi_{\delta,k}$ refer to the astrometric displacements due to parallax in the α and δ directions⁹ during observation k , which are given by [cite Supplement to Astronomical Almanac here]:

$$\Pi_{\alpha,k} = r_x(\tau_k) \sin \alpha - r_y(\tau_k) \cos \alpha \quad (53)$$

$$\Pi_{\delta,k} = (r_x(\tau_k) \cos \alpha + r_y(\tau_k) \sin \alpha) \sin \delta - r_z(\tau_k) \cos \delta \quad (54)$$

Here (r_x, r_y, r_z) represent the Cartesian components in equatorial coordinates of the position of the observatory, \vec{r} , at time τ with respect to the Solar System barycenter (in units of AU when ϖ is in arcsec). These values for the Earth are available from the NASA Jet Propulsion Laboratory Solar System ephemerides,¹⁰ but for μ as and spaceborne work the precise position of the observatory itself is required.

Note that since a is the apparent semi-major axis of the star's orbit in units of arc, its relationship to the mass of the secondary depends on the method of astrometry used. For astrometric perturbations due to an unseen planet, (that is, absolute astrometric displacements with

⁹ In this paper the bare symbols α and δ will always refer to the nominal right ascension and declination of a star at t_0 , absent the effects of parallax and astrometric displacement from companions.

¹⁰ <http://ssd.jpl.nasa.gov>

respect to the sidereal frame, as measured by SIM Lite) we have from Kepler's Third Law

$$a^3 = \frac{\varpi^3 m^3}{(m_* + m)^2} P^2 \quad (55)$$

where a is measured in arcseconds when P is measured in years, ϖ is the parallax in arcseconds, and m is the mass of the unseen companion and m_* is the mass of the star in solar masses.¹¹

We can now extend Eq.16 to the case of 2-D data by defining our vector of N measurements taken at times τ :

$$[\Delta\delta_1, \Delta\delta_2 \dots \Delta\delta_N, \Delta\alpha_1 \cos \delta, \Delta\alpha_2 \cos \delta \dots \Delta\alpha_N \cos \delta] \quad (56)$$

and our model with linear parameters for n planets:

$$\vec{\beta} = [A_1, B_1, F_1, G_1 \dots A_n, B_n, F_n, G_n, \Delta\delta_0, \Delta\alpha_0 \cos \delta, \mu_\delta, \mu_\alpha, \varpi] \quad (57)$$

and matrix $\mathbf{F} =$

$$\begin{bmatrix} X_{1,1} & X_{1,2} & \dots & X_{1,N} & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & X_{1,1} & X_{1,2} & \dots & X_{1,N} \\ Y_{1,1} & Y_{1,2} & \dots & Y_{1,N} & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & Y_{1,1} & Y_{1,2} & \dots & Y_{1,N} \\ X_{2,1} & X_{2,2} & \dots & X_{2,N} & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & X_{2,1} & X_{2,2} & \dots & X_{2,N} \\ Y_{2,1} & Y_{2,2} & \dots & Y_{2,N} & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & Y_{2,1} & Y_{2,2} & \dots & Y_{2,N} \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\ X_{n,1} & X_{n,2} & \dots & X_{n,N} & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & X_{n,1} & X_{n,2} & \dots & X_{n,N} \\ Y_{n,1} & Y_{n,2} & \dots & Y_{n,N} & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & Y_{n,1} & Y_{n,2} & \dots & Y_{n,N} \\ 1 & 1 & \dots & 1 & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 1 & 1 & \dots & 1 \\ \tau_1 - t_0 & \tau_2 - t_0 & \dots & \tau_N - t_0 & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & \tau_1 - t_0 & \tau_2 - t_0 & \dots & \tau_N - t_0 \\ \Pi_{\delta,1} & \Pi_{\delta,2} & \dots & \Pi_{\delta,N} & \Pi_{\alpha,1} & \Pi_{\alpha,2} & \dots & \Pi_{\alpha,N} \end{bmatrix} \quad (58)$$

The nonzero components of $d\mathbf{F}/dx$ can be calculated from:

$$\frac{dX}{dP} = -\frac{dE}{dP} \sin E \quad (59)$$

$$\frac{dX}{dt_p} = -\frac{dE}{dt_p} \sin E \quad (60)$$

$$\frac{dX}{de} = -\frac{dE}{de} \sin E - 1 \quad (61)$$

$$\frac{dY}{dP} = \sqrt{1 - e^2} \cos E \frac{dE}{dP} \quad (62)$$

$$\frac{dY}{dt_p} = \sqrt{1 - e^2} \cos E \frac{dE}{dt_p} \quad (63)$$

$$\frac{dY}{de} = \sqrt{1 - e^2} \cos E \frac{dE}{de} - \frac{e \sin E}{\sqrt{1 - e^2}} \quad (64)$$

and Eqs. 28–30.

