Bayesian Parameter Estimation of Photosynthesis Biochemical Models and Its Application to Grapes in Arid Regions (Postprint)

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Abstract

Using Thompson Seedless grapes as experimental material, net photosynthetic rates were measured at different intercellular CO concentrations across seasons (June–September), and parameters of the photosynthetic biochemical model were estimated using Bayesian methods combined with the Markov Chain Monte Carlo (MCMC) algorithm to obtain seasonal parameter values and compare them with results from the least squares method, thereby exploring the feasibility of Bayesian methods for solving high-dimensional complex model parameter estimation problems and the seasonal variation patterns of key photosynthetic parameters in grapes. The results indicated that maximum carboxylation rate (Vcmax), maximum electron transport rate (Jmax), and triose phosphate utilization rate (TPU) all exhibited distinct seasonal variation patterns, with a trend of initially increasing and subsequently decreasing, peaking in August at 54.30 mol · m ^{2} · s ^{1}, 88.45 mol · m ^{2} · s ^{1}, and 6.56 mol · m ^{2} · s ^{1}, respectively, and reaching minima in September at 34.66 mol · m ^{2} · s ^{1}, 58.86 mol · m ^{2} · s ^{1}, and 4.38 mol · m ^{2} · s ^{1}, respectively. Mesophyll conductance (gm) remained relatively stable across months, with values of 5.16, 5.29, 5.39, and 5.41 mol · m ^{2} · s ^{1} · Pa ^{1} from June to September, respectively. Compared with the traditional least squares method, the Bayesian method yielded slightly lower Vcmax estimates, while no significant differences were observed for Jmax, TPU, and gm. Furthermore, model parameters estimated using the Bayesian method were obtained by incorporating prior parameter information, thereby enhancing their biochemical significance. The study demonstrated that when applying the photosynthetic biochemical model (FvCB model) to simulate photosynthesis, the seasonal variability of its parameters should be fully accounted for; Bayesian parameter estimation combined with the Markov Chain Monte Carlo (MCMC) algorithm provides a more effective solution for parameter estimation in the FvCB model.

Full Text

Biochemically-Based Model for Photosynthetic Parameter Estimation Using Bayesian Method and Its Application in Grapes in Arid Region

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Abstract

Taking Thompson Seedless grape as experimental material, this study measured net photosynthetic rates under different intercellular CO concentrations across different seasons (June–September). Based on the Bayesian method combined with Markov Chain Monte Carlo algorithm, photosynthetic biochemical model parameters were estimated to obtain seasonal model parameter values. These were compared with results from the least squares method to explore the feasibility of the Bayesian method in solving high-dimensional complex model parameter estimation problems and the seasonal variation patterns of key photosynthetic parameters in grapes. Results showed that maximum carboxylation rate (Vcmax), maximum electron transport rate (Jmax), and triose phosphate utilization rate (TPU) all exhibited clear seasonal variation characteristics, showing a trend of first increasing then decreasing, reaching maximum values in August (54.30 μmol·m ^{2}·s ^{1}, 88.45 μmol·m ^{2}·s ^{1}, and 6.56 μmol·m ^{2}·s ^{1} respectively) and minimum values in September (34.66 μmol·m ^{2}·s ^{1}, 58.86 μmol·m ^{2}·s ^{1}, and 4.38 μmol·m ^{2}·s ^{1} respectively). Mesophyll conductance (gm) showed little fluctuation across months, with values of 5.16, 5.29, 5.39, and 5.41 μmol·m ^{2}·s ^{1}·Pa ^{1} from June to September respectively. Compared with the traditional least squares method, Vcmax values estimated by the Bayesian method were smaller, while Jmax, TPU, and gm showed no significant differences. Meanwhile, model parameters estimated by the Bayesian method were obtained based on consideration of prior parameter information, making their biochemical significance more pronounced. The experiment demonstrated that when applying the photosynthetic biochemical model (FvCB model) to photosynthesis simulation, the seasonal variability of its parameters should be fully considered; Bayesian parameter estimation combined with Markov Chain Monte Carlo algorithm can more effectively solve parameter estimation problems in the FvCB model.

