Xsec: the cross-section evaluation code

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Abstract The evaluation of higher-order cross-sections is an important component in the search for new physics, both at hadron colliders and elsewhere. For most new physics processes of interest, total cross-sections are known at next-to-leading order (NLO) in the strong coupling $\alpha_s$, and often beyond, via either higher-order terms at fixed powers of $\alpha_s$, or multi-emission resummation. However, the computation time for such higher-order cross-sections is prohibitively expensive, and precludes efficient evaluation in parameter-space scans beyond two dimensions. Here we describe the software tool xsec, which allows for fast evaluation of cross-sections based on the use of machine-learning regression, using distributed Gaussian processes trained on a pre-generated sample of parameter points. This first version of the code provides all NLO Minimal Supersymmetric Standard Model strong-production cross-sections at the LHC, for individual flavour final states, evaluated in a fraction of a second. Moreover, it calculates regression errors, as well as estimates of errors from higher-order contributions, from uncertainties in the parton distribution functions, and from the value of $\alpha_s$. While we focus on a specific phenomenological model of supersymmetry, the method readily generalises to any process where it is possible to generate a sufficient training sample.

1 Introduction

The determination of cross-sections beyond leading order (LO) is typically very computationally expensive because of the evaluation of tensorial loop integrals. This is especially so for hadronic interactions, where the loop integrals must themselves be numerically integrated over the relevant parton distribution functions (PDFs).

The computational cost of evaluation per parameter point restricts the usage of next-to-leading order (NLO) cross-sections to (simplified) new physics models with only one or two relevant parameters. However, higher-order contributions can be very important in many other models. This is especially true for strong interactions, where NLO contributions can be of comparable size to the LO contribution. The physics impact of...
In addition to the processes found in Prospino, cross-sections for gaugino and slepton pair production, as well as the selection of cross-sections and models will be extended in future versions.

The increasing sparsity of training data in models with larger numbers of free parameters means that a lot of care must go into performing the regression, and that reliable regression errors can only be determined on a point-by-point basis. We choose to use Gaussian process (GP) regression [4], a highly flexible Bayesian method for modelling functions. It is not restricted to pre-determined functional shapes with a set number of parameters, and is instead directly informed by the data together with some prior understanding of the underlying correlation structure of the function that it is used to model. Moreover, a point-specific regression uncertainty follows naturally from the posterior predictive distribution, which is straightforward to compute in closed form.

Training GP models involves the inversion of a matrix of the size of the number of training points. This means that while GPs are a very powerful regression tool, single GPs scale very badly with increasing training data, and training becomes infeasible beyond $O(10^4)$ data points. To overcome this difficulty we use a model with factorised and distributed training, where the data are split into manageable subsets each assigned to a single GP. The regression prediction is subsequently determined by a combination of the predictions of the individual GPs [5, 6].

Current codes that can evaluate a broad collection of MSSM cross-sections at NLO include Prospino 2.1 [7–12] and MadGraph 5 [13]. However, the evaluation time per parameter point on a modern CPU is in the range of minutes for a single final state. This does not include the calculation of scale, $\alpha_s$, nor PDF errors, which increase the evaluation time by orders of magnitude. A test of the calculation time per parameter point for all strong-production cross-sections in Prospino, including the evaluation of scale, $\alpha_s$, and PDF errors, when Prospino has been heavily optimised with the ifort compiler, takes around two and a half hours on a single Intel Xeon-Gold 6138 (Skylake) core running at 2.0 GHz.

Fast evaluation of strong-production cross-sections in the MSSM at NLO, with next-to-leading (NLL) and next-to-next-to-leading (NNLL) logarithmic resummation, already exists in the form of the NLL-fast and NNLL-fast codes [14–24], which add NLL and NNLL corrections to existing NLO results from Prospino. However, these results are restricted to interpolation in a two-dimensional subspace spanned by the gluino mass and a common squark mass, and results are given as a sum over outgoing squark flavours.

In this work we present $\mathbf{xsec}$, an attempt at a general solution to the speed problem irrespective of the type of cross-section being evaluated, the size of the parameter space of the model, and the underlying precision of the calculation. We achieve this by performing machine-learning regression on a pre-generated training dataset consisting of cross-sections sampled from a model. In this first version of $\mathbf{xsec}$, we will be focusing on strong-production cross-sections in the MSSM, but the selection of cross-sections and models will be extended in future versions.

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In addition to the processes found in Prospino, cross-sections for gaugino and slepton pair production, as
well as gaugino-gluino production, can be evaluated at
NLO+NNLL precision by the Resummino code \cite{resummino}. Here, the total running time for all chargino and neu-
tralino production processes at NLO (again on a single
2.0 GHz Intel Xeon-Gold 6138 Skylake core) is around
three hours, with no evaluation of scale, \( \alpha_s \), nor PDF
errors. Combined NLO+NNLL precision takes four days.

Recently, the DeepXS package \cite{deepxs} appeared, which
performs a fast evaluation of neutralino and chargino
pair production using neural networks. This is currently
limited to a small set of the most phenomenologically
relevant processes in the MSSM-19, and does not in-
clude uncertainties arising from PDFs, or the value
of \( \alpha_s \).

The xsec 1.0 code is currently designed to reproduce
all the NLO results of Prospino 2.1 for strong production
in the MSSM in a small fraction of the time, in-
cluding scale errors, and with the addition of PDF and
\( \alpha_s \) errors based on a modern PDF set. It does not in-
clude NNLL or even NLL resummation as can be found
in NNLL-fast and NLL-fast, however, unlike those codes
it provides reliable results for non-degenerate squark
masses, within the inherent limitations of the training
set generated with Prospino. We intend to extend the
code to also include NLL resummation in future re-
leases.

Unlike NNLL-fast, xsec performs a separate evalua-
tion of the cross-section for all distinct flavour com-
binations of the first two generations of squarks. The xsec code also treats sbottom and stop pair-production
processes separately, but this has limited impact as the
two cross-sections are the same at LO (for the same
masses),\(^1\) as Prospino — and therefore our training set
— is limited to light quark initial states. A complete list of available processes can be found in Table 1.

The code is written in Python with heavy use of the
NumPy \cite{numpy} package for numerical calculations, and is
compatible with both Python 2 and 3. It can be installed
using the pip package manager and run as a set of func-
tions from a self-contained module. We also provide in-
terfaces through SLHA files \cite{slha} and a command-line
tool.

The rest of this paper is structured as follows. We begin in Sec. 2 with an introduction to the GP regression
framework that we employ. In Sec. 3 we describe our GP training regime, including how we compute the
required training sets of NLO cross-sections. In Sec. 4, we perform a thorough validation of the results from
xsec, with a comparison to results from existing codes.

Section 5 covers the structure of the code and its inter-
faces, and we conclude in Sec. 6.

2 Regression framework

2.1 Gaussian process regression

The basic objective in regression is to estimate an un-
known function value \( f(x) \) at some new \( x \) point, given
that we know the function values at some other \( x \) points.
A Bayesian approach to this task is provided by Gauss-
ian process regression, in which we express our degree
of belief about any set of function values as a joint
Gaussian pdf. We underline here that this pdf should
be understood in a purely Bayesian sense — it does not imply any randomness in the true function we are
approximating.

We begin by defining some notation and terminol-
ogy, indicating in italics the terminology commonly used
in the GP and machine learning literature. Each input
point \( x \) has \( m \) components (features), which in our
case will correspond to masses and mixing angles from
the MSSM squark and gluino sector. We denote by \( x_n \)
the new input point (test point) for which we will es-
timate the unknown, true function value \( f_n \equiv f(x_n) \),
here an NLO production cross-section. We let \( x_i \), with
\( i = 1, \ldots, n \) denote the \( n \) input points (training points)
at which we know the function values \( f_i \equiv f(x_i) \) (tar-
gets). The combined set \( D = \{ x_i, f_i \}_{i=1}^n \) is referred to
as the training set. The complete set of input compo-
ents in our training set can be expressed as an \( n \times m \)
matrix \( X = [x_1, \ldots, x_n]^T \). Similarly, the complete set
of known function values can be collected in a vector \( f = [f_1, \ldots, f_n]^T \). Thus, our training set can also be
expressed as \( D = \{ X, f \} \).

The starting point for GP regression is the formul-
ation of a joint Gaussian prior pdf\(^2\)

\[
p(D, f_n | x_n) \equiv p(f, f_n | X, x_n),
\]

which formally describes our degree of belief for possible
function values at both the training points \( X \) and the
test point \( x_n \), before we look at the training data. This
prior is chosen indirectly by choosing a mean function \( m(\cdot) \) and a covariance function or kernel \( k(\cdot, \cdot) \), defined to
specify the following expectation values for arbitrary
input points:

\[
m(x) = \mathbb{E}[f(x)] = \int_{-\infty}^{\infty} f p(f | x) \, df
\]

\(^1\)Considering only QCD corrections, corrections that de-
pend on the mixing angles contribute only through \( t_\beta \tilde{g} \) and \( t_1 t_2 t_3 t_4 \) vertices (and similarly for sbottoms) at NLO and are
typically small.

\(^2\)We always treat the input \( x \) points in a dataset \( D \) as
known. Thus, the pdf \( p(D) \) should be understood as the pdf
\( p(f_1, \ldots, f_n | x_1, \ldots, x_n) = p(f | X) \), and similarly for other
pdfs involving \( D \).
asurement error, we shall refer to the prediction error, keeping in mind that it should be interpreted "literally" as the regression error or GP prediction error, or GP predictive variance, the latter being a term in the Gaussian posterior pdf. We will refer to the prediction variance simply as the regression error or GP prediction error, or GP predictive variance, the latter being a term in the Gaussian posterior pdf.

