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INTERNATIONAL SOCIETY FOR BAYESIAN ANALYSIS

# THE ISBA BULLETIN Official bulletin of the International Society for Bayesian Analysis

#### **MESSAGE FROM THE PRESIDENT**

#### Sudipto Banerjee president@bayesian.org

With the year winding down and the holidays upon us, I wish all of you the very best for the season as I write my last message as 2022 ISBA President for this bulletin. Let me reiterate what a privilege and honour it has been for me to serve this incredible Society together with my remarkable colleagues on the Executive Committee. I absorbed much from the wisdom and leadership of my predecessor, Igor Pruenster, and from the invigorating energy and enthusiasm of my successor, Amy Herring, who will begin her term on January 01, 2023. While I look forward to working with President Herring in the coming year, I wish to express my deepest appreciation to Igor as he completes his term as Past President and retires from the ISBA leadership. It is difficult for me to imagine an Executive Committee without Igor's presence, but his "retirement" is welldeserved and I am confident that he will always be there for ISBA whenever needed.

It has also been my pleasure serving with Executive Secretary Donatello Telesca, who will continue serving in this capacity until 2024, and Treasurer Marian Farah, who completes her service at the end of the year. I have never hesitated to pester them with questions and clarifications and they have always responded with patience and promptitude. The ISBA leadership considers the financial health of the Society of utmost importance and the Treasurer undertakes a significant amount of responsibility in keeping our accounts updated. The biennial World Meetings see this role accentuated and this year was especially demanding, given the organisation and conduct of the 2022 World Meeting in Montreal amid unprecedented uncertainties because of the pandemic. Marian has been splendid in conducting her affairs and I thank her deeply for the service she has rendered in this crucial year.

I take this opportunity to thank all the ISBA officers who have contributed immensely with their service throughout the past year. In particular, I wish to thank Francois Caron (University of Oxford), Miguel de Carvalho (University of Edinburgh), Nial Friel (University College, Dublin) and Laura Ventura (University of Padova) for their dedicated service over the last three years as members of ISBA's Board of Directors. It has been a pleasure working closely with them in an environment of shared governance as we strive to ensure that the intellectual pursuits and global synergies that ISBA aims to foster and support across the world continues unabated.

> IN THIS ISSUE FROM THE EDITOR SOFTWARE HIGHLIGHT UPDATES FROM BA JUNIOR ISBA FROM THE PROGRAM COUNCIL NEWS FROM THE WORLD

Let us welcome our two newly elected officers in the Executive Committee, President-Elect Aad van der Vaart (Delft Institute of Applied Mathematics) and ISBA Treasurer Yanxun Xu (Johns Hopkins Whiting School of Engineering), and newly elected directors to the ISBA Board: Tamara Broderick (Massachussetts Institute of Technology), Subhashis Ghoshal (North Carolina State University), Claire Gormley (University College, Dublin) and Matteo Ruggiero (University of Torino). The transition of the newly elected officials into their new roles is being facilitated by the tireless efforts of the Executive Secretary Donatello Telesca.

Reflecting on this past year, I distinctly recall the discussions and meetings we held in the first half of the year over the uncertainties surrounding the 2022 World Meeting in Montreal, Canada. That the meeting was successfully held on site (see my message in the September 2022 Bulletin) is a massive testament to the tenacity and relentless efforts of the local organising committee (chaired by Alexandra Schmidt), the scientific committee (chaired by Botond Szabo) and all our members who grappled with and overcame the challenges presented by an ongoing pandemic and geopolitical uncertainties to attend the meeting. This event, along with several other regional meetings, workshops and conferences held throughout the year, affirms the vibrancy present in our Society.

In my September 2023 message carried by this bulletin I pointed out an impressive growth in ISBA's membership and the vivacity and exuberance exhibited by several of ISBA's sections including, perhaps most prominently, by j-ISBA (short form for Junior ISBA). This section stands today as the section with the highest membership. Among numerous impressive initiatives that have have helped ISBA register an impressive growth in its membership, j-ISBA administers the Blackwell-Rosenbluth Awards to recognise six outstanding junior Bayesian researchers based on their overall contribution to the field and to the community. I am extremely pleased to congratulate the winners Sharmistha Guha (Texas A&M University), Simon Mak (Duke University) and Akihiko Nishimura (John Hopkins University) from coordinated universal time-zones UTC-12 to UTC-1 (the Americas); and Jeremy Heng (ESSEC Business School, Singapore), Swapnil Mishra (University of Copenhagen); and Leah South (Queensland University of Technology) from UTC+0 to UTC+13 (Africa, Asia, Europe and Oceania). These talented early-career scholars will, I am sure, contribute immensely to the future growth of ISBA.