Keywords: Arid region; Grape; Bayesian parameter estimation; Biochemical photosynthesis model; Photosynthetic parameter; Seasonal variation

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Abstract: The response of photosynthesis to CO concentration can provide a number of important parameters related to environmental factors. Using white seedless grape as the tested material in this study, net photosynthetic rates of leaves were measured for different intercellular CO concentrations during two typical growing seasons from June to September in 2014 and 2015. A widely used biochemical model (FvCB model) in the simulation of CO and H O gas exchange at the leaf scale was parameterized using data obtained from situ leaf-scale observations. In order to obtain the photosynthetic parameters values, to explore seasonal variations in the photosynthetic parameters in different seasons and to discuss the feasibility and advantage of the Bayesian method in solving high dimensional and complex model parameters estimation, the Bayesian approach was used to estimate the parameters of the FvCB model. In order to generate the Bayesian posterior probability distribution, a version of the Markov Chain Monte Carlo (MCMC) technique was used. In contrast, the least square procedure was used in the application of the same set of observational data. The results showed that maximum ribulose 1.5-bisphosphate carboxylase/oxygenase (Rubisco) carboxylation rate (Vcmax), potential light-saturated electron transport rate (Jmax) and the rate of use of triose-phosphates utilization (TPU) had evident seasonal variations which increased from June to August, and then decreased in September. The maximum values were observed in August (54.30 µmol · m ^{2} · s ^{1}, 88.45 µmol · m ^{2} · s ^{1} and 6.56 µmol · m ^{2} · s ^{1}, respectively) and minimum values in September (34.66 µmol · m ^{2} · s ^{1}, 58.86 µmol · m ^{2} · s ^{1} and 4.38 µmol · m ^{2} · s ^{1}, respectively). The trend in mesophyll conductance (gm) was relatively stable in different months, with respective values of 5.16 µmol · m ^{2} · s ^{1} · Pa ^{1}, 5.29 µmol · m ^{2} · s ^{1} · Pa ^{1}, 5.39 µmol · m ^{2} · s ^{1} · Pa ^{1}, 5.41 µmol · m ^{2} · s ^{1} · Pa ^{1} from June to September. In comparison with traditional least square method, the values of Vcmax estimated by the Bayesian method were relatively small and those of Jmax, TPU and gm had no obvious difference. Also because the estimated parameters by the Bayesian method were obtained after adequate consideration of prior information, each parameter was in biological sense obviously more meaning. As a consequence, it indicated that the Bayesian approach combined with Markov Chains and Monte Carlo (MCMC) sampling algorithm was an effective way of estimation of the parameters in the FvCB model. As the parameters in the FvCB model were different in different seasons, it was necessary to consider these variations in using the parameters in the FvCB model.

Keywords: Arid region; Grape; Bayesian parameter estimation; Biochemical photosynthesis model; Photosynthetic parameter; Seasonal variation

Introduction

In recent years, modeling studies of photosynthesis have attracted increasing attention [1-2]. Among these, the mechanistic photosynthesis model developed by von Caemmerer et al. [3-6] (hereinafter referred to as the FvCB model) has been widely applied in photosynthesis research due to its clear biological significance and has been adopted by most carbon cycle models (such as SiB, CLM, etc.). In this model, maximum carboxylation rate (Vcmax), maximum electron transport rate (Jmax), and triose phosphate utilization rate (TPU) are key parameters characterizing plant photosynthetic capacity. How to estimate these parameters using measured net photosynthetic rate/intercellular CO concentration response curves (A/Ci curves) is not only a hot topic in plant ecology research but also crucial for improving the accuracy of terrestrial carbon cycle simulations [7].