Choosing the kernel, Eq. (3), is the main modeling step in GP regression. It effectively determines what types of functional structure the GP will be able to capture. In particular, it encodes the smoothness and the periodicity (if applicable) of the function that is being modelled, as it controls the expected correlation between function values at two different points. The choice of prior mean function, Eq. (2), is typically much less important, as we discuss at the end of this section.

The kernel choice and optimisation

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The question of the optimal kernel choice is covered in more detail in Refs. [4, 37]. The squared-exponential kernel

\[
k(x, x') = \sigma_f^2 \exp \left( -\frac{(x - x')^2}{2\ell^2} \right),
\]

is the standard choice. It results in an exponentially decreasing correlation as the Euclidean distance between two input points increases with respect to a length-scale hyperparameter \(\ell\). The signal variance \(\sigma_f^2\) is a hyperparameter containing information about the amplitude of the modeled function. This is a universal kernel [38], which means that it is in principle capable of approximating any continuous function given enough data. The infinite differentiability and exponential behaviour of this kernel typically result in a very smooth posterior mean.

However, for our purposes, the squared-exponential has some problems. Its sensitivity to changes in the function means that the length scale \(\ell\) is usually determined by the smallest ‘wiggle’ in the function [37]. We hence consider also the Matérn kernel family: the squared-exponential, these are universal and stationary, i.e., only functions of the relative positions of the two input points, but additionally incorporate a smoothness hyperparameter \(\nu\) following the basic form

\[
k_M(x, x'; \nu, \ell) = 2^{1-\nu} \frac{\Gamma(\nu)}{\sqrt{2\pi}} \left(\frac{2|\mathbf{x} - \mathbf{x}'|}{\ell}\right)^\nu K_\nu \left(\sqrt{2|\mathbf{x} - \mathbf{x}'|}/\ell\right),
\]

where \(\Gamma(\nu)\) is the gamma function and \(K_\nu\) is a modified Bessel function of the second kind. For the modelling of cross-section functions, we adopt the Matérn kernel class on the basis of its superior performance. This has followed significant testing and cross-validation across a number of different problems [39–41]. During testing we found \(\nu = 3/2\) to be optimal for our purposes, in which case Eq. (13) simplifies to

\[
k_M(x, x'; \nu, \ell) = 2^{1-\nu} \frac{\Gamma(\nu)}{\sqrt{2\pi}} \left(\frac{2|\mathbf{x} - \mathbf{x}'|}{\ell}\right)^\nu K_\nu \left(\sqrt{2|\mathbf{x} - \mathbf{x}'|}/\ell\right).
\]
To account for the fact that some directions in the input space of masses and mixing angles may have more impact on the cross-section values than others, we use an anisotropic, multiplicative Matérn kernel,

\[ k_{\text{AMM}}(\mathbf{x}, \mathbf{x}'; \nu, \sigma_f^2, \ell) = \sigma_f^2 \prod_{d=1}^{m} k_M(x^{(d)}, x'^{(d)}; \nu, \ell_d), \tag{15} \]

where we have also included a signal variance hyperparameter \( \sigma_f^2 \), similar to the one in Eq. (12). Here \( x^{(d)} \) denotes the \( d \)th component of the input vector \( \mathbf{x} \), and \( \ell \), with components \( \ell_d \), is a vector containing one length scale per \( \mathbf{x} \) component. The product over the dimensions of the parameter space results in points only being strongly correlated if in each dimension, their distance is small with respect to the relevant length scale.

So far we have focused on the “noise-free” case, in which the training targets \( \mathbf{f} \) are the exact values of the true function at the training points. In this case the predictive posterior \( p(\mathbf{f}_*|\mathcal{D}, \mathbf{x}_*) \) collapses to a delta function when \( \mathbf{x}_* \) equals a training point. In theory this is a reasonable approach, since what we seek is a surrogate model for an expensive, but precise and deterministic numerical computation. In practice, however, allowing for some uncertainty also at the training points typically results in a more well-behaved and stable regression model. The main reason for this is that the additional wiggle-room in the modelling can ease the challenging matrix numerics of GP regression, as we will discuss in some detail in Sect. 2.3. We therefore add a “white-noise” term,

\[ k_{\text{WN}}(\mathbf{x}, \mathbf{x}'; \nu, \sigma^2_\epsilon) = \delta_{\mathbf{x}\mathbf{x}'} \sigma^2_\epsilon, \tag{16} \]

to our kernel, where \( \sigma^2_\epsilon \) is the hyperparameter that sets the amount of “noise”. The effect of this term is simply to add \( \sigma^2_\epsilon \) along the diagonal of the covariance matrix \( \Sigma \), as well as to the prior variance at the test point, \( k(\mathbf{x}_*, \mathbf{x}_*) \). It is known as homoscedastic noise, as it is the same for all data points.

In GP terminology, to include this additional variance term corresponds to going from the noise-free case to a scenario with noisy training data. The targets are then considered measurements \( y_i \equiv y(\mathbf{x}_i) = f(\mathbf{x}_i) + \epsilon_i \), with the noise \( \epsilon_i \), introduced in the process of performing the \( i \)th measurement, modelled by a Gaussian distribution \( \mathcal{N}(0, \sigma^2_\epsilon) \). However, we remind the reader that for our case this Gaussian pdf represents an adopted effective Bayesian degree of belief in the accuracy of the training data, rather than an expression of actual random noise.

Conceptually we should then make the substitution \( f \rightarrow y \) in our definitions from Sect. 2.1. Our training set becomes \( \mathcal{D} = \{ \mathbf{X}, \mathbf{y} \} \), with \( \mathbf{y} = [y_1, \ldots, y_n]^\top \), and the GP prior becomes a joint pdf for \( \mathbf{y} \) and \( y_* \):

\[ p(\mathcal{D}, y_*|\mathbf{x}_*) = p(\mathbf{y}, y_*|\mathbf{X}, \mathbf{x}_*). \tag{17} \]

The prior mean function and kernel now specify expectation values in \( y \) space,

\[ m(\mathbf{x}) = \mathbb{E}[y(\mathbf{x})] \tag{18} \]

\[ k(\mathbf{x}, \mathbf{x}') = \mathbb{E}[(y(\mathbf{x}) - m(\mathbf{x}))(y(\mathbf{x}') - m(\mathbf{x}'))], \tag{19} \]

where we note that \( \mathbb{E}[y(\mathbf{x})] = \mathbb{E}[f(\mathbf{x})] \) since the Gaussian noise term has zero mean. Likewise, the predictive posterior pdf becomes

\[ p(y_*|\mathcal{D}, \mathbf{x}_*) = \mathcal{N}(\mu_*, \sigma^2_\epsilon), \tag{20} \]

with mean and variance

\[ \mu_* = m(\mathbf{x}_*) + k(\mathbf{x}_*, \mathbf{X})\Sigma^{-1}(\mathbf{y} - m(\mathbf{X})) \tag{21} \]

\[ \sigma^2_* = k(\mathbf{x}_*, \mathbf{x}_*) - k(\mathbf{x}_*, \mathbf{X})\Sigma^{-1}k(\mathbf{X}, \mathbf{x}_*). \tag{22} \]

Our complete kernel is then given by

\[ k(\mathbf{x}, \mathbf{x}') = k_{\text{AMM}}(\mathbf{x}, \mathbf{x}'; \nu, \sigma^2_f, \ell) + k_{\text{WN}}(\mathbf{x}, \mathbf{x}'; \nu, \sigma^2_\epsilon). \tag{23} \]

Fixing \( \nu = \frac{1}{2} \), as discussed above, we are left with the set \( \Theta = \{ \sigma^2_f, \ell, \sigma^2_\epsilon \} \) of undetermined hyperparameters. To be fully Bayesian, one would introduce a prior pdf \( p(\theta) \) for the hyperparameters and obtain the GP posterior \( p(y_*|\mathcal{D}, \mathbf{x}_*) \) by marginalising over \( \theta \),

\[ p(y_*|\mathcal{D}, \mathbf{x}_*) = \int p(y_*|\mathcal{D}, \mathbf{x}_*; \theta) p(\theta|\mathcal{D}, \mathbf{x}_*) \ d\theta \]

\[ = \int p(y_*|\mathcal{D}, \mathbf{x}_*) p(\theta|\mathcal{D}) \ d\theta \]

\[ \propto \int p(y_*|\mathcal{D}, \mathbf{x}_*) p(D|\theta) p(\theta) \ d\theta. \tag{24} \]

In our high-dimensional case with large datasets, such integration would come at a steep computational expense, even with MCMC methods. We therefore follow the common approach of using a point estimate for the hyperparameters, found by maximising the log-likelihood function \[4\]

\[ \log p(D|\theta) = \log p(\mathbf{y}|\mathbf{X}, \theta) \]

\[ = \frac{1}{2} (\mathbf{y} - m(\mathbf{X}))^\top \Sigma^{-1} (\mathbf{y} - m(\mathbf{X})) \]

\[ - \frac{1}{2} \log |\Sigma| - \frac{n}{2} \log 2\pi. \tag{25} \]

Finding an adequate set of hyperparameters constitutes the model training step in the GP approach. It is complicated by the fact that each optimisation step requires the computation of the inverse and determinant of the \( n \times n \) covariance matrix \( \Sigma \), which scales
poorly with the number of training points $n$. To increase speed and numerical stability, $\Sigma$ is generally not directly inverted in practice, and its Cholesky decomposition is used instead. In an attempt to avoid local optima, we employ the SciPy implementation of the differential evolution method \cite{42,43}, rather than performing a gradient-based search.