While much of the this year was devoted to the planning and successful conduct of the World Meeting, the months since have witnessed discussions surrounding future ISBA initiatives. Notably, the Program Committee comprising Matthias Katzfuss (Chair), Sinead Williamson and Botond Szabo have solicited and reviewed pre-proposals for the 2026 and 2028 World Meetings. In my own interactions with members in different parts of the world—from the Americas to Japan to South Africa—I have witnessed keen interest in hosting these World Meetings. There is, now, a template available for applicants to construct their proposals for hosting World Meetings. New proposals will be expected to address (i) facilities for childcare, which was officially introduced as a conference facility in Montreal, and is expected to become a regular feature for World Meetings going forward); and (ii) the possibility for holding the conference in hybrid format. In addition to matters of hosting the World Meetings, the ISBA leadership will continue to brainstorm on how to assist the different chapters and sections to conduct their affairs including the hosting of regional meetings.

ISBA has registered impressive growth in membership over the last year with currently over 1230 members and is also in robust financial health. Nevertheless, I believe we have a long road ahead to fulfil our potential for further growth. Therefore, allow me to remind you to renew your membership and also encourage your students, collaborators and colleagues to join ISBA. ISBA is a truly special association that has served our profession admirably since its inception in 1992 and has witnessed the massive growth of Bayesian statistics over the years. Student memberships are available at a very reasonable USD 5/- per year. I especially encourage you to join and participate in the different Sections of ISBA listed under https://bayesian.org/. The vitality of these Sections ensures the growth and expansion of the synergistic scholarly activities that our Society strives to achieve. I hope ISBA will see many new faces in the coming year among its members. The link to renew your membership and join the Sections is available from the ISBA homepage (https://bayesian.org/) or at https://bayesian.org/poinrenew.

#### FROM THE EDITOR

#### Gregor Kastner

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Just in time before the year comes to an end and daylight hours are longest/shortest, I present to you with pleasure 2022's final ISBA Bulletin. Let me take the chance to thank all contributors for their dedicated service and their timely deliveries; what a delight it is to be editor with such a marvelous team of collaborators! And finally, from snowy Klagenfurt, Austria, my best wishes go out to all of you and those close to your hearts.

#### SOFTWARE HIGHLIGHT

# Annie Sauer

## deepgp: AN R-PACKAGE FOR BAYESIAN DEEP GAUSSIAN PROCESSES

The deepgp package provides a fully-Bayesian implementation of deep Gaussian process (DGP) regression models via Markov Chain Monte Carlo (MCMC). The package was designed with an eye towards surrogate modeling of computer experiments. It supports several acquisition criteria for strategic sequential design and offers optional Vecchia-approximation for faster computations with larger data sizes. Computations are performed in C/C++ under-the-hood, with optional parallelization through OpenMP and SNOW. Here, I provide an overview of the package's features; see Sauer et al. (2022b) and Sauer et al. (2022a) for methodological details.

Traditional Gaussian processes (GPs) are popular nonlinear regression models, preferred for their closed-form posterior predictive moments, with relevant applications to Machine Learning (ML; Rasmussen and Williams, 2005) and computer experiment surrogate modeling (Santner et al., 2018; Gramacy, 2020). In their canonical form, GPs suffer from the limitation of stationarity due to reliance on covariance kernels that are strictly functions of Euclidean distance. Deep Gaussian processes (Damianou and Lawrence, 2013) address this stationarity limitation through functional compositions of Gaussian layers. Intermediate layers act as warped versions of the original inputs, allowing for non-stationary flexibility. A "two-layer" DGP may be formulated as