¹¹ In the case where the binary orbit is measured as a separation and position angle of one star with respect to another (i.e., relative astrometry) the measured separation is given by $a^3 = \varpi^3 (m_* + m) P^2$. The application of the techniques here for multiple-planet systems with relative astrometry is not straightforward, and is beyond the scope of this manuscript.

3.2. Astrometry in Arbitrary Coordinates

Astrometry does not always deliver contemporaneous $(\Delta\alpha \cos \delta, \Delta\delta)$ pairs at a common time t . In the general case, a baseline determines the 1-D displacement of a star from some reference at an intermediate position angle on the sky (i.e., not necessarily 0 [as in the case for $\Delta\delta$] or $\pi/2$ [as for $\Delta\alpha \cos \delta$]). We can combine Eqs. 49 & 50 to a more general form to accommodate a heterogeneous set of such data :

$$\begin{aligned} \rho_{\theta,k} = & \sum_{j=1}^n [(A_j X_{j,k} + F_j Y_{j,k}) \cos \theta_k + \\ & (B_j X_{j,k} + G_j Y_{j,k}) \sin \theta_k] + \\ & (\Delta\delta_0 + \varpi \Pi_{\delta,k} + \mu_\delta (\tau_k - t_0)) \cos \theta_k + \\ & (\Delta\alpha_0 \cos \delta + \varpi \Pi_{\alpha,k} + \mu_\alpha (\tau_k - t_0)) \sin \theta_k \end{aligned} \quad (65)$$

where ρ is the separation and θ the position angle of the measurement.

Interestingly, we could also use the other two Thiele-Innes constants to achieve the same result by defining a new linear parameter scheme where the astrometric displacements are described as:

$$\begin{aligned} \rho_{\theta,k} = & \sum_{j=1}^n [H_j S_{j,k} + C_j T_{j,k}] + \\ & (\Delta\delta_0 + \varpi \Pi_{\delta,k} + \mu_\delta (\tau_k - t_0)) \cos \theta_k + \\ & (\Delta\alpha_0 \cos \delta + \varpi \Pi_{\alpha,k} + \mu_\alpha (\tau_k - t_0)) \sin \theta_k \end{aligned} \quad (66)$$

where S and T are defined for the k th measurement and j th planet as

$$\begin{bmatrix} S_{j,k} \\ T_{j,k} \end{bmatrix} = \begin{bmatrix} \cos(\Omega_j - \theta_k) \csc i_j & -\sin(\Omega_j - \theta_k) \cot i_j \\ -\sin(\Omega_j - \theta_k) \cot i_j & -\cos(\Omega_j - \theta_k) \csc i_j \end{bmatrix} \begin{bmatrix} X_{j,k} \\ Y_{j,k} \end{bmatrix} \quad (67)$$

This scheme uses only two linear parameters, instead of four, per planet, and so will not be as efficient, but it is still useful because it can be easily combined with the radial velocity scheme of §2.2. We demonstrate this in §3.3 with a procedure that can accommodate any combination of radial velocity and astrometric data.

We can recover the parameters a and ω from the linear parameters C and H given the nonlinear parameter i by:

$$a_j^2 = \frac{C_j^2 + H_j^2}{\sin^2 i_j} \quad (68)$$

$$\tan \omega_j = \frac{-C_j}{-H_j} \quad (69)$$

where ω_j is chosen so $\sin \omega_j$ has the same sign as $-C_j$.

3.3. Combining Astrometry with Radial Velocities

Combining astrometric data with radial velocity data is not as simple as combining the RV-only and astrometry-only schemes outlined above, because the six linear parameters (A, B, F, G , and c and h) are a combination of only five Keplerian elements (K, a, Ω, ω , and i), and the problem is thus overconstrained. One solution would be to minimize χ^2 subject to the appropriate constraints using Lagrange multipliers, but the resulting set of nonlinear equations may not be guaranteed to have a unique solution and would be difficult to solve for the case of an arbitrary number of planets.