Previous studies have conducted considerable research on model parameter estimation using different plants. Harley et al. [8] and Wullschleger [9] used piecewise estimation methods to estimate Vcmax, dark respiration rate (Rd), and mesophyll conductance (gm) for cotton (Gossypium spp.) and 109 C plant species. However, such methods empirically partition data using an intercellular CO partial pressure of 20 Pa as the node, which is not only subject to large human interference but also difficult to converge when the dataset is small. Dubois et al. [10] and Miao et al. [11] combined grid search with nonlinear least squares methods to simultaneously estimate Vcmax, Jmax, TPU, and Rd. However, this approach approximates the true parameter values by minimizing errors and is more suitable for parameter estimation of continuous functions, making it difficult to obtain globally optimal results for the piecewise discontinuous and high-dimensional FvCB model. Su et al. [12] applied genetic algorithms to estimate the main parameters of the FvCB model, overcoming the drawback of traditional iterative methods that easily fall into local optimal solutions. However, this algorithm tends to have consistent fitness in later stages, making the advantage of superior individuals in producing offspring less obvious and resulting in lower search efficiency in the later stages of algorithm evolution. In recent years, Zhu et al. [13] and Feng et al. [14] have applied Bayesian methods to photosynthetic model parameter estimation, which shows significant advantages over other methods. Compared with other parameter estimation methods, the Bayesian method obtains the distribution range of parameters based on full consideration of observation errors and model structural errors, greatly improving fitting accuracy. However, studies applying this method to photosynthetic biochemical model parameter estimation to obtain model parameters suitable for grapes in the arid regions of northwestern China are still rare.

This study takes grape (Vitis vinifera), an economic crop in typical farmland ecosystems in the arid oases of northwestern China, as the research object. Using a portable photosynthesis-fluorescence measurement system to obtain data on grape net photosynthetic rate varying with intercellular CO concentration in different seasons, we applied the Bayesian method to estimate FvCB model parameters and analyze their relationship with leaf characteristics. This was done to verify the feasibility of the Bayesian method in solving high-dimensional complex model parameter estimation problems, estimate model parameters with biochemical significance, reveal seasonal variation patterns of key photosynthetic parameters in grapes and their relationship with leaf characteristics, enhance understanding of photosynthetic characteristics of grapes as a typical economic crop in arid oases, provide scientific guidance for improving yield in farmland ecosystems, and promote the application of Bayesian methods.

1. Study Area

The experimental site is located in the southwestern part of Nanhu Oasis in Yangguan Town, Dunhuang City, Gansu Province, approximately 70 km from the city center. It is surrounded by mountains on three sides (Sanwei Mountain, Qilian Mountain, and Beisai Mountain) to the east, south, and north, and adjacent to the Taklamakan Desert to the west. The observation point has geographic coordinates of 39°53 N, 94°07 E, at an altitude of 1,100–1,297 m. The region is inland with a warm temperate arid climate, characterized by long sunshine hours, large diurnal temperature variations, scarce precipitation, and high evaporation. The average annual precipitation is 36.9 mm, while the average annual potential evaporation reaches 2,486 mm [15]. The annual sunshine duration is 3,115–3,247 h, and the average annual temperature is 9.3°C. The soil is mainly azonal, including swamp soil, meadow soil, and saline soil. The observation point is located in the southwestern part of Nanhu Oasis, belonging to a farmland ecosystem with oasis irrigation soil. The vineyard undergoes manual flood irrigation once per month in the late ten-day period to ensure plants grow under fully watered conditions.

2.1 Experimental Materials

The experimental material was 'Thompson Seedless' grape (Vitis vinifera), with an average canopy height of 1.84 m, average diameter at breast height of 3.2 cm, and tree age of 13 years. Four plants were randomly selected for measurement of CO response curves (A/Ci) using a portable photosynthesis-fluorescence measurement system (GFS-3000). Observation dates were in June, July, August, and September 2014, covering four typical growth stages: flowering, fruit set, berry growth, and berry maturation. Observation times were on sunny days from 10:00–16:00 during the middle and late ten-day periods of each month. Observation leaves were selected as mature sun-exposed leaves in the upper-middle canopy for in situ measurements under natural conditions in different seasons, with three leaves selected per plant for repeated experiments.

Before measurement, leaves were adapted under saturated light conditions (PARtop = 1,200 μmol · m ^{2} · s ^{1}) for 30 minutes to fully activate enzyme activity. Leaf chamber temperatures (Tcuv) were set to 25°C, 30°C, 30°C, and 20°C for June, July, August, and September respectively, ensuring consistency with natural environmental temperatures of each month. Ambient atmospheric pressure (Pamb) was 86 kPa, leaf temperature (Tleaf) ranged from 24–34°C, sample chamber relative humidity (RH) was controlled at 40%–65% (all within the optimal range for photosynthesis in each month), and air flow rate was 750 µmol · s^{1} to ensure sufficient CO absorption. With these settings unchanged, the absolute CO concentration (CO abs) was adjusted to complete A/Ci curve measurements for different plants and leaves in different seasons. CO abs was initially set to 120 kPa, then sequentially to 100, 80, 60, 50, 40, 30, 20, 10, and 5 kPa (10 levels total). Adaptation at each CO concentration lasted 2–3 minutes before measurement, with three recordings per gradient averaged.