Recent work has demonstrated that the theoretical prediction error $\sigma^2_c$ in Eq. (22) systematically underestimates the mean-squared prediction error when the hyperparameters are learned from the data \cite{44}. As proposed there, we account for the uncertainty on the point estimate of the hyperparameter by adding a correction term to $\sigma^2_c$, derived from the Hybrid Cramér-Rao bound. In our case, with a constant prior mean function, this extra term amounts to

$$\Delta \sigma^2_c = \left(1 - \mathbf{1} \Sigma^{-1} k(X, x_i)\right)^2 \sum_{i,j=1}^{n} [\Sigma^{-1}]_{ij}, \quad (26)$$

where $\mathbf{1} = [1, \ldots, 1]$. In particular, this increases the prediction error at test points far from the training data.

Compared to the choice of kernel, the choice of the prior mean function, Eq. (18), is typically less important. Following conditioning on a sufficiently large training set, the prior gets overpowered and the posterior mean is primarily influenced by the training data through the second term in Eq. (21). For this reason the prior mean function is commonly taken to be zero everywhere. Nevertheless, it is sensible to incorporate our knowledge of the mean, and we therefore use the sample mean of the target values $y$ as a prior mean function that is constant in $x$.

2.3 Regularisation of the covariance matrix

A practical challenge when training GPs is to ensure numerical stability when inverting the covariance matrix $\Sigma$. The precision of the result is controlled by the condition number $\kappa$ of $\Sigma$, which can be considered a measure of the sensitivity of the inversion to roundoff error. It is computed as the ratio $\lambda_{\text{max}}/\lambda_{\text{min}}$ between the highest and lowest eigenvalues of $\Sigma$, and becomes infinite for a singular matrix. The loss of numerical precision at high $\kappa$ becomes most obvious when the predictive variance, computed according to Eq. (22), evaluates to a negative number. In order to prevent this problem, it is essential to understand how to control $\kappa$.

When the target values of training points are strongly correlated, their corresponding rows and columns in $\Sigma$ are nearly identical. This leads to eigenvalues close to zero and a very large condition number. It has been shown that in the worst case, $\kappa$ can grow linearly with the number of training points and quadratically with the signal-to-noise ratio $\text{SNR} = \sigma_f/\sigma_e$ \cite{45}.

Increasing the noise level improves numerical stability, as a larger diagonal contribution $\sigma^2_e$ to $\Sigma$ enhances the difference between otherwise similar rows and columns. Therefore, we add a term to the log likelihood in Eq. (25) that penalises hyperparameter choices with extremely high signal-to-noise ratios, as suggested in Ref. \cite{45}. Our objective function for training GPs then becomes

$$\log p(y|X, \theta) \equiv \log(\sigma_f/\sigma_e)^{\Delta \sigma^2}
\log(\text{SNR}_{\text{max}})\). \quad (27)$$

The large exponent guarantees that situations where SNR > SNR$_{\text{max}}$ are the only ones where the penalty term has a significant effect. We use SNR$_{\text{max}} = 10^4$.

In some cases the likelihood penalty in Eq. (27) does not decrease the condition number sufficiently to stabilise the inversion. However, choosing a lower overall value for SNR$_{\text{max}}$ dilutes the information in the training data to an extent that it can sometimes be fitted by noise, even when unnecessary. We therefore check the condition number after the optimisation with the penalty term, and proceed to increase the homoscedastic noise $\sigma^2_e$ just for the inversion step until the condition number drops below a reasonable value $\kappa_{\text{max}}$ \cite{46}:

$$\Delta \sigma^2_e = \frac{\lambda_{\text{max}} - \kappa_{\text{max}} \lambda_{\text{min}}}{\kappa_{\text{max}} - 1}. \quad (28)$$

We set $\kappa_{\text{max}} = 10^9$, roughly corresponding to a maximal loss of nine digits accuracy from the total of 16 in a 64-bit double-precision floating-point number.

These measures may seem to deteriorate the performance of our regression model, but they are necessary to ensure the numerical stability. The underlying reason is that we have essentially noiseless data, and are hitting the limits of floating-point precision in the process of calculating the GP predictions. In comparison to the scale and PDF uncertainties on the cross-sections, the resulting regression errors nevertheless remain small, as we demonstrate in Sec. 4.

2.4 Distributed Gaussian processes and prediction aggregation

With $n$ training points, the complexity of the matrix inversion operations in Eqs. (21) and (22) scales as $n^3$, making standard GP regression unsuitable for problems

\footnote{This is a power, not a footnote.}
that require large training sets. To overcome this challenge we construct a regression model based on distributed Gaussian processes (DGP) [5]. We partition the total training set $D$ into $d$ manageable subsets $D_i$, and for each $D_i$ we train a new GP $M_i$. These GPs are referred to as experts. The prediction from our regression model is obtained by aggregating the predictions from the individual experts. For this prediction aggregation we follow the approach known as the Generalised Robust Bayesian Committee Machine (GRBCM) [6], for which we summarise the main steps below.

First we construct a data subset $D_1 \equiv D_c$, randomly chosen from $D$ without replacement, which will be used to train a single communication expert $M_c$. Next, we partition the remaining data into subsets $\{D_i\}_{i=2}^d$, each of which will serve to train one expert $M_i$. Following Refs. [5, 6], all experts are then trained simultaneously, such that they share a common set of hyperparameters. The GRBCM approach places no restrictions on how to partition the data to form the subsets $\{D_i\}_{i=2}^d$. Compared to using a simple random partition, we have noticed minor improvements with a disjoint partition, where the data is split into local subsets based on the mass parameter with the smallest length-scale hyperparameter.

The special role of the communication expert $M_c$ becomes evident at the prediction stage. For each of the experts $\{M_i\}_{i=2}^d$, we construct an improved expert $M_{+i}$ by replacing the corresponding dataset $D_i$ with the extended set $D_{+i} = \{D_1, D_c\}$. That is, for prediction the communication dataset $D_c$ is shared by all the experts $M_{+i}$. The communication expert $M_c$ serves as a common baseline to which the experts $M_{+i}$ can be compared. In the final combination, the prediction from expert $M_{+i}$ will be weighted according to the differential entropy difference between its predictive distribution and that of $M_c$.

The central approximation that allows for computational gains in DGP s and related approaches is an assumption that the individual experts can be treated as independent, which corresponds to approximating the kernel matrix of the combined problem, i.e. without partition into experts, as block-diagonal. In the GRBCM approach, this approximation is expressed as the conditional independence assumption $D_i \perp D_j|D_c, y_s, x_s$ for $2 \leq i \neq j \leq d$, which enables the approximation $p(D_i|D_j, D_c, y_s, x_s) \approx p(D_i|D_c, y_s, x_s)$. That is, when the information contained in the communication set $D_c$ is known, we assume that the predictive distribution for points in subset $D_i$ should not be strongly influenced by the additional information contained in subset $D_j$.

Using Bayes’ theorem and the above independence assumption, the exact predictive distribution $p(y_s|D, x_s)$ can now be approximated as

$$p(y_s|D, x_s) \propto p(y_s|x_1) p(D_c|x_s) \prod_{i=2}^d p(D_i|D_1, \ldots, D_{i-1}, y_s, x_s)$$

$$\approx p(y_s|x_1) p(D_c|x_s) \prod_{i=2}^d p(D_i|D_c, y_s, x_s)$$

$$= p(y_s|x_1) p(D_c|y_s, x_s) \prod_{i=2}^d \frac{p(D_i|D_c, y_s, x_s)}{p(D_i|D_c, y_s, x_s)}$$

$$= \frac{p(y_s|x_1) \prod_{i=2}^d p_D(\hat{D}_i|y_s, x_s)}{p(D_c|y_s, x_s)} \prod_{i=2}^d \frac{p_c(D_i)}{p(D_i|D_c, y_s, x_s)},$$

(29)

where we have introduced the weights $\beta_i$ for the predictions from different experts, and defined $\beta_1 = -1 + \sum_{i=2}^d \beta_i$. By applying Bayes’ theorem again, we can express our approximation for $p(y_s|D, x_s)$ in terms of the corresponding predictive distributions from the individual experts, $p_{+i}(y_s|D_{+i}, x_s)$ and $p_i(y_s|D_i, x_s)$. Leaving out normalisation factors, the distribution for the aggregated prediction becomes

$$p_A(y_s|D, x_s) \propto \prod_{i=2}^d \frac{p_{+i}(y_s|D_{+i}, x_s)}{p_i(y_s|D_i, x_s)},$$

(30)

with mean $\mu_{DGP}$ and variance $\sigma^2_{DGP}$ at $x_s$ given by

$$\sigma_{DGP}^2(x_s) = -\beta_1 \sigma_c^{-2}(x_s) + \sum_{i=2}^d \beta_i \sigma_{+i}^{-2}(x_s)$$

(31)

$$\mu_{DGP}(x_s) = -\beta_1 \sigma_c^{-2}(x_s) \mu_c(x_s)$$

$$+ \sum_{i=2}^d \beta_i \sigma_{+i}^{-2}(x_s) \mu_{+i}(x_s).$$

(32)

Following Ref. [6], we set the weights $\beta_i$ to

$$\beta_2 = 1,$$

(33)

$$\beta_{i \geq 3} = 0.5 \left[ \log \sigma_{+i}^2(x_s) - \log \sigma_{+i}^2(x_s) \right].$$

(34)

The reason for assigning weight $\beta_2 = 1$ for expert $M_{+2}$ is that the transition

$$p(D_i|D_1, \ldots, D_{i-1}, y_s, x_s) \rightarrow p_{+2}(D_i|D_c, y_s, x_s)$$

(35)

in Eq. (29) is exact for $i = 2$, $\beta_2 = 1$. For each remaining expert $M_{+i > 2}$, the weight is taken to be the difference in differential entropy between the baseline predictive distribution of the communication expert, $p_i(y_s|D_i, x_s)$, and that of the given expert, $p_{+i}(y_s|D_{+i}, x_s)$. Thus, if an expert $M_{+i}$ provides little additional predictive
power over $\mathcal{M}_c$, its relative influence on the aggregated prediction is low.