Another solution is to adapt the C and H constants to accommodate general astrometric data, and these constants are closely related to the scheme for RV data used in §2.2. To do this, we define our vector of measurements to be

$$[\vec{v}, \vec{\rho}_{\vec{\theta}}] \quad (70)$$

where the velocities are taken at times \vec{t} and the astrometry at times $\vec{\tau}$, and define our model, as in Eq. 16:

$$\vec{\beta} = [H_1, C_1, H_2, C_2 \dots H_n, C_n, v_0, d, \Delta\delta_0, \Delta\alpha_0 \cos \delta, \mu_\delta, \mu_\alpha, \varpi] \quad (71)$$

From Eqs. 5, 6, 41, & 55 we have:

$$h_j = -\lambda_j H_j \quad (72)$$

$$c_j = \lambda_j C_j \quad (73)$$

where we have introduced a λ , a combination of nonlinear orbital parameters of planet j which has units of velocity and has the value

$$\lambda_j = \frac{2\pi \text{AU}}{\tilde{\omega} P_j \sqrt{1 - e_j^2}} \quad (74)$$

when the estimated parallax, $\tilde{\omega}$, is expressed in arcseconds.

The parameters H_j , C_j , and v_0 can be transformed into $m_j^3/(m_* + m_j)^2$, ω_j , and γ with Eqs. 8–11 & 72–73.

The appearance of ϖ in the definition of λ_j (and therefore in C_j and H_j) indicates a fundamental nonlinearity in the combined RV-astrometry problem: the parallax is not a truly linear parameter. However, because it is nearly linear, if a good estimate of the parallax is available then this can be used in the formula for λ_j (we indicate the approximate nature of the parallax term with a tilde). Once the parallax is solved for more precisely, the fit can be re-run with an improved estimate of ϖ . This procedure should converge very quickly, and we will use it again to deal with other, smaller nonlinear terms in §4.

The first columns of the \mathbf{F} matrix, corresponding to the radial velocity measurements, now read

$$\begin{bmatrix} -\cos f_{1,1}\lambda_1 & -\cos f_{1,2}\lambda_1 & \dots \\ \sin f_{1,1}\lambda_1 & \sin f_{1,2}\lambda_1 & \dots \\ -\cos f_{2,1}\lambda_2 & -\cos f_{2,2}\lambda_2 & \dots \\ \sin f_{2,1}\lambda_2 & \sin f_{2,2}\lambda_2 & \dots \\ \vdots & \vdots & \\ -\cos f_{n,1}\lambda_n & -\cos f_{n,2}\lambda_n & \dots \\ \sin f_{n,1}\lambda_n & \sin f_{n,2}\lambda_n & \dots \\ 1 & 1 & \dots \\ t_1 - t_0 & t_2 - t_0 & \dots \\ 0 & 0 & \dots \end{bmatrix} \quad (75)$$

and the rest of the columns, corresponding to the astro-

metric measurements, read

$$\begin{bmatrix} S_{1,1} & S_{1,2} & \dots \\ T_{1,1} & T_{1,2} & \dots \\ S_{2,1} & S_{2,2} & \dots \\ T_{2,1} & T_{2,2} & \dots \\ \vdots & \vdots & \\ S_{n,1} & S_{n,2} & \dots \\ T_{n,1} & T_{n,2} & \dots \\ 0 & 0 & \dots \\ 0 & 0 & \dots \\ \cos \theta_1 & \cos \theta_2 & \dots \\ \sin \theta_1 & \sin \theta_2 & \dots \\ (\tau_1 - t_0) \cos \theta_1 & (\tau_2 - t_0) \cos \theta_2 & \dots \\ (\tau_1 - t_0) \sin \theta_1 & (\tau_2 - t_0) \sin \theta_2 & \dots \\ \Pi_{\delta,1} \cos \theta_1 + \Pi_{\alpha,1} \sin \theta_1 & \Pi_{\delta,2} \cos \theta_2 + \Pi_{\alpha,2} \sin \theta_2 & \dots \end{bmatrix} \quad (76)$$

For the nonlinear parameters P_j , $T_{p,j}$, and e_j , the two nonzero rows of $d\mathbf{F}/dx$ can be calculated from:

$$\frac{d}{dx}(\cos f(t)\lambda) = -\sin f(t)f'(t)\lambda + \cos f(t)\frac{d\lambda}{dx} \quad (77)$$

$$\frac{d}{dx}(-\sin f(t)\lambda) = -\cos f(t)f'(t)\lambda - \sin f(t)\frac{d\lambda}{dx} \quad (78)$$

where

$$\frac{d\lambda}{dP} = -\frac{\lambda}{P} \quad (79)$$

$$\frac{d\lambda}{de} = \frac{e\lambda}{1 - e^2} \quad (80)$$

$$\frac{d\lambda}{d\Omega} = \frac{d\lambda}{di} = \frac{d\lambda}{dt_p} = 0 \quad (81)$$

and

$$\begin{bmatrix} dS/dx \\ dT/dx \end{bmatrix} = \begin{bmatrix} \cos(\Omega - \theta) \csc i & -\sin(\Omega - \theta) \cot i \\ -\sin(\Omega - \theta) \cot i & -\cos(\Omega - \theta) \csc i \end{bmatrix} \begin{bmatrix} dX/dx \\ dY/dx \end{bmatrix} \quad (82)$$

and Eqs. 27–34, 59–64. Now we have introduced two additional nonlinear parameters, Ω and i .