2.2 Model Description

The FvCB model divides the entire photosynthesis process into three limiting stages: the ribulose-1,5-bisphosphate carboxylase/oxygenase (Rubisco) limitation stage, the ribulose-1,5-bisphosphate (RuBP) regeneration limitation stage, and the triose phosphate utilization (TPU) limitation stage. The expressions are [3-5]:

$$A_c = V_{cmax} \times (C_c - \Gamma^*)/[C_c + K_c \times (1 + O/K_o)] - R_d \tag{2}$$

$$\theta \times J^2 - (\alpha \times Q + J_{max})J + \alpha \times Q \times J_{max} = 0 \tag{5}$$

Where: A_n is net photosynthetic rate (µmol · m^{2} · s^{1}); A_c, A_j, and A_p are net CO assimilation rates (µmol · m^{2} · s^{1}) under Rubisco limitation, RuBP limitation, and TPU limitation stages, respectively; V_{cmax} is maximum carboxylation rate (µmol · m^{2} · s^{1}); J is electron transport rate (µmol · m^{2} · s^{1}); TPU is triose phosphate utilization rate (µmol · m^{2} · s^{1}); R_d is dark respiration rate (µmol · m^{2} · s^{1}); Γ^* is CO compensation point (Pa); A is photosynthetic rate (µmol · m^{2} · s^{1}); K_c and K_o are Michaelis-Menten constants for carboxylation and oxygenation (kPa and Pa), respectively; C_c and O are CO partial pressure (Pa) and O partial pressure (21 kPa) in Rubisco [16], respectively; J_{max} is maximum electron transport rate (µmol · m^{2} · s^{1}); g_m is mesophyll conductance (µmol · m^{2} · s^{1} · Pa^{1}); C_i is intercellular CO concentration (Pa); θ is the light response curve slope (0.90); α is the quantum yield of electron transfer (0.30); Q is photosynthetic photon flux density (0.093 µmol · m^{2} · s^{1}) [7].

2.3 Parameter Estimation Methods

Bayes' theorem states that the posterior distribution of parameters is proportional to the product of the prior distribution and the probability density function [17], expressed as:

$$p(\beta|D) \propto p(D|\beta) \times p(\beta) \tag{8}$$

Where: β is the parameter vector composed of parameters to be estimated (including V_{cmax}, J_{max}, TPU, and g_m); D is observation data; $p(\beta|D)$ is the posterior distribution; $p(D|\beta)$ is the probability density function of the sampling distribution; $p(\beta)$ is the prior probability distribution of parameters β; and $p(D)$ is the marginal distribution of random variables. The Markov Chain Monte Carlo (MCMC) method was used for sample extraction [18-20].

The least squares method has been applied earlier in FvCB model parameter estimation. Its basic principle is to find the best functional match for data by minimizing the sum of squared errors [10]. Assuming a dataset $(x_i, y_i), i = 1, 2, ..., N$, and knowing that this dataset satisfies $y = f(a, x)$, where a is the vector of parameters to be determined, the least squares method aims to find a set of parameter values that defines an optimization problem as follows: $\min \sum_{i=1}^{N} [y_i - f(a, x_i)]^2$.

3.1 Photosynthetic Parameter Estimation Results

Using Thompson Seedless grape as the research object, both least squares and Bayesian methods were used to estimate parameters of the FvCB model using the same observational dataset (Figure 1 [Figure 1: see original paper]). The figure shows that parameters varied significantly across seasons for both methods. For parameters V_{cmax}, J_{max}, and TPU, values showed a trend of first increasing then decreasing, reaching maximum values in August and minimum values in September. In contrast, g_m was slightly larger in June and September than in July and August, with consistent seasonal variation patterns between the two parameter estimation methods. Notably, parameter estimation results obtained by the traditional least squares method are single values, while Bayesian method estimation results can provide not only median values but also parameter distribution ranges. Additionally, Table 1 shows that V_{cmax} estimated by the least squares method was greater than that estimated by the Bayesian method across all four months, with the maximum difference reaching 15.51 µmol • m ^{2} • s ^{1} (in September), while parameters J_{max}, TPU, and g_m did not show this pattern.