Requiring the experts to share a common set of hyperparameters effectively disfavours overfitting of individual experts. Moreover, the risk of overfitting is alleviated by the fact that after training, each expert is coupled with the communication dataset $\mathcal{D}_c$ that it did not see during training, and its weight in the prediction aggregation is regularised through the comparison to the communication expert.

The GRBCM split of the dataset into $d$ experts reduces the complexity of training from $n^3$ to $\mathcal{O}(d(n/d)^3 = n^3d^{-2})$. The memory, storage space, and evaluation all depend directly on the size of the matrix, and scale as $\mathcal{O}(n^2)$ for a regular GP, but as $\mathcal{O}(n^2/d)$ in the GRBCM approach.

3 Training

3.1 Sample generation

We generate the inputs for our training data calculations by sampling the physical gluino and squark masses and (for third-generation squarks) the angles describing mass mixing between gauge eigenstates. The only other parameters involved in the production of gluinos and squarks to NLO QCD are the strong coupling $\alpha_s$ and the SM quark masses. The cross-sections depend on $\alpha_s$ both through the matrix element and the PDF.

To capture the cross-section variation due to the uncertainty on $\alpha_s$, we generate separate input points with $\alpha_s$ set to 0.1180 (central value), 0.1165 (1σ lower value) and 0.1195 (1σ upper value), using the corresponding PDF sets, and train separate GPs on the ratio of cross-sections obtained with the central and $\pm1\sigma$ values. For the SM masses we use a fixed value for the bottom and top quark masses, and assume the other quark masses to be zero.

In the sample generation we do not simply sample over a regular grid of parameter values, for three reasons:

1. Grid sampling is inefficient when one parameter is more important than the others: too many evaluations are spent on varying the less influential parameters whilst keeping the important one at a fixed value.

2. The curse of dimensionality renders this sampling technique infeasible for processes that depend on more than three or four parameters.

3. The complexity of sampling and cross-section calculation for the large number of processes that we consider (in terms of final-state squark flavours) means that it is more efficient to evaluate multiple cross-sections for every parameter combination than to generate separate samples for each final state.

We sample individual baseline masses for the gluino, $m_{\tilde{g}}$, and the first and second-generation (gauge eigenstate) squarks, $m_{\tilde{u}}$, $m_{\tilde{d}}$, $m_{\tilde{b}}$, $m_{\tilde{t}}$, $m_{\tilde{e}}$, $m_{\tilde{\mu}}$, and $m_{\tilde{\tau}}$, and for the third-generation (mass eigenstate) squarks $m_{\tilde{t}}$, $m_{\tilde{b}}$, $m_{\tilde{c}}$, and $m_{\tilde{\tau}}$. We do this in two different ways: either drawing from a uniform distribution on the interval [50, 3500] GeV, or from a hybrid distribution uniform on the interval [50, 150] GeV and logarithmic on the interval [150, 3500] GeV. We order the third-generation squark masses in mass after sampling, so that $\tilde{t}_1$ and $\tilde{b}_1$ are by definition the lightest. We intentionally allow these sampling ranges to be slightly beyond our final claimed region of validity for the regression — typically 200–3000 GeV — in order to try to avoid large regression errors at the edges. The regions where our regression has been validated more than cover the ranges of masses of interest for the LHC. We sample the cosines of the sbottom and stop mixing angles, $\cos\theta_{\tilde{b}}$ and $\cos\theta_{\tilde{t}}$, uniformly on the interval $[-1, 1]$.

On top of our baseline sampling, we employ further sub-sampling of the particle masses in order to properly include cross-section resonances within our training set. This ensures that our training dataset is more densely sampled where the cross-sections of interest vary the most. To do this, we generate and then combine five different training sets:

i) All masses sampled from the uniform prior.

ii) All masses sampled from the hybrid prior.

iii) Employing the uniform prior for both the mass of the gluino and for a common squark mass scale, and taking a Gaussian prior with width 50 GeV for the difference between the common squark mass scale and the masses of the individual squarks.

iv) Employing the uniform prior for the mass of the gluino, the hybrid prior for a common squark mass scale, and the same Gaussian prior as in iii) to draw values for the squark masses around the common scale.

v) Employing the uniform prior for a common mass scale, and using the same Gaussian prior as in iii) to draw a gluino mass and the individual squark masses around the common scale.

By joining these samples, we are able to achieve both good sampling of low masses (where cross-sections are large) via the logarithmic mass prior, and acceptable sampling of large masses via the uniform prior.

Because $R$-parity is assumed in the MSSM, there are no new $s$-channel resonances in the mass range where we train our GPs, and SM resonances are too light to
Table 1 List of all available cross-sections in *xsec*. Explicit first and second-generation squarks \( \tilde{q}_i \) can be \( u_L, d_L, c_L, s_L, u_R, d_R, c_R \) or \( s_R \), whilst \( \bar{m}_\tilde{q} \) denotes the average over all eight of these masses. Where the charge-conjugate process is distinct from the original, \( xsec \) returns the sum of the cross-section for the process and its conjugate (as indicated; for \( q_i \tilde{q}_j \), the conjugate is only distinct when \( i \neq j \)).

| Final state | Variables |
|-------------|-----------|
| \( \tilde{g}\tilde{g} \) | \( m_{\tilde{g}}, \bar{m}_\tilde{g}, m_{\tilde{u}_L}, m_{\tilde{u}_R}, m_{\tilde{c}_L}, m_{\tilde{c}_R}, m_{\tilde{s}_L}, m_{\tilde{s}_R} \) |
| \( \tilde{g}\tilde{q}_i + \text{c.c.} \) | \( m_{\tilde{g}}, m_{\tilde{q}_i}, \bar{m}_\tilde{q} \) |
| \( \tilde{q}_i\tilde{q}_j + \text{c.c.} \) | \( m_{\tilde{q}_i}, m_{\tilde{q}_j}, \bar{m}_\tilde{q} \) |
| \( \tilde{q}_i\tilde{q}_j^* (+ \text{c.c.}) \) | \( m_{\tilde{q}_i}, m_{\tilde{q}_j}, \bar{m}_\tilde{q} \) |
| \( \tilde{b}_i \tilde{b}_j^* \) | \( m_{\tilde{b}_i}, m_{\tilde{b}_j}, m_{\tilde{b}_i}, \cos \theta_R \) |
| \( \tilde{t}_i \tilde{t}_j^* \) | \( m_{\tilde{t}_i}, m_{\tilde{t}_j}, m_{\tilde{t}_i}, \cos \theta_L \) |

have any impact. Therefore, we do not have to worry directly about sampling densely in the region of resonances. However, at LO there are potential effects for gluino pair production near threshold from destructive interference between diagrams with s-channel gluons and those with t-channel squarks. For squark production, the chirality of the final-state squarks affects the contribution from t-channel gluino exchange, so that for example in squark–squark production for equal chiralities the matrix element has a zero at \( m_{\tilde{g}} \to 0 \), and a maximum around \( m_{\tilde{g}} \approx \bar{m}_\tilde{g} \), where \( \bar{m}_\tilde{g} \) is the average mass of the first and second-generation squarks. Both these effects can lead to non-monotonous behaviour of the cross-section as a function of masses (bumps and dips). In Sec. 4 we shall see this particularly for gluino pair production. This necessitates the separate samples with (near) degenerate masses, where such effects are larger.

Even though all non-degenerate squark masses enter into the LO cross-sections, to the precision of our training sample (see Sec. 3.2), only two mass parameters enter into the NLO corrections to gluino and first/second-generation squark production: the gluino mass \( m_{\tilde{g}} \) and the averaged first and second-generation squark mass \( \bar{m}_\tilde{q} \). Therefore, any additional interference structures present in the NLO corrections to these processes must be visible in the \( (m_{\tilde{g}}, \bar{m}_\tilde{q}) \) slice of the parameter space. For stop/stopbottom production, such structures should be similarly visible in the \( (m_{\tilde{g}}, m_{\tilde{t}_i/\tilde{b}_i}) \) slice. As a result, we shall spend some time below in validation (Sec. 4) looking at gluino and first/second-generation squark production cross-sections in terms of \( m_{\tilde{g}} \) and \( \bar{m}_\tilde{q} \), and third-generation squark production in terms of \( m_{\tilde{g}} \) and \( m_{\tilde{t}_i} \).