$$\begin{array}{ll} Y \mid W \sim \mathcal{N}\left(0, \Sigma(W)\right) \\ W_i \sim \mathcal{N}\left(0, \Sigma(X)\right) \quad \text{for} \quad i = 1, \dots, p \end{array} \quad \text{with} \quad \Sigma(X)^{ij} = \Sigma(x_i, x_j) = \tau^2 \left(k \left(\frac{||x_i - x_j||^2}{\theta}\right) + g\mathbb{I}_{i=j}\right) \end{array}$$

where  $k(\cdot)$  represents a stationary kernel function (deepgp offers both the squared exponential and Matérn). Note, each of the two layers is a typical GP with a stationary covariance. These covariances depend on hyperparameters  $\tau^2$ ,  $\theta$ , and g controlling the scale, lengthscale, and noise respectively. Latent layers are noise-free with unit scale (i.e. g = 0 and  $\tau^2 = 1$  for each  $W_i$ ). The intermediate latent layer W is unobserved and presents an inferential challenge (it can not be marginialized from the posterior analytically). Many have embraced variational inference for fast, thrifty approximations (Salimbeni and Deisenroth, 2017; Marmin and Filippone, 2022). The deepgp package offers an alternative, fully-Bayesian sampling-based inferential scheme as detailed in Sauer et al. (2022b). This sampling approach provides full uncertainty quantification (UQ), which is crucial for sequential design.



Figure 1: (Left/middle) Trace plots of outer/inner lengthscales. (Right) ESS samples of W.

# **Model Fitting**

Latent Gaussian layers are sampled through elliptical slice sampling (ESS; Murray et al., 2010). Kernel hyperparameters are sampled through Metropolis Hastings sampling (except  $\tau^2$  which can be marginialized analytically under an inverse gamma reference prior, see Gramacy (2020), Chapter 5). All of these are iterated in a Gibbs scheme. MCMC sampling for one-, two-, and three-layer models is wrapped in the fit\_one\_layer, fit\_two\_layer, and fit\_three\_layer functions respectively, each creating unique S3-class objects (the one layer model is not deep, rather it is a typical stationary GP used for benchmarking).

As a simple example, consider a one-dimensional step function (visualized momentarily in Figure 2).

```
library(deepgp)
x <- seq(0, 1, length = 8)
y <- as.numeric(x > 0.5)
x_pred <- seq(0, 1, length = 100) # predictive grid</pre>
```

The following code "trains" a two-layer DGP model by conducting MCMC sampling of W (with dimension matching the dimension of X as default) and lengthscale hyperparameters for each layer. I specify the squared exponential kernel and, presuming I know the data is noiseless, I fix the noise parameter using true\_g = 1e-6 (if this input is not specified, the g parameter on the outermost layer is estimated through MCMC). After sampling, I generate trace plots of the two lengthscales and plot some sampled W curves.

```
fit <- fit_two_layer(x, y, nmcmc = 10000, cov = "exp2", true_g = 1e-6)
plot(fit, trace = TRUE, hidden = TRUE)</pre>
```

The resulting plots are shown in Figure 2. Each line in the rightmost pane represents a single ESS sample of W. Since 10,000 lines would make for a dense plot, an evenly spaced subset of samples is shown. The samples are colored on a gradient – red lines are the earliest iterations and yellow lines are the latest. By default, W is initialized at the identity mapping, shown by the red line along the diagonal W = X. The samples quickly settle in to a step pattern to accommodate the nature of the response surface, flipping back and forth between mirror images which are equivalent in terms of pairwise Euclidean distance. While burn-in is hard to visualize in this functional form, we can see that the yellow lines (later samples) have settled in after some adjustments from the red lines (earlier samples).



Figure 2: Posterior mean and 95% prediction intervals for one-, two-, and three-layer models.

Burning/thinning of samples is implemented in trim, with posterior predictions generated by predict.

```
fit <- trim(fit, 5000, 2) # cut-off burn-in, thin by half
fit <- predict(fit, x_pred)
plot(fit)</pre>
```

The predictive surface for the two-layer DGP is shown in the middle panel of Figure 2. To compare models, I repeated the above code after swapping out fit\_two\_layer with fit\_one\_layer and fit\_three\_layer to fit a one-layer GP and three-layer DGP. The resulting predictions are shown in the left and right panels. The stationary one-layer GP is un-able to adapt to the step-wise nature of the surface. The two-layer and three-layer DGPs are flexible enough to handle the abrupt regime shift.