Unlike the least squares method, the Bayesian method is a parameter interval estimation approach. Its objective is not to find an optimal parameter combination within the feasible parameter interval that yields the best model simulation, but rather to estimate the distribution interval of model parameters at a certain confidence level while fully considering prior information errors. From the prior information and posterior distribution results of parameters in different months (Table 1), it can be seen that the Bayesian parameter estimation method based on prior information can effectively narrow the given prior distribution range of parameters. Defining UR (uncertainty reductions) as the relative reduction in parameter uncertainty (UR = 1 - CI_posterior/CI_prior, where CI_posterior and CI_prior are the 95% confidence intervals of posterior and prior distributions, respectively) [21], for parameters V_{cmax}, J_{max}, and TPU, the relative uncertainty reduction was nearly 50% across different months, reaching up to 72%. In contrast, UR values for g_m were relatively small, only slightly greater than 10% (Table 2). This indicates that parameters V_{cmax}, J_{max}, and TPU converged well and could be well estimated under the Bayesian method.

3.2 Model Evaluation Based on Observed and Simulated Values

The linear regression between net photosynthetic rate estimates based on the Bayesian method ($A_{n,sim}$) and observed net photosynthetic rate values ($A_{n,obs}$) under different intercellular CO concentrations is shown in Figure 2 [Figure 2: see original paper]. The results show high correlation coefficients for all four months, with R^2 values above 0.90. Simultaneously, the observed/fitted trend lines approached the 1:1 line, particularly significantly in August and September (Table 3). Moreover, compared with the least squares method, data points of observed/fitted values from the Bayesian method were distributed overall in regions closer to the 1:1 line, fully demonstrating that the Bayesian method has stronger convergence and obtains higher-precision parameter estimation results.

The response curve of photosynthesis to intercellular CO concentration (A/Ci curve) is an important indicator for analyzing photosynthesis mechanisms. Applying parameter estimation results from different methods to the FvCB model, the A/Ci curve fitting results are shown in Figure 3 [Figure 3: see original paper]. For the Bayesian method fitting results, net photosynthetic rate (A_n) showed three distinct stages with increasing intercellular CO concentration (C_i), consistent with the FvCB model structure: when C_i was relatively low, A_n increased rapidly and linearly with C_i, representing the first stage of photosynthesis—the Rubisco limitation stage; as C_i increased, the rate of increase of A_n with C_i gradually decreased, representing the second stage—the RuBP limitation stage; when C_i continued to increase to a certain value, A_n no longer increased with C_i but stabilized, representing the third stage—the TPU limitation stage. The C_i values corresponding to the transition points between stages 1 and 2 were 31.68 Pa, 48.19 Pa, 50.82 Pa, and 35.67 Pa for the four months, respectively, showing clear seasonal differences. Additionally, the maximum net photosynthetic rates for different months were 13.49, 15.32, 18.49, and 12.28 μmol · m ²· s ¹, respectively, showing the same seasonal variation pattern as the parameter estimation results. For the least squares method fitting results, although ensuring root mean square error remained within a small range, due to interactions between parameters during estimation, only the RuBP regeneration limitation stage and TPU limitation stage were fitted, resulting in less obvious physiological and ecological significance. Thus, compared with the least squares method, the Bayesian method can estimate model parameters with biochemical significance, and the parameter-optimized FvCB model can be used to simulate photosynthetic rates of crops in the arid oases of northwestern China.