Table 1 gives the list of cross-sections available from *xsec*, and their parameter dependencies. The reader may wonder at this point why we train our GPs on the total cross-section in terms of all the non-degenerate masses, rather than simply on the NLO corrections (in terms of just \( m_{\tilde{g}} \) and \( \bar{m}_\tilde{q} \) for gluino/first/second-generation squark production, supplemented with the three relevant third-generation parameters each for stop and sbottom production). One reason is that we have designed *xsec* to be more general than *Prospino*: in future releases we intend to make use of training data from other tools able to move beyond the degenerate-squark-mass approximation. The other reason is that we feel it is more convenient for a user to simply obtain full LO+NLO (and future +NNL+NNLL+) cross-sections from *xsec*, rather than needing to install the correct LO cross-section calculator and PDF set, call them, and then combine the results. Similarly, training on and returning the full cross-section will make simultaneously including cross-sections from different calculators (chosen e.g. as most appropriate for different theories or processes) far more straightforward.

3.2 Calculation of NLO training cross-sections

We use *Prospino* 2.1 to generate cross-sections for our training samples. This calculates, amongst other things, NLO cross-sections for strong production processes in the MSSM for proton-proton collisions at a given centre-of-mass (CoM) energy, and for a choice of renormalisation/factorisation scales. We have modified the code to set \( \alpha_s \) accordingly, and to accept generic PDF sets from LHAPDF 6.2 \([47]\). For the current version of *xsec* we have used the PDF4LHC15_nlo30_pdfas symmetric Hessian NLO PDF set with 30 eigenvector members and two members with varied strong coupling \( \alpha_s(m_Z) = 0.1180 \pm 0.0015 \) \([48]\).

*Prospino* performs the PDF integral of the partonic process using the VEGAS \([49]\) importance sampling algorithm for Monte Carlo integration. The convergence criterion leaves some numerical noise in the result, typically of the order of \( 10^{-3} \) relative to the central cross-section value.

In order to obtain \( K \)-factors for gluino and first/second-generation squark production, *Prospino* first calculates the LO and NLO cross-sections using a single squark mass, obtained as the average over the masses of all first and second-generation squarks, i.e. eight in total; this mass is employed even for any internal third-generation squark propagators. The ratio of the LO and NLO results gives the \( K \)-factor for the process in question. *Prospino* then recomputes the cross-section at LO, without the assumption of an average mass, and the corresponding NLO value is found by multi-
plying this LO result by the $K$-factor calculated for the average squark mass. The calculation proceeds similarly for stop and sbottom production, except that the third-generation squark masses are kept non-degenerate for all steps of the calculation, meaning that first and second-generation masses are still averaged in the $K$-factor calculation. The final cross-sections should thus be viewed as an approximation to a fully non-degenerate squark mass NLO calculation. The effect of this assumption was investigated in Ref. [50] and found to be relatively small in most parts of parameter space.

In total, Prospino allows 141 final states containing gluinos and different flavour squarks. However, due to charge conjugation relations and NLO QCD identities in the cross-section (relating certain combinations of left and right-handed final-state squarks under the exchange of masses), only 49 distinct final states are needed to represent all processes calculated by Prospino in our training sample. These relationships are handled internally in xsec, and therefore need not directly concern the user. A list of the available cross-sections from the user’s side can be found in Table 1.

For every parameter point and every process in the training sample, we calculate 34 different cross-section values. These include: i) a central value, ii) 30 values using the PDF eigenvectors, iii) one value where $\alpha_s$ is taken to its lower value, iv) one where $\alpha_s$ is taken to its upper value, v) a value where the renormalisation/factorisation scale is doubled, and, vi) a value where the renormalisation/factorisation scale is halved.

From the values in i) and ii) we follow the PDF4LHC guidelines to calculate the symmetric PDF uncertainty on the central value, understood to be a 68% confidence level bound. Similarly, we follow the PDF4LHC prescription to calculate the 68% confidence level bound from varying $\alpha_s$ alone, using the results from iii) and iv). We do not add the PDF and $\alpha_s$ errors, but train different DGPs for the two errors. We note that these errors should be added in quadrature after evaluation if the user wishes to obtain a single 68% confidence bound incorporating both effects.

Further, we follow the standard lore of estimating an uncertainty associated with missing higher-order corrections by calculating the spread in cross-section values under scale variation coming from v) and vi). In xsec this is referred to as the scale uncertainty. Choosing exactly how to interpret this asymmetric uncertainty as a probability distribution (flat, Gaussian or otherwise), and whether/how to combine it with the (Gaussian) $\alpha_s$ and PDF uncertainties, is left to the user.

In total this leaves us with seven cross-sections: the central value and the two-sided PDF, $\alpha_s$ and scale uncertainties.

### 3.3 Training implementation details

For each final state, we train one large DGP with multiple experts on the central cross-section value, and five smaller regular DGPs: one each on the upper and lower values arising from regularisation and factorisation scale variation, one each on the cross-sections for the variation of $\alpha_s$ (and corresponding PDFs) to its upper and lower limit in its $68\%$ confidence interval (these values are later symmetrised), and a single GP on the symmetric $68\%$ confidence level PDF variation.

To improve the training, we try to simplify the target model. The span of some ten orders of magnitude in cross-sections across the sampled parameter space means that it is numerically challenging to train the DGPs on the raw cross-section numbers. Before training, we scale out part of the dependence on the final-state masses by first multiplying the central input cross-section by the square of the (average) final-state mass, and then take the logarithm of the result. For the remaining five ‘error’ values, we train on the logarithm of the ratio to the central cross-section, such that after the reverse transformation, the final predictions for the ratios are strictly positive. As noted in section 2.2, we choose a constant prior mean equal to the sample average of the transformed target values, which results in DGPs effectively modelling the deviation from this mean value. We also rescale all input parameters to the interval $[0, 1]$ before training, to improve numerical stability and precision.

The transformations during training are automatically recorded and reversed at the time of evaluation. As the DGPs are trained on the logarithm of the (mass-rescaled) cross-section, the resulting predictive distribution for the absolute cross-section is a log-normal distribution. Due to the positive skew of this distribution, we base the central cross-section estimate on the median. Specifically, let $\mathcal{N}(\mu_{\text{DGP}}(x), \sigma_{\text{DGP}}^2(x))$ denote the aggregated DGP predictive distribution for the log-transformed cross-section at point $x$, after accounting for the constant prior shift and the mass scaling applied to the training data. The central cross-section value $y_{\text{sec}}(x)$ returned by xsec is then

$$y_{\text{sec}}(x) = \exp[\mu_{\text{DGP}}(x)],$$

with associated asymmetric regression uncertainties $\Delta_{\text{sec}}^-$ and $\Delta_{\text{sec}}^+$. These are constructed from the bounds of the
More generally, the range $n \Delta n$ so that

$$
\Delta \sigma = \exp[\mu_{\text{DGP}}(x_\epsilon)] - \exp[\mu_{\text{DGP}}(x_\epsilon) - \sigma_{\text{DGP}}(x_\epsilon)],
$$

$$
\Delta \sigma^+ = \exp[\mu_{\text{DGP}}(x_\epsilon) + \sigma_{\text{DGP}}(x_\epsilon)] - \exp[\mu_{\text{DGP}}(x_\epsilon)].
$$

More generally, the range $y_{\text{sec}} \pm m \Delta y_{\text{sec}}$ corresponds to an $n \sigma$ credible interval, where $n$ is given by

$$
n = \frac{\log\left(1 + \frac{m \Delta y_{\text{sec}}}{y_{\text{sec}}^\ast}\right)}{\log\left(1 + \frac{\Delta y_{\text{sec}}}{y_{\text{sec}}^\ast}\right)},
$$

so that $n = m$ to first order in $(m \Delta y_{\text{sec}}/y_{\text{sec}})$ and $(\Delta y_{\text{sec}}/y_{\text{sec}})$.

We train the GPs with the union of the five training sets discussed in Sec. 3.1. In order to choose the optimal training parameters (relative sizes of the five different training samples, total number of training points, and experts per process), we have carried out a long programme of testing and cross-validation, in which we optimised training parameters separately for each process type, e.g. separately for gluino pair production and gluino–squark production. Our goal was to achieve good performance in terms of the regression error estimated by the DGP, while keeping disk size, memory footprint, training and evaluation time down to acceptable levels.

4 Validation

To validate the $\sigma$ cross-section results we generate three main test sets: $D_{\text{test}}$, $D_{\text{test-tb}}$ and $D_{\text{MSSM-24}}$. The set $D_{\text{test}}$ is used for testing all cross-sections except for the stop/sbottom pair-production processes, which are tested with the set $D_{\text{test-tb}}$. The sets $D_{\text{test}}$ and $D_{\text{test-tb}}$ contain 10000 and 5000 points, respectively, and in both cases the input points are sampled in the same way as for the corresponding training sets. The third set, $D_{\text{MSSM-24}}$, contains 19000 points. We use this in the validation of all cross-sections. Here we draw the input points from the MSSM-24, as defined at $Q = 1$ TeV, using uniform priors for the MSSM parameters. Our definition of the MSSM-24 follows that in Ref. [3], except that we parameterise the Higgs sector using the higgsino mass parameter $\mu$ and the tree-level mass of the $A^0$ boson $m_{A^0}$, instead of the soft-breaking mass parameters $m^2_{H_u}$ and $m^2_{H_d}$. For the samples in $D_{\text{MSSM-24}}$ we use SoftSUSY 4.0 to calculate the physical mass spectrum from the MSSM input parameters [51, 52]. In addition to the three main test sets, we also generate a number of process-specific two-dimensional parameter grids for further validation.