$$\begin{bmatrix} dS/d\Omega \\ dT/d\Omega \end{bmatrix} = \begin{bmatrix} -\sin(\Omega - \theta) \csc i & -\cos(\Omega - \theta) \cot i \\ -\cos(\Omega - \theta) \cot i & \sin(\Omega - \theta) \csc i \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} \quad (83)$$

and

$$\begin{bmatrix} dS/di \\ dT/di \end{bmatrix} = \begin{bmatrix} -\cos(\Omega - \theta) \csc i \cot i & \sin(\Omega - \theta) \csc^2 i \\ \sin(\Omega - \theta) \csc^2 i & \cos(\Omega - \theta) \csc i \cot i \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} \quad (84)$$

4. NONLINEAR TERMS

4.1. Sources of Nonlinearity

There are several small nonlinear terms which are important at the m/s and μas level, especially for the

nearby and high-proper motion stars likely to be observed by SIM Lite.

Secular acceleration — A star with significant proper motion will have the radial component of its space velocity change with position on the sky, resulting in a secular change in the radial velocity up to ~ 1 m/s/yr for the most extreme cases. Secular acceleration is given, to first order, by:

$$\dot{v}_r = D\mu^2 \quad (85)$$

where, v_r is the bulk radial velocity of the star,¹² D is the star's distance¹³ and μ is the total proper motion in radians per unit time. This term will be absorbed into the linear parameter d , if present, and so could be ignored.

Parallax changes — The change in parallax of nearby stars due to their radial velocity may be of order $0.3 \mu\text{as/yr}$. The shape of the parallactic motion is also a function of position on the sky, and thus of the proper motion. These changes can be of order $5 \mu\text{as/yr}$. The radial velocity term is given by:

$$\dot{\varpi} = -\varpi \frac{v_r}{D} \quad (86)$$

Proper motion changes — The flip side of secular acceleration is proper motion change due to change in distance. This effect can be of order $3 \mu\text{as/yr}$ and is given by:

$$\dot{\mu} = -\mu \frac{v_r}{D} \quad (87)$$

Curvilinear effects — The curvilinear nature of spherical coordinates can produce what are essentially nonlinear terms depending on how astrometric displacements are defined. These effects are on the same order as the above proper motion changes, and more pronounced near the poles. For μas astrometry, it suffices to handle these effects by employing a rectilinear grid:

In this work, astrometric displacements labeled $\Delta\alpha \cos \delta$ and $\Delta\delta$ do not strictly refer to changes in the right ascension and declination of the star, but refer to displacements along rectilinear axes along those dimensions at the nominal position of the star. That is, if the unit vector pointing to the nominal position of the star from the Solar System barycenter is defined:

$$\hat{p} = [\cos \alpha \cos \delta, \sin \alpha \cos \delta, \sin \delta] \quad (88)$$

then the unit vectors pointing east and north are given by

$$\hat{\alpha} = [0, 0, 1] \times \hat{p} \quad (89)$$

$$\hat{\delta} = \hat{p} \times \hat{\alpha} \quad (90)$$

and the astrometric displacements are given by

$$\Delta\delta \equiv \hat{p}' \cdot \hat{\delta} \quad (91)$$

$$\Delta\alpha \cos \delta \equiv \hat{p}' \cdot \hat{\alpha} \quad (92)$$

¹² This quantity v_r defines the true radial velocity of the system with respect to the Solar System barycenter. It differs from the spectroscopic parameter γ in that the latter is often measured with respect to a fiducial frame and can include non-Doppler effects such as instrumental offsets, gravitational redshift, and convective blueshift.

¹³ D is distinguished here from the inverse parallax ϖ^{-1} simply for convenience of units.

where \hat{p}' is the displaced position of the star and $\hat{\delta}$ and $\hat{\alpha}$ are constant.

Interferometric cross terms — The 1-D interferometric measurement of astrometric displacement on the sky may be complicated by the motion of the reference and target stars. That is, the calculation of θ in Eq. 65 may require proper motion advanced or parallax corrected positions in a manner specific to the details of a particular instrument's measurement of θ . These cross terms are likely to be small, and so they can be estimated and refined in the same manner as the other nonlinear terms, if necessary.

RV-astrometry cross terms — The RV semi-amplitude K is related to the astrometric semi-major axis, a , by the parallax, and so ϖ is not strictly a linear parameter in the combined astrometry-RV problem. This effect can be large if the parallax is small or not known, and should not be ignored for any system.