# **Sequential Design**

Sequential design (also called "active learning") is the process of sequentially selecting training locations using a statistical "surrogate" model to inform acquisitions. Acquisitions may target specific objectives including minimizing posterior variance or optimizing the response. The non-stationary flexibility of a DGP, combined with full UQ through Bayesian MCMC, is well-suited for sequential design tasks. Where a typical stationary GP may end up space-filling, DGPs are able to target areas of high signal/high interest (Sauer et al., 2022b).

The deepgp package implements the Integrated Mean Squared Error (IMSE) acquisition criterion (Sacks et al., 1989), targeting minimal posterior variance, in the IMSE function. The following code evaluates this criterion for the model above using the predictive grid as candidates and plots the resulting values. Results are shown in the right panel of Figure 3. The next acquisition is chosen as the candidate that produced the minimum IMSE (highlighted by the blue triangle).

```
imse <- IMSE(fit, x_pred)
plot(x_pred, imse$value, type = "l", ylab = "IMSE")
points(x_pred[which.min(imse$value)], min(imse$value), pch = 17, cex = 1.5, col = 4)</pre>
```

Again, to provide some contrast, I repeated the above code with the one-layer GP (left panel of Figure 3). Whereas the one-layer model is inclined to space-fill with low IMSE across most of the



Figure 3: IMSE criterion with minimum marked by a blue triangle.

domain, the two-layer model appropriately targets acquisitions in the middle region, where uncertainty is highest. The sum approximation to IMSE, referred to as Active learning Cohn (ALC; Cohn, 1994) in the ML literature, is similarly implemented in the ALC function.

If the sequential design objective is instead to minimize the response, the expected improvement criterion (EI; Jones et al., 1998) is offered by specifying the argument EI = TRUE within the predict function. See Gramacy et al. (2021) for discussion on EI with DGPs.

# **Vecchia Approximation**

The Bayesian DGP suffers from the computational bottlenecks that are endemic in typical GPs. Inverses of dense covariance matrices experience  $O(n^3)$  costs. The Vecchia approximation (Vecchia, 1988) circumvents this bottleneck by inducing sparsity in the precision matrix (Katzfuss et al., 2020; Katzfuss and Guinness, 2021). The sparse Cholesky decomposition of the precision matrix is easily populated in parallel, making for fast evaluation of Gaussian likelihoods and posterior predictive moments. In addition to the original, un-approximated implementation, the deepgp package offers the option to utilize Vecchia approximation in all under-the-hood calculations. Vecchia approximation is triggered by specifying vecchia = TRUE in any of the fit functions.

```
fit <- fit_two_layer(x, y, nmcmc = 10000, vecchia = TRUE)</pre>
```

Details are provided in Sauer et al. (2022a). While the original implementation was only suitable for data sizes in the hundreds, the Vecchia option allows for feasible computations with data sizes up to a hundred thousand.

# **More Information**

The deepgp package is supported by a git repository of examples.<sup>1</sup> While I showcased a simple one-dimensional step function, the simulated examples provided in the repository span up to six dimensions, with training data sizes up to tens of thousands. Real-world applications to computer

<sup>&</sup>lt;sup>1</sup>https://bitbucket.org/gramacylab/deepgp-ex/

experiments include a three-dimensional simulation of the Langley Glide Back Booster (LGBB; Pamadi et al., 2004) and the seven-dimensional Test Particle Monte Carlo Simulator (TPM) of a satellite in low earth orbit (Sun et al., 2019), with training data sizes ranging from n = 300 to n = 100,000.

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### UPDATES FROM BA

# Mark Steel

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I only have a brief update, in which I would like to report on an upcoming change of the Managing Editor and on webinars.

Following the usual term of appointment, Jing Cao (Southern Methodist University; https://www. smu.edu/Dedman/Academics/Departments/Statistics/People/FacultyDirectory/JCao) will step down as Managing Editor of the journal. As of January 1, 2023, she will be succeeded by Maria Kalli (King's College, London; https://www.kcl.ac.uk/people/maria-kalli). I want to take the opportunity to thank Jing very much for her dedication to this crucial role and all the hard work she put in over the last three years in support of the journal and I greatly look forward to working with Maria in the near future.