As part of the validation we will discuss two simple error measures and their distributions for our sets of test points. The first measure is just the relative error,

$$
\epsilon(x_\epsilon) = \frac{y_{\text{prop}}(x_\epsilon) - \sigma_{\text{sec}}(x_\epsilon)}{y_{\text{prop}}(x_\epsilon)};
$$

which measures the relative deviation of the $\sigma$ result $y_{\text{sec}}$ from the true Prospino value $y_{\text{prop}}$. By assuming some sampling prior $\pi(x_\epsilon)$ for the test points $x_\epsilon$ and looking at the resulting distribution of $\epsilon(x_\epsilon)$ values, we can get a global picture of how well $\sigma$ performs for the different supersymmetric production processes included in $\sigma$.

One of the strengths of GP regression is that the method directly provides point-wise uncertainty estimates, here in terms of $\Delta \sigma_{\text{sec}}(x_\epsilon)$ and $\Delta \sigma_{\text{sec}}(x_\epsilon)$, which are based on the width $\sigma_{\text{DGP}}(x_\epsilon)$ of the DGP predictive distribution (see Eq. 37). As discussed in Sec. 2, the point-wise regression uncertainty is connected to a Bayesian degree of belief regarding the unknown function value at $x_\epsilon$, given the particular training set $D$ and the modelling choices made in constructing and optimising the kernel.

An interesting question is then how this point-wise uncertainty compares to the actual deviation between $y_{\text{sec}}$ and the true Prospino value $y_{\text{prop}}$ across the input feature space. That is, we should also investigate the distribution of the standardised residual

$$
z(x_\epsilon) = \frac{y_{\text{prop}}(x_\epsilon) - \sigma_{\text{sec}}(x_\epsilon)}{\Delta \sigma_{\text{sec}}(x_\epsilon)},
$$

in our sets of test points. Here the notation $\Delta \sigma_{\text{sec}}$ is shorthand for using $\Delta \sigma_{\text{sec}}$ when $y_{\text{prop}} - \sigma_{\text{sec}} > 0$ and $\Delta \sigma_{\text{sec}}$ when $y_{\text{prop}} - \sigma_{\text{sec}} < 0$. By studying the distribution of $z(x_\epsilon)$ values for our test sets, and comparing to the unit normal distribution, we will obtain a global picture of the extent to which the point-wise regression errors are conservative or not, compared to the true deviations.

In cases where the main source of GP regression uncertainty is actual random noise in the training data, and we learn this noise level from the data by including a white-noise term, Eq. (16), in the GP kernel, we expect the residual in Eq. (40) to be distributed as $N(0,1)$. We can understand this from a simple example with single-component input points $x$. Assume that

---

4 As detailed in Sec. 5, $\sigma$ returns these regression errors in the form of the signed, relative errors $(-\Delta \sigma_{\text{sec}}/\sigma_{\text{sec}})$ and $(\Delta \sigma_{\text{sec}}/\sigma_{\text{sec}})$.

5 That is, at least up to log-normal corrections implied by Eq. (38) for $n \neq 1$. 

---
the target data are noisy measurements of the form
\[ y(x) = f(x) + \delta, \]
where the noise \( \delta \) is distributed as \( \mathcal{N}(0, \sigma_{\text{noise}}^2) \). Let the GP posterior predictive distribution for \( y(x_u) \) be given by \( \mathcal{N}(\mu_{\text{GP}}(x_u), \sigma_{\text{GP}}^2(x_u)) \). If the noise is the dominant uncertainty we have \( \sigma_{\text{GP}}(x_u) \approx \sigma_{\text{noise}} \), and we can express the residual as
\[ z(x_u) = \frac{y(x_u) - \mu_{\text{GP}}(x_u)}{\sigma_{\text{GP}}(x_u)} \approx \frac{y(x_u) - f(x_u)}{\sigma_{\text{noise}}} + \frac{f(x_u) - \mu_{\text{GP}}(x_u)}{\sigma_{\text{GP}}(x_u)}. \tag{41} \]

Given the generative model for the data, the first term will follow an \( \mathcal{N}(0, 1) \) distribution. The second term is the number of standard deviations (as measured by the GP’s own uncertainty) by which the GP prediction \( \mu_{\text{GP}} \) differs from the true value of the underlying function \( f \). While this term can in general not be expected to be normally distributed, the assumption of noise-dominated uncertainty implies that its contribution to the residual is \( \ll 1 \), and hence, that the \( z \) distribution is close to \( \mathcal{N}(0, 1) \).

On the other hand, if the true noise level is tiny and some other source of uncertainty dominates \( \sigma_{\text{GP}} \), i.e., if \( y \approx f \) and \( \sigma_{\text{GP}} \gg \sigma_{\text{noise}} \), we get
\[ z(x_u) \approx \frac{f(x_u) - \mu_{\text{GP}}(x_u)}{\sigma_{\text{GP}}(x_u)}. \tag{42} \]

Thus, in this limit it is the generally small, and potentially non-Gaussian, second term from Eq. (41) that dominates the residual.

The latter scenario is most similar to the case we have for the \( \text{xsec} \) residual in Eq. (40). The actual noise level in the \text{Prospino} training data is very small, as typically is the additional error in Eq. (26) accounting for uncertainty in the hyperparameter choice. Assuming some reasonably uninformative sampling prior \( \pi(x_u) \), this means that for most points the widths \( \Delta_{\text{xsec}}(x_u) \) are dominated by the homoscedastic error contribution that we include to stabilise the numerics (see Sec. 2.3). As this is a global error contribution, we can expect the resulting regression error for most test points to be larger than the actual error, \( y_{\text{prosp}}(x_u) - y_{\text{xsec}}(x_u) \). We therefore in general expect the \( z(x_u) \) distributions to be narrow compared to \( \mathcal{N}(0, 1) \), and not necessarily Gaussian. For comparison, we will include a graph of \( \mathcal{N}(0, 1) \) in all our plots of residual distributions.

In the coming subsections, much of our focus will be on the regression errors and the related relative error \( \epsilon \) and residual \( z \). However, we remind the reader that the regression errors that we find are typically far subdominant to the cross-section uncertainties coming from the scale and PDF errors.

4.1 Gluino pair production

The gluino pair-production cross-section to NLO in QCD depends on the gluino mass and all the other squark masses. Naturally, the gluino mass is the dominant feature of the DGP after training. The mass-averaging approximation that \text{Prospino} uses (see Sec. 3.2) means that the average first/second-generation squark mass \( \bar{m}_\tilde{q}_i \) is a strong predictor of the NLO contribution. We therefore provide it to the GPs as a separate feature, i.e. as if it were part of the vector of parameters \( \mathbf{x} \). The importance of the individual first and second-generation squark masses roughly follows the PDF contributions from their corresponding quarks, due to LO \( t \)-channel squark exchange diagrams.

Given that the mass range of parameters (features) in the training samples is [100, 3500] GeV, we validate the cross-section on the sub-interval [200, 3000] GeV for both gluino and squark masses, where the cross-section regression has solid support from training data and the regression error is small.

In Fig. 2 we compare the gluino pair-production cross-sections predicted by \text{xsec}, presented as a function of the gluino mass, with values taken directly from \text{Prospino} (but not in the training set). For this comparison we fix the squark masses to a common value of 1 TeV. We also show the associated \text{xsec}-predicted uncertainty from the renormalisation scale and the PDFs as bands. The uncertainties from the regression provided by \text{xsec} and from \( \alpha_s \) are too small to be visible on the logarithmic scale. However, below the plot we show the residual between the \text{xsec} prediction and the \text{Prospino} value (Eq. 40), as a multiple of the \text{xsec} regression uncertainty. We observe good agreement overall with the \text{Prospino} result. As expected, the scale error dominates at low gluino masses, and the PDF error at high masses.

A particular phenomenon occurs in gluino pair production due to destructive interference between LO diagrams when \( m_{\tilde{g}} \approx m_{\tilde{q}_j} \), resulting in a vanishing partonic cross-section at threshold [7]. This can be found as a significant dip in the total pair-production cross-section when one or more of the squark masses become degenerate with the gluino. We show that \text{xsec} reproduces this behaviour to very good precision in Fig. 3. Here the gluino mass is fixed to 1 TeV while the squark masses are run together as a common squark mass \( \bar{m}_\tilde{q} \). This figure also clearly demonstrates how subdominant the regression error is compared to the scale and PDF errors. Finally, Fig. 3 compares the results of \text{xsec} to the corresponding NLO result from \text{NNLL-fast} based on the same PDF set. We observe a slight systematic
Fig. 2 Gluino pair-production cross-section as a function of gluino mass, with all squark masses fixed at 1 TeV. The central value is shown in light green, the scale error in pink, and the PDF error in violet. The $\alpha_s$ error is too small to be visible on the scale of the plot. Superimposed on the prediction are the Prospino values (dots). Inset is a close-up of the region at low gluino mass, and below we show the residual between the xsec prediction and the Prospino values.

Fig. 3 Gluino pair-production cross-section as a function of average first and second-generation squark mass. The gluino mass is fixed at 1 TeV. Shown are the central xsec prediction (solid line), the $1\sigma$ regression error band (light green), the scale error (pink), the PDF error (violet), the Prospino values (dots) and the corresponding NNLL-fast NLO result (crosses).