Relativistic Terms — Gravitational deflection by Solar System objects and relativistic stellar aberration produce large, time dependent astrometric displacements that depend on the position of the star, and are therefore slightly nonlinear. Because these displacements can be calculated to better than μas precision given an estimate of the star's true position to arcsecond precision, these effects are ignored here.

4.2. Incorporating Nonlinear Terms

Implementing these small nonlinear effects in our model requires good estimates of the astrometric parameters (when astrometric data is available, these parameters can be estimated from a first-pass solution assuming no planetary companions). The system is then solved using these estimates to calculate the second-order terms above. Below, we indicate these estimated astrometric parameters with a tilde to distinguish them from the solved parameters. These estimates can then be iteratively refined if necessary, but convergence should be very fast for SIM Lite data.

We can include these nonlinear terms by making the following substitutions to the bottom 3 rows of the matrix \mathbf{F} in Eqs. 58 & 76:

$$\tau_k - t_0 \rightarrow \left(1 - (\tau_k - t_0) \frac{v_r}{2\tilde{D}}\right) (\tau_k - t_0) \quad (93)$$

$$\Pi_{\alpha,k} \rightarrow \left(1 - (\tau_k - t_0) \frac{v_r}{\tilde{D}}\right) \Pi_{\alpha,k} \quad (94)$$

$$\Pi_{\delta,k} \rightarrow \left(1 - (\tau_k - t_0) \frac{v_r}{\tilde{D}}\right) \Pi_{\delta,k} \quad (95)$$

and in the definitions of Π_k (Eqs. 53 & 54):

$$\Pi_{\alpha,k} \rightarrow \Pi_{\alpha,k} + (\Delta\tilde{\alpha}_0 \cos \delta + (\tau_k - t_0)\tilde{\mu}_{\alpha})\tilde{r} \cdot \hat{p} \quad (96)$$

$$\Pi_{\delta,k} \rightarrow \Pi_{\delta,k} + (\tilde{\Delta}\delta_0 + (\tau_k - t_0)\tilde{\mu}_{\delta})\tilde{r} \cdot \hat{p} \quad (97)$$

where the quantities in parentheses have units of radians. The estimated terms $\Delta\tilde{\alpha}_0 \cos \delta$ and $\tilde{\Delta}\delta_0$ will likely be zero at first, but may be iteratively refined with the other estimated parameters.

Finally, the secular acceleration can be accommodated by simply subtracting off the appropriate, approximate linear trend to the RV data, or, if the trend parameter is present, allowing it to be absorbed in d .

This procedure of estimating and refining linear astrometric terms will also work for the nonlinear term introduced by the appearance of ϖ in H and C in Eqs. 72 &

72. Alternatively, the parallax can be treated as a non-linear parameter from the outset and eliminated from the linear coefficients in $\vec{\beta}$ entirely.

5. IMPLEMENTATION

5.1. *Public code*

We have implemented these algorithms into a set of IDL software routines which we have made available publicly for the fitting of radial velocity data.¹⁴ The software package includes RVLIN, the user-defined function that may be passed to MPFIT, and RV_FIT_MP, a “wrapper” routine that employs MPFIT to fit a multi-planet Keplerian model to a user-supplied set of radial velocity data. We anticipate maintaining and improving this package, and eventually incorporating astrometric and transit data analysis. This code, or components of it, are currently used by members of the California Planet Search. Below, we discuss our software package’s performance.

5.2. *Speed-up From the Use of Explicit Derivatives*

The use of explicit derivatives above in an LM code significantly speeds up the algorithm by avoiding unnecessary calculation of numerical derivatives. To quantify this improvement, we tested two cases with published RV data, the 2-planet system HD 217107 (Vogt et al. 2005) and the 5-planet system 55 Cnc (Fischer et al. 2008) (in both cases assuming no jitter). We combined the Lick and Keck RV data sets for both cases, solving for all $5n + 2$ parameters (including the RV offset between the two telescopes). We ran over 2,500 trials, where in each trial we started the search with different initial guesses for the orbital elements, each randomly drawn from a normal distribution with a width given by the uncertainty in each parameter and centered on its best-fit value.¹⁵ We compared the total time taken for these trials on a 2.6 GHz Intel Core 2 Duo MacBook Pro running IDL 7.0 using explicit derivatives to the time taken on the same machine with same initial guesses using numerical derivatives.

In the case of HD 217107, the use of explicit derivatives sped up the calculation by a factor of 2.3. The improvement in the case of 55 Cnc was even larger, a factor of 4. The total number of steps taken by MPFIT to converge on a solution was similar in the cases with and without explicit derivatives, indicating that our step sizes for the numeric derivatives were well chosen.