Bayesian Analysis regularly publishes papers with discussion. These are normally presented in webinars shortly before publication where the author(s) present their main findings and the invited discussants provide comments. In addition, other participants also have an opportunity to ask questions or participate in the discussion. On December 6 we had a very successful webinar (with over 80 participants from around the world) focused on the paper "Deep Gaussian Processes for Calibration of Computer Models" by Sébastien Marmin and Maurizio Filippone. A recording of this event can be found at https://www.youtube.com/watch?v=K\_hPbvoo0\_M. The next webinar will be devoted to the paper "Evaluating Sensitivity to the Stick-Breaking Prior in Bayesian Nonparametrics" by Ryan Giordano, Runjing Liu, Michael I. Jordan and Tamara Broderick. The manuscript can be accessed at https://doi.org/10.1214/22-BA1309 and I would like to invite all of you to participate in the webinar. Date and time will be advertised closer to the event (probably in March 2023). In this context, I want to convey my sincere thanks to Tommaso Rigon, the ISBA Social Media Manager for his invaluable help in organising and technically supporting the webinars.

Finally, I wish you all a wonderful Christmas break and a happy, healthy and productive New Year!

# JUNIOR ISBA

#### Cecilia Balocchi cecilia.balocchi@ed.ac.uk

#### Blackwell-Rosenbluth Award

Please, join me in congratulating the recently announced winners of the Blackwell-Rosenbluth Award! This is the second edition of the award, which recognizes outstanding junior Bayesian researchers, based on their overall contribution to the field and to the community. The award is assigned to three winners from the UTC+ region (based on the time zones UTC+0 to UTC+13) and three winners from

the UTC- region (based on the time zones UTC-12 to UTC-1).

#### UTC+ winners

- Jeremy Heng, ESSEC Business School, Singapore
- Swapnil Mishra, University of Copenhagen
- Leah South, Queensland University of Technology

#### UTC- winners

- Sharmistha Guha, Texas A&M University
- Simon Mak, Duke University
- Akihiko Nishimura, John Hopkins University

The winners presented their work at two special events of Junior Bayes Beyond the Borders (JB<sup>3</sup>) on November 28th and 29th, hosted by Universidad Nacional Autónoma de México (UNAM), Mexico and by Bocconi University, Italy. The abstract of their very interesting talks are still available at https://j-isba.github.io/blackwell-rosenbluth\_abstracts2022.html. Finally, let us recognize the important work of the members of the Scientific Committees:

**UTC+ Scientific Committee**: Daniele Durante (Chair), Sylvia Frühwirth-Schnatter (Vice-Chair), Xenia Miscouridou (j-ISBA Liaison), Federico Camerlenghi, François Caron, Ismael Castillo, Marta Catalano, Cathy W. Chen, Jim Griffin, Maria de Iorio, Samuel Livingstone, Gael Martin, Brendan Murphy, Jouchi Nakajima, Sonia Petrone, Sylvia Richardson, Dootika Vats.

**UTC- Scientific Committee**: Lorin Crawford (Chair), Ramses Mena (Vice-Chair), Fan Bu (j-ISBA Liaison), Kate Calder, Trevor Campbell, Merlise Clyde, Daniel Kowal, Rosangela Helena Loschi, Li Ma, Peter Mueller, Raquel Prado, Fernando Quintana, Abhra Sarkar, Yixin Wang.

### j-ISBA Elections

With the 2022 ISBA election being recently complete, it is also time to congratulate the incoming j-ISBA officers! The newly elected Chair-elect is Beatrice Franzolini (A\*STAR, Singapore), and the new Treasurer is Beniamino Hadj-Amar (Rice University), and they will join the j-ISBA board from January 2023.

Our gratitude goes to the departing officers, Xenia Miscouridou and Sally Paganin, who have contributed to make j-ISBA a larger, stronger and all-welcoming community.

### j-ISBA has grown!

A final thanks goes to all members of our growing j-ISBA community. We have now reached 298 members! Given that we started the year with the goal to grow and hit 200 members, I'd say this is a huge success, and you are all to thank!