Fig. 4 Gluino pair-production cross-section as a function of average first and second-generation squark mass for a set of different gluino masses. Shown is the central xsec prediction (solid line), the $1\sigma$ and $2\sigma$ regression error bands (shaded regions), and the Prospino values (dots). We also show the residuals of the comparison to Prospino.
difference at the ~1% level. This is at the level of the interpolation error quoted by NNLL-fast.

The same gluino pair-production cross-section as a function of a common squark mass for a selection of different gluino masses can be found in Fig. 4, showing that xsec reproduces the feature across the whole assumed range of validity for the regression. As expected, the regions in which the cross-section changes most rapidly are the most difficult to predict, but we see that with one exception the prediction is always within 2σ of the Prospino value, over a large number of test points.

In Figs. 5 and 6, we show the potential importance of being able to deal with non-degenerate squark masses in xsec. Here, we vary the t̄L and d̄R mass alone, respectively, with all other squarks fixed at 1 TeV and the gluino at 1.5 TeV for t̄L, and 2 TeV for the plot with d̄R. While less pronounced, qualitatively the same dip feature due to the t-channel interference as discussed above can be seen here as well. In this example, the NNLL-fast NLO result fails to reproduce the feature, as expected from its inherent assumption of degenerate squark masses.

Figure 7 shows the distributions of the relative error (left) and the residual (right) for the test sets Dtest and DMSSM-24. All distributions are normalised to unity, and the y-axis range is set to show all bins with non-zero values. In both sets the relative error is well below 5% for most points, and in fact there is only a single point, in the DMSSM-24 set, with an error greater than 5%. From the comparison to the unit normal distribution we see that, as expected, the xsec regression error is somewhat larger than the true error, but with no apparent bias. The xsec prediction is also robust under a change of the test sample to the MSSM-24.

It is also instructive to perform two-dimensional grid scans of mass planes to show the relative error and residual as a function of two of the features at a time. Two examples of this are found in Fig. 8, where we show the result in the planes of (m̃g, m̃q) and (m̃g, m̃dR). We see that the relative errors and residuals are correlated in the mass planes, as should be expected from Gaussian processes when the dominant uncertainty is not due to random noise in the training data, but rather due to the lack of information in regions where the function is changing quickly. We also note that the regression uncertainty is largest when m̃g ≈ m̃q. This shows that the destructive interference dip seen in Figs. 3–5 is the part of this cross-section function that is the most challenging to capture in the regression. Further improvements could be made by adding extra training points, but only at significant cost to the evaluation speed, which seems unwarranted given the small regression errors compared to the other errors. Naive counting of the number of bins in the residual plots (right panels) above the 1, 2, and 3σ levels indicates that the quoted xsec regression error is in general conservative compared to the actual error (i.e. fewer bins show large residuals than expected from Gaussian statistics).
Fig. 7 The relative error (left) and residual (right) distributions for the gluino pair-production cross-section in the test sets $D_{\text{na}}$ (solid) and $D_{\text{MSSM-24}}$ (dashed). The input points in $D_{\text{na}}$ are sampled from the same distribution as the training set, while the points in $D_{\text{MSSM-24}}$ are sampled from the MSSM-24 using flat priors for the MSSM parameters. All distributions are normalised to unity. The unit normal distribution is shown for comparison as a dotted black line.

Fig. 8 The relative error (left) and residual (right) for the gluino pair-production cross-section as a function of the gluino mass versus a common squark mass (top) and the $d_R$ mass (bottom). All other masses are fixed at 1 TeV.
4.2 Pair production of gluinos with first or second-generation squarks

The data that we employ for training \texttt{xsec 1.0} are limited by the fact that \texttt{Prospino} assumes flavour conservation and neglects heavy quarks in the proton PDFs. It therefore offers gluino–squark pair-production cross-sections only for processes with first and/or second-generation squarks in the final state. However, cross-sections for gluino–squark production with sbottoms or stops in the final state are expected to be very small. We also note that \texttt{Prospino} returns the cross-section for the sum over charge-conjugate final states, i.e. $\tilde{g}\tilde{q}_L + \tilde{g}\tilde{q}_R^*$, making it pointless to train \texttt{xsec} separately on the two final states. In addition to these limitations, at NLO QCD the numerical value of the cross-section is identical for left and right-handed squark final states, as long as their masses are identical. Although we use this fact internally in \texttt{xsec} to reduce the total file size of the DGPs, the user can freely request any first or second-generation final-state squark.

The sizes of the gluino–squark production cross-sections are naturally dominated by the gluino and final-state squark masses. Because of flavour conservation, to the level of approximation used in \texttt{Prospino}’s $K$-factor calculation, the only additional property of the model parameter space (i.e. feature) used by \texttt{xsec} is the average squark mass $\tilde{m}_q$. The range of sparticle masses over which we assume this cross-section evaluation to be valid is the same as for gluino pair production, i.e. $[200, 3000]$ GeV.

In Fig. 9 we show the predicted gluino–squark production cross-sections as a function of the gluino mass (left) and squark masses (right), for production of first and second-generation squarks. Shown are individual (left-handed) squark final states (colours) and the sum of all first and second-generation final states (black). In the left-hand plot all squark masses are fixed at 1 TeV. In the right-hand plot all masses except for the final-state squark mass are fixed at 1 TeV. The central-value $\text{xsec}$ prediction is shown with error bands from regression (solid line), scale error (dashed) and PDF error (dotted). The $\alpha_s$ error is too small to be visible. Also shown are the \texttt{Prospino} values (dots).

For the $\tilde{g}\tilde{d}_L$ and $\tilde{g}\tilde{u}_L$ processes, the scale error is the dominant uncertainty across the full mass range in both the gluino mass and the final-state squark mass. For the $\tilde{g}\tilde{s}_L$ and $\tilde{g}\tilde{c}_L$ processes it is generally the PDF error that dominates the uncertainty, except at low gluino masses, where the scale error is more important. The fact that the regression error residuals comparing the \texttt{xsec} and \texttt{Prospino} values seem correlated between the four processes shown is due to the same training sample being used for all processes, causing the distances to the nearest, most influential training points to be the same in all cases.
In Fig. 10 we show the distributions of the relative error between the \texttt{xsec} prediction and the corresponding \texttt{Prospino} results, as well as the residual, for each individual flavour final state. We use the same two test sets, \( \mathcal{D}_{\text{test}} \) and \( \mathcal{D}_{\text{MSSM-24}} \), as for the gluino pair-production cross-section in Fig. 7. All the distributions are normalised to unity.

The relative errors and residuals are similar across all squark flavours. There are no obvious differences in performance with the two sets of test points. The relative error distributions show that for almost all points in the test sets, the true regression error is below 10%, and \texttt{xsec} tends to overestimate the \texttt{Prospino} cross-section by a few percent. Comparing the residual and \( \mathcal{N}(0,1) \) distributions, we see that the predicted \texttt{xsec} regression uncertainty is conservative; indeed, notably more so than for the gluino pair-production cross-section (Fig. 7).

We can also compare the relative error across mass planes, which is shown in Fig. 11 separately for all \( \tilde{q}q_L \) processes, in terms of the gluino mass and the average first and second-generation squark mass. Here the final-state squark mass for each plotted cross-section is set equal to the average squark mass. We see that the regression error is below 8% across this plane for all four of the \( \tilde{g}d_L, \tilde{g}u_L, \tilde{g}s_L, \) and \( \tilde{g}c_L \) production cross-sections.

4.3 First and second-generation squark–anti-squark pair production

We now look at the production cross-sections for squark–anti-squark pairs \( \tilde{q}_L/\tilde{q}_R \). The flavours of the pair may be identical or different, and all four combinations of squark handedness are treated as separate processes.

If the flavours of the two squarks are different, the process is assumed to include the charge-conjugate state. In this section we discuss only final states with first and second-generation (anti-)squarks, where the final-state flavour may come from first and second-generation (anti-)squarks sampled from the proton.

Within the limitations set by the training data from \texttt{Prospino}, the LO first and second-generation squark–anti-squark cross-sections depend on the masses of the gluino and the final-state squark(s), and the NLO corrections further on the mean mass of all first and second-generation squarks. Again, we validate the cross-section on the sub-interval \([200,3000]\) GeV of the training data (in both gluino and squark mass). For squark–anti-squark production, one should keep in mind that masses below the lower end of this range may be affected by resonant production through \( Z \) and \( W \), and while \texttt{xsec}’s reported regression error increases below 200 GeV, it cannot take these resonances into account, as they are not included in its training data. The resulting cross-sections reported by \texttt{xsec} must thus be seen as wholly unreliable for squark masses below 50 GeV.

In NLO QCD, cross-sections for the two sets of process pairs \((\tilde{q}_L\tilde{q}_L, \tilde{q}_R\tilde{q}_R)\) and \((\tilde{q}_R\tilde{q}_L, \tilde{q}_R\tilde{q}_L)\) differ within each set only by an exchange of the appropriate squark masses. Removing also charge-conjugate states, an initial number of 64 independent processes \( \tilde{q}_L/\tilde{q}_R \) therefore reduces to 20 unique cross-sections. To save training time and user disk space, we reuse the DGPs for the identical processes in \texttt{xsec} simply by employing symbolic links and mapping the masses accordingly. This is however invisible to the user.

In Fig. 12 we show the predicted first and second-generation squark–anti-squark production cross-sections.
Fig. 11 The relative error of the production cross-section for gluinos and first or second-generation squarks, as a function of the average mass of first and second-generation squarks and the mass of the gluino. Shown are results for the production of $\tilde{g}_d^L$ (top left), $\tilde{g}_u^L$ (top right), $\tilde{g}_s^L$ (bottom left), and $\tilde{g}_c^L$ (bottom right). The final-state squark mass for each process is set equal to the average squark mass.