5.3. *Convergence Benefits of Exploiting Linear Parameters*

We employed a custom version of the multi-planet fitting routine often employed by the California and Carnegie Planet search as a baseline to test the improvement in convergence of the algorithm described in this work. This routine, which derives from code described in Marcy & Butler (1992) and Valenti, Butler, & Marcy (1995), is essentially an LM algorithm for searching all

$5n + 1$ parameters with carefully chosen step-sizes for numerical derivatives.¹⁶

Using the same hardware described above, we again fit the Fischer et al. (2008) 55 Cnc RV data from two telescopes. We drew the initial guesses for every parameter from normal distributions centered on the Keplerian best-fit values and with width given by $s\sigma_x$, where σ_x is the parameter uncertainty quoted in Fischer et al. (2008) and s is a scale factor. We varied s smoothly from 0 (where the initial guesses were the best-fit values exactly) to 10 (where every parameter is independently, randomly altered by $10\sigma_x$) over 4000 trials.

We did not attempt to fit for the telescope offset at each trial, as this particular routine was not optimized for such a task. We also did not vary the γ parameter from its best-fit value (though we did fit for it), as no uncertainties were given for γ in Fischer et al. (2008).

We compared the results of this custom code to our LM code employing linear parameters (§5.1) with both explicit and numerical derivatives. In some sense, this is not a fair test since the linear parameter models do not require or accept initial guesses for K and ω , and thus the initial guesses are closer to the best-fit values (since they differ in only 15 dimensions space, whereas the guesses for the nonlinear routine they differ in 25 dimensions.) We thus also ran an additional test, where the fully-nonlinear routine was provided the best-fit values for K and ω for each planet, and thus had only 15 parameters varied (but still had all 26 parameters to fit). With this exception, we provided the same initial guesses to each of the four schemes in each trial.

We recorded the final χ^2 reported by each routine for each trial and compared this with χ_{\min}^2 , the best-fit value. We deemed any trial for which $(\chi^2 - \chi_{\min}^2) < 2$ to be a “successful” convergence on the correct parameters.¹⁷ At each tested value of s , we weighted the full set of trials by a Gaussian window 75 trials wide (corresponding to $\sim 0.19\sigma$) and calculated the fraction on trials that were successful.

In Figure 1 we plot the fraction of successful tests as a function of s . The use of numerical derivatives had no overall effect on the convergence of the linear parameter routine, but was slower, on average, by a factor of 4.

Even with initial guesses $10\sigma_x$ from the best-fit values in all 15 parameters, the linear parameter routine found the global minimum of χ^2 in roughly half of all trials. The fully-nonlinear routine, searching a 26-dimensional space, required much better initial guesses to achieve convergence. With the same 15 parameters varied, fits with initial parameters off by $3\sigma_x$ had only a 20% chance of properly converging. With all 25 orbital parameters varied, the initial guesses had to be within $1.5\sigma_x$ of their proper value to have a 50% chance of convergence. With 26 dimensions to search, there are many wrong paths for the LM algorithm to follow away from the global χ^2 minimum.

6. CONCLUSIONS

¹⁶ That is to say, the only significant differences between the baseline code and the code described in § 5.1 is the exploitation of linear parameters.

¹⁷ $\chi_{\min}^2 \sim 2910$. Our results are only weakly sensitive to the precise definition of “successful”

¹⁴ Available at <http://exoplanets.org/code/>

¹⁵ Although dynamical fits are more precise, here we are only concerned with the algorithm’s convergence in the region of the global χ^2 minimum for a purely Keplerian fit. The initial guesses for the parameters in this and the test in § 5.3 were thus drawn near their values at this (presumed) global minimum.

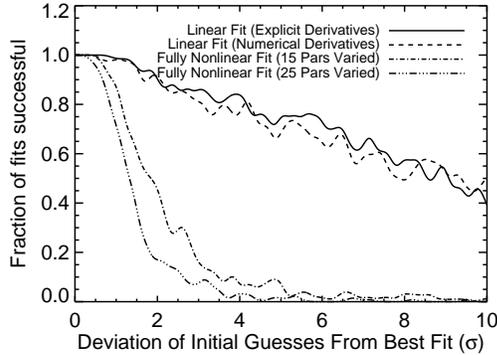


FIG. 1.— Sensitivity of RV-only fitting algorithms to initial guesses on the 5-planet, two-telescope RV data for 55 Cnc (Fischer et al. 2008). Initial guesses to four fitting routines were randomly varied from their best-fit values by various factors of their respective uncertainties. The linear parameter fitting algorithm described in this work converged on the best solution for a wide range of initial guesses, including $\sim 50\%$ of cases with guesses 10σ from nominal. A full, 26-parameter nonlinear fit required guesses within 1.5σ of the best-fit value, or within 2σ if only the 15 truly nonlinear parameters were varied.