And if there are 2 more junior Bayesians out there willing to join our great community, you can join our section with only 5\$ with your ISBA membership (which now is only 5\$ for students and 30\$ for early career researchers)!

As for our beloved members, we hope you will join us again in the new year, so remember to renew your membership this January! We are excited to keep working for and with you.

## FROM THE PROGRAM COUNCIL

# Matthias Katzfuss

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(Co-)Sponsorship/Endorsement Requests. If you are planning a meeting and would like to request financial sponsorship (or co-sponsorship) or non-financial endorsement from ISBA, please submit your request to the program council at program-council@bayesian.org. Detailed information on how to submit a request for either sponsorship or endorsement can be found at https://bayesian.org/events/request-sponsorshipendorsement/.

#### Upcoming ISBA-Sponsored/Endorsed Events:

- BayesComp, March 15–17, 2022, Levi, Finland
- 13th Workshop on Bayesian Inference in Stochastic Processes, May 22–24, 2023, Madrid, Spain
- Seventh Symposium on Games and Decisions in Reliability and Risk, May 24–26, 2023, Madrid, Spain

## NEWS FROM THE WORLD

#### Francesco Denti francesco.denti@unicatt.it

#### Announcements

**New Bayesian group in the Société Française de Statistique** by *Robin Ryder* 

We are pleased to announce that a Bayesian group has recently been created in the **French Statistical society** (Société Française de Statistique, SFdS).

There is a large and strong community of Bayesian statisticians in France, but until now, there was no national structure to coalesce them. Our hope is that the Bayesian SFdS group will help develop scientific exchanges around Bayesian inference. In particular, the group will (help) organize training in Bayesian Statistics in public and private sectors as well as Bayesian conferences or sessions within larger conferences.

The initial officers are **Julien Stoehr** (president), **Sophie Ancelet** (vice-president), **Sylvain Le Corff** (treasurer), **Robin Ryder** (secretary & ISBA liaison) and **Guillaume Kon Kam King** (webmaster). The extended board also includes **Julyan Arbel**, **Pierre Barbillon**, **Sophie Donnet** and **Pierre Gloaguen**.

Membership is open to all SFdS members. We hope that many Bayesians in France will consider joining the group!

We have also created a newsletter on Bayesian events in France, to which anyone can subscribe. These events are also publicized on our Twitter account. Please email ryder@ceremade.dauphine.fr with any information you think should be broadcast there.

## Upcoming Meetings, Conferences, and Workshops

• The **Applied Bayesian Statistics school** is back! ABS23 will be held in Florice on June 12-16, 2023.

The school is organized by CNR IMATI (Institute of Applied Mathematics and Information Technologies at the Italian National Research Council in Milan), this year in cooperation with the Florence Center for Data Science and the Department of Statistics, Computer Science and Applications at the University of Florence. The topic will be **Bayesian causal inference**. The lecturer will be **Fan Li** (Duke University) with the support by researchers at the University of Florence.

• The **Joint Statistical Meetings** (JSM) is the largest gathering of statisticians and data scientists held in North America. The 2023 JSM will be held in Toronto, CA. The conference is scheduled for August 5-10, 2023.

With a focus on the 2023 theme, *One Community: Informing Decisions and Driving Discovery*, the JSM program consists not only of invited, topic-contributed, and contributed technical sessions but also poster presentations, roundtable discussions, professional development courses and workshops, award ceremonies, and countless other meetings and activities. The abstract submission is open and closes on February 1, 2023. More info at this link

### And don't forget:

• **Bayes Comp 2023** is the biennial conference of the Bayesian Computation Section of the International Society for Bayesian Analysis. Bayes Comp will take place in Levi, Finland, on March 15-17, 2023.

If you have any questions, please email bayescomp2023@gmail.com. There will also be three satellite events on 12-14 March 2023. More information at this link.

• Don't miss the **series of monthly webinars** organized by the Bayesian nonparametric section of ISBA (**BNP-ISBA**).

The next speakers are **Judith Rousseau** (January 11, 2023), **Fernando Quintana** (February 2, 2023), and **Matteo Ruggiero** (April 5, 2023). Check this link for more details.

#### **EXECUTIVE COMMITTEE**

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