Thompson Seedless grape is a perennial woody plant. The estimated ranges of parameters V_{cmax}, J_{max}, and TPU are similar to the results of Wullschleger [9], who selected 109 C plant species and estimated parameter values for different vegetation types based on nonlinear regression techniques of A/Ci curves, providing parameter ranges: V_{cmax} of 6–94 μmol · m ²· s ¹, J_{max} of 17-372 μmol · m ²·

s $^{-1}$, and TPU of 4.9–20.1 μmol · m $^{-2}$ · s $^{-1}$, with annual herbaceous plants having greater parameter values than perennial woody plants. This study accurately estimated model parameters using the Bayesian method, with results within the ranges given by previous studies. Meanwhile, traditional parameter estimation methods, such as Harley et al. [8] who used piecewise methods to estimate V_{cmax}, R_d, and g_m, set the transition point between Rubisco limitation and RuBP limitation stages in A/Ci curves as a fixed value. In contrast, Bayesian fitting results in this study showed clear seasonal differences in transition points, reflecting that piecewise estimation methods are subject to large errors due to artificial partitioning. Sharkey et al. [7] used Microsoft Excel to simultaneously estimate V_{cmax}, J_{max}, TPU, R_d, and g_m; Dubois et al. [10] and Miao et al. [11] combined grid search with nonlinear least squares methods to estimate V_{cmax}, J_{max}, TPU, and R_d. These methods are derived optimization approaches that not only involve large computational loads and are highly sensitive to initial value settings, but are also suitable for parameter estimation of continuous functions, making it difficult to obtain globally optimal results for the piecewise discontinuous FvCB model. In contrast, the Bayesian method does not require minimizing objective functions through derivative functions while incorporating prior information, giving it great superiority in solving parameter estimation problems for high-dimensional complex discontinuous functions. This study is the first to apply this method in the extremely arid Dunhuang Oasis of western China, accurately estimating model parameters for the main local economic crop grape during typical growing seasons (June, July, August, and September) and different stages (flowering, fruit set, berry growth, and berry maturation), providing guidance for improving yield in farmland ecosystems and offering insights for terrestrial ecosystem carbon cycle model research.

The parameter estimation results for different months showed clear seasonal differences, related to nitrogen allocation strategies in grapes across seasons. Thompson Seedless grape is a C_3 plant, with approximately 60%–80% of leaf nitrogen existing in leaves in the form of nucleic acids and enzymes [22-23]. Previous studies have shown that leaf nitrogen content is positively correlated with photosynthetic capacity [24-25]. In months with stronger photosynthetic capacity, more nitrogen is required and enzyme activity is stronger; conversely, in months with weaker photosynthetic capacity, less nitrogen is consumed and enzyme activity is weaker [26-27]. V_{cmax} is the most important parameter in the Rubisco limitation stage, where CO_2 fixation is constrained by Rubisco activity. Therefore, in August, parameter V_{cmax} also reached its maximum value. In September, representing the berry maturation stage, leaves tended to senesce with weaker enzyme activity. When large amounts of nitrogen were not consumed, leaf nitrogen was transferred to and stored in the xylem, and parameter V_{cmax} showed lower values. Similarly, parameters J_{max} and TPU, acting in the RuBP limitation stage and TPU limitation stage respectively, also showed the same seasonal variation characteristics. Parameter g_m, however, is more affected by temperature and solar radiation. July and August had higher temperatures and stronger solar radiation compared with June and September. During these periods, leaves closed stomata to prevent excessive water loss through evaporation, resulting in smaller stomatal conductance.

Conclusion

The main conclusions of this study are as follows:

1) Based on the Bayesian method, the ranges of four main parameters in the FvCB model were estimated: maximum carboxylation rate (V_{cmax}) of 23.76–90.69 µmol · m ² · s ¹, maximum electron transport rate (J_{max}) of 47.26–123.98 µmol · m ² · s ¹, triose phosphate utilization rate (TPU) of 3.14–8.61 µmol · m ² · s ¹, and mesophyll conductance (g_m) of 1.42–9.40 µmol · m ² · s ¹ · Pa ¹.

2) Parameter values showed clear seasonal variation patterns. Maximum carboxylation rate (V_{cmax}), maximum electron transport rate (J_{max}), and triose phosphate utilization rate (TPU) showed a trend of first increasing then decreasing, with maximum values in August and minimum values in September. Stomatal conductance (g_m) was slightly larger in June and September than in July and August.

3) Compared with the traditional least squares method, Bayesian parameter estimation can effectively solve parameter estimation problems for high-dimensional complex discontinuous models and can effectively estimate reasonable parameter values with biochemical significance based on observational data.

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Note: Figure translations are in progress. See original paper for figures.