Applying linear parameters to the problem of fitting Keplerian curves to radial velocity and astrometry data significantly improves the efficiency and reliability of multi-planet Keplerian fitting routines. This technique can be applied to many methods of searching this complex, nonlinear, multi-parameter χ^2 space, including the Levenberg-Marquardt method, Markov chain Monte Carlo algorithms, and brute force approaches. Table 1 summarizes the various schemes used in this work.

We have identified the nonlinear terms relevant for μ as astrometry and m/s radial velocity work (such as that by SIM Lite and its supporting RV data), and shown how to incorporate these terms into a linear parameter scheme. In §2.4 we have provided analytic forms for explicit derivatives relevant to various applications of the Kepler problem.

In the case of RV-only data, use of explicit derivatives can speed up a fitting routine by a factor of 2–4, depending on the number of planets being fit. Use of linear parameters greatly improves the convergence properties of a multi-planet fitting routine. In the case of an actual 5-planet fit, a linear parameter model requires initial guesses within $10\sigma_x$ of their correct values in only 15 parameters to have a 50% chance of convergence, while

a full, 26-parameter search requires all 26 parameters to be specified within $1.5\sigma_x$.

The principle improvement from use of linear parameters comes from reducing the search space for an n -planet model. In the case of RV fitting, the reduction is from exploiting the linearity of $2n + 1$ of the $5n + 1$ fitted parameters, leaving only $3n$ nonlinear parameters to be fit algorithmically. The problem of fitting astrometric orbits can be similarly treated by exploiting the linearity of $4n + 5$ of the $7n + 5$ parameters, leaving, again, only $3n$ nonlinear parameters to be with a nonlinear fitting routine. When combining RV and astrometric data, as will be the case for SIM Lite, only $2n + 6$ of the $7n + 6$ model parameters are usefully linear under the scheme described here, leaving $5n$ nonlinear parameters.

We have derived a general expression for the explicit model derivatives for models employing linear parameters in nonlinear fits, appropriate for application in the LM method. This result is general and can be applied to problems beyond Keplerian fitting – indeed to any model with both linear and nonlinear parameters.

Eric Agol inspired §2 by pointing out how to exploit the linear parameters in the problem of RV fitting in the context of MPFIT. He has provided substantial guidance and ideas for this and future versions of our code. We thank him, Eric Ford, Matthew Muterspaugh, Tom Loredo, and Alessandro Sozzetti for careful readings of this manuscript and their many substantive and constructive suggestions.

Our membership on a SIM Planet-Finding Astrometry Analysis Team (PI Matthew Muterspaugh) motivated §§3 & 4 of this work, and we are grateful to all of the Teams involved for their efforts and insights into the problem. We thank Jeff Valenti and Nikolai Piskunov for encouraging us to calculate the explicit derivatives for a general linear least-squares problem. Nikolai Piskunov provided insight into the sources of instability in the LM search algorithm. Matthew Muterspaugh provided guidance with the problem of fitting astrometric orbits and understanding the small astrometric cross terms. We thank Martin Sirk, Sam Halverson, and John Asher Johnson for their work employing and debugging various versions of our code. J.T.W received support from NSF grant AST-0504874, and A.W.H. received support from NASA contract NAS7-03001 (JPL#1336910).

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TABLE 1
SUMMARY OF LINEARIZATION SCHEMES

	Radial Velocities	Astrometry	Radial Velocities & Astrometry
Inputs	$\vec{v}(t), \tilde{\mu}, \tilde{\omega},$	$\vec{\Delta}\alpha(\vec{\tau}), \vec{\Delta}\delta(\vec{\tau}), \tilde{\mu}_\alpha, \tilde{\mu}_\delta, v_r, \tilde{\omega}$	$\vec{v}(t), \vec{\rho}_\beta(\vec{\tau}), \tilde{\mu}_\alpha, \tilde{\mu}_\delta, v_r, \tilde{\omega}$
Nonlinear parameters	$P_j, t_{p,j}, e_j$	$P_j, t_{p,j}, e_j$	$P_j, t_{p,j}, e_j, \Omega_j, i_j$
Transformed linear parameters	$c_j, h_j, v_0 \rightarrow \omega_j, K_j, \gamma$	$A_j, B_j, F_j, G_j \rightarrow \omega_j, \Omega_j, i_j, a_j$	$C_j, H_j, v_0 \rightarrow \omega_j, \frac{m_j^3}{(m_* + m_j)^2}, \gamma$
Linear parameters	d	$\Delta\delta_0, \Delta\alpha_0, \mu_\delta, \mu_\alpha, \varpi$	$d, \Delta\delta_0, \Delta\alpha_0, \mu_\delta, \mu_\alpha, \varpi$

NOTE. — The transformed linear parameters v_0 and γ and all of the linear parameters appear once per system. The subscript j on the other parameters indicates that there are n such parameters, one for each companion in the system.

TABLE 2
 VARIABLES AND SYMBOLS USED IN THIS MANUSCRIPT

Symbol	Meaning	Example equation
-	A tilde indicates a first approximation as opposed to a fitted parameter	93
A, B, C, F, G, H	Thiele-Innes constants	41
a	Astrometric semi-major axis of a star's orbit in units of arc	55
α	Nominal right ascension of a system at the epoch of observations, t_0	
$\hat{\alpha}$	Constant unit east vector	89
$\vec{\beta}$	Vector of linear parameters	12
c	Linear parameter in RV fitting corresponding to a component of a planet's RV signature	6
d	Linear parameter in RV fitting corresponding to an RV trend	6
D	Distance to a system	93
$\Delta\alpha \cos \delta, \Delta\delta$	Measured astrometric displacements in units of arc in the $\hat{\alpha}$ and $\hat{\delta}$ directions	49 & 50
δ	Nominal declination of a system at the epoch of observations, t_0	
$\hat{\delta}$	Constant unit north vector	90
δ_{kl}	Kronecker delta	17
γ	Constant (and often instrument dependent) offset in a set of RV data	1
E	Eccentric anomaly of a planet (a function of time)	2
e	Eccentricity of a planet	1
\mathbf{F}	Matrix defined such that the model $\vec{u} = \vec{\beta}\mathbf{F}$	15 & 58
f	True anomaly of a planet (a function of time)	2
θ	Position angle of astrometric displacement such that $\theta = 0$ refers to $\Delta\delta$	42
h	Linear parameter in RV fitting corresponding to a component of a planet's RV signature	5
i	Inclination of a planet's orbit with respect to the sky	41
j	Subscript indicating a quantity corresponds to the j th planet	1
K	RV semi-amplitude of a star's orbit due to planet	1
k	Subscript indicating a quantity corresponds to the k th observation	14
λ	A combination of nonlinear orbital parameters	72
M	Mean anomaly	3
m_*	Mass of the primary component of a binary or planetary system	55
m	Mass of a smaller component of a binary or planetary system	55
$\mu, \mu_\alpha, \mu_\delta$	Proper motion. The total proper motion is given by $\mu^2 = \mu_\alpha^2 + \mu_\delta^2$	58
n	Number of planets in a system	1
N	Number of observations being fit	15
χ^2	The statistic	14
P	Period of a planet	3
\hat{p}	Unit nominal position vector of a star in barycentric equatorial coordinates	88
Π_α, Π_δ	Functions (of time and \vec{r}) describing unit parallactic motion	53 & 54
π	The mathematical constant	
ϖ	Parallax of a system	55 & 58
$R_x(\omega), R_z(\omega)$	The 3-D rotation matrix about the x - or z -axis.	42
\vec{r}, r_x, r_y, r_z	Observatory position in barycentric equatorial coordinates (a function of time)	53 & 54
ρ_θ	Measured astrometric displacement in the direction of position angle θ	65
s	Scale of random deviation of initial guesses from nominal in units of σ_x	§5.3
S, T	Astrometric terms in the \mathbf{F} matrix	67
σ	Measurement uncertainty	14 & 17
σ_x	Uncertainty in an orbital parameter, x	14 & 17
t	Time of a radial velocity observation	1
t_0	Fiducial time at the epoch of the observations	93
t_p	Time of periastron passage of a planet	3
τ	Time of an astrometric observation	
u	Model values, such as velocities or astrometric displacements	1 & 16
v	Measured radial velocities	14
v_0	Linear parameter corresponding to a constant offset in a set of RV data	7
v_r	Radial velocity of a system's barycenter with respect to Solar System barycenter	85
\mathbf{W}	Diagonal matrix containing weights of measured data	17
X, Y	Elliptical rectangular coordinates of a planet (functions of time)	51 & 52
x	As a variable, can stand for any parameter, such as $P_j, t_{p,j}$, or e_j	21
Ω	Position angle of the ascending (approaching) node of a planet	41
ω	Argument of periastron of a planet's orbit	1
ω_*	Argument of periastron of a star's orbit due to a planet. $\omega = \omega_* + \pi$	41