Fig. 12 Squark–anti-squark pair-production cross-sections for first and second-generation squarks. Panels show cross-sections as a function of the average of all first and second-generation squark masses (left) and gluino mass (right), for a selection of final states (colours) and the total cross-section for production of first and second-generation squark–anti-squark pairs (black).
as a function of the mean first and second-generation squark mass $m_{\tilde{q}}$ (left) and the gluino mass (right). We show results for a selection of sub-processes, and for the total cross-section (black, rescaled for readability). All other masses are kept at 1 TeV. We see that $\sigma_{\text{sec}}$ reliably predicts the contribution from individual squark final states, although at high squark masses the PDF error (dotted line) for some processes is consistent with zero cross-section. We also see that $\sigma_{\text{sec}}$ correctly captures the contribution of the gluino $t$-channel diagram, which controls the cross-section when the final-state squarks have different chirality, leading to the peak in Fig. 12 (right) for L-R combinations when $m_{\tilde{q}} \simeq m_{\tilde{g}}$.

In Fig. 13 we show the distributions of the relative regression error and residual (Eqs. (39) and (40)) for the points in the test sets $D_{\text{test}}$ and $D_{\text{MSSM-24}}$. We have normalised all distributions to unity. The comparison to the unit normal distribution included in Fig. 13 (right column) shows that for both test sets, and all processes, the $\sigma_{\text{sec}}$ regression error is conservative with respect to the true error.

The relative regression error in Fig. 13 (left column) is below 10% for all processes for the vast majority of test points. There is again a slight tendency for $\sigma_{\text{sec}}$ to overestimate the Prospino cross-section values, in particular for the $D_{\text{MSSM-24}}$ test set. As this set has individual flat priors for all the squark (soft) masses, which only a subset of $D_{\text{test}}$ has, we expect it to be more challenging to reproduce as its points are more likely to lie on the outskirts of the validation region.

The relative error distributions are most narrow for the processes producing a squark–anti-squark pair of the same type, i.e., for the four $\tilde{q}_{L}\tilde{q}_{L}$ processes and the corresponding $\tilde{q}_{R}\tilde{q}_{R}$ processes (not shown). These cross-sections are easier to model, as the final state involves only a single mass parameter. The $\tilde{s}_{L}\tilde{s}_{L}$ and $\tilde{c}_{L}\tilde{c}_{L}$ processes have particularly small relative errors. This is likely due to the smallness of the proton PDFs for the $s$ and $c$ quarks, which effectively makes the gluino $t$-channel diagram irrelevant and thus further simplifies the parameter dependence.

Again, we discuss only final states with first and second-generation squarks, where at LO the final-state flavour comes from first and second-generation quarks in the proton.

As for squark–anti-squark production, within the limitations set by the design of Prospino, the LO first and second-generation squark–squark pair-production cross-sections depend on the mass(es) of the final-state squarks and the gluino mass, and the NLO corrections further depend on the mean mass of the first and second-generation squarks. We again validate our cross-sections on the sub-interval $[200, 3000]$ GeV of the training data, for both gluino and squark masses.

If the squark masses are interchanged appropriately, the cross-sections for the process pairs $(\tilde{q}_{L}\tilde{q}_{L}, \tilde{q}_{R}\tilde{q}_{R})$ are identical in Prospino, as are those for the process pairs $(\tilde{q}_{R}\tilde{q}_{L}, \tilde{q}_{L}\tilde{q}_{R})$. The 64 independent processes $\tilde{q}_{L/R}\tilde{q}_{L/R}$ can therefore be reduced to 20 unique cross-sections. Again we use symbolic links to reuse DGPs for processes with identical cross-sections.

In Fig. 14 we show the predicted first and second-generation squark–squark production cross-sections for a selection of sub-processes, as a function of $m_{\tilde{q}}$ and $m_{\tilde{g}}$. All other masses are kept at 1 TeV. For readability, the total cross-section is rescaled. We see that $\sigma_{\text{sec}}$ reliably predicts the contribution from individual squark final-state flavours, and captures the contribution of the gluino $t$-channel diagram, which depends on the chirality of the final-state squarks, giving the qualitatively different behaviour of the cross-section as a function of the gluino mass seen in the right panel of Fig. 14.

In Fig. 15 we show the corresponding distributions of the relative error and residual between the $\sigma_{\text{sec}}$ prediction and the Prospino central cross-section values in $D_{\text{test}}$ and $D_{\text{MSSM-24}}$, for each individual squark–squark process. The residuals indicate that the regression errors from $\sigma_{\text{sec}}$ across all squark–squark processes are generally conservative compared to the actual difference between the true and predicted cross-sections. The relative errors are below 10% for the large majority of test points, across all processes. There is some interesting process-dependent structure, however. For processes with two identical final-state squarks, e.g. $\tilde{u}_{L}\tilde{u}_{L}$ or $\tilde{s}_{L}\tilde{s}_{L}$, the relative error is quite small, due to the dependence of the cross-section upon only three instead of four masses, making it easier to predict reliably. Processes with chirally-matched squarks, i.e. LL or RR final states, have smaller errors than LR final states. This is due to a difference in the LO matrix element, where the LR final states depend on $(t - m_{\tilde{g}}^2)(u - m_{\tilde{g}}^2) - m_{\tilde{g}}^2 s$, whereas LL and RR final states are proportional to $m_{\tilde{g}}^2 s$ [39]. This more complicated kinematic dependence
Fig. 13 The relative error (left) and residual (right) distributions for the first and second-generation squark–anti-squark cross-sections for the test sets $\mathcal{D}_{\text{test}}$ (solid) and $\mathcal{D}_{\text{MSSM-24}}$ (dashed).
Fig. 14 First and second-generation squark–squark pair-production cross-section as a function of the average first and second-generation squark mass (left) and gluino mass (right), for a selection of final states (colours) and the (rescaled) total cross-section for first and second-generation squark–squark production (black).

means that the LR final states are harder to train and show larger relative errors.

4.5 Stop and sbottom pair production

**Prospino** includes PDF contributions only from light quarks and gluons. This means that production of third-generation squarks is purely s-channel in our training samples, so only flavour-neutral squark–anti-squark final states are available, i.e. there are no processes with third-generation squarks in gluino–squark nor squark–squark production. However, the third-generation mass eigenstates used by Prospino include left-right mixing, quantified through the sbottom and stop mixing angles $\cos \theta_t$ and $\cos \theta_{\tilde{t}}$, where $\cos \theta_t = 1$ implies that $\tilde{t}_1, \tilde{t}_2 = \tilde{t}_L, \tilde{t}_R$, and similarly for sbottoms. Furthermore, Prospino does not calculate cross-sections for the production of mixed $\tilde{t}_1 \tilde{t}_2^* + \text{c.c.}$ (or $\bar{b}_1 \bar{b}_2^* + \text{c.c.}$) states, as their cross-sections are of order $\alpha_s^4$, resulting in negligibly small rates [9]. As a result, xsec is limited to training the third-generation processes $\tilde{b}_1 \tilde{b}_1^*, \tilde{b}_2 \tilde{b}_2^*, \tilde{t}_1 \tilde{t}_1^*$, and $\tilde{t}_2 \tilde{t}_2^*$.

For the stop and sbottom pair-production cross-sections, only the final-state mass enters at LO as a parameter (feature). To NLO in QCD, i.e. up to $\mathcal{O}(\alpha_s^3)$, the cross-sections depend on the stop or sbottom final-state mass, the gluino mass, the averaged first and second-generation squark mass, and the stop or sbottom mixing angle, in roughly descending order of importance. Unlike the processes involving first and second-generation squarks, the sbottom and stop cross-sections also include the dependence on all the individual sbottom and stop masses in loops. However, for sbottom (stop) final states, the dependence on the stop (sbottom) masses was found to be very small, and we do not use them as features in the GPs.

For the NLO contributions involving heavy-quark loops, we have used top and bottom masses of $m_t = 172.0 \text{ GeV}$ and $m_b = 4.6 \text{ GeV}$. However, we have checked that the effect of changing these within current experimental uncertainties is numerically irrelevant.

Due to the symmetry of the cross-section expressions at NLO, $\sigma_{\tilde{t}_1 \tilde{t}_1^*} \leftrightarrow \sigma_{\tilde{t}_2 \tilde{t}_2^*}$ under the combined interchange

$$\begin{align*}
\begin{cases}
  m_{\tilde{t}_1} \\
  \cos \theta_{\tilde{t}_1} \\
  \sin \theta_{\tilde{t}_1}
\end{cases} & \leftrightarrow 
\begin{cases}
  m_{\tilde{t}_2} \\
  \cos \theta_{\tilde{t}_2} \\
  -\sin \theta_{\tilde{t}_2}
\end{cases},
\end{align*}
$$

(43)

and similarly for sbottoms. There is also very little difference between the sbottom and stop cross-sections for the same masses. Nevertheless, xsec contains separate DGPs for all four non-zero stop and sbottom pair-production processes included in Prospino, in preparation for future extensions. Here we will focus our validation tests on the $\tilde{t}_1 \tilde{t}_1^*$ cross-sections, and only discuss the other cross-sections when there are significant differences. We validate the xsec output for the third-generation squarks over a slightly larger mass range than for the other processes ([100, 3000] GeV), as there is still considerable interest in light stops.

In Fig. 16, we show the stop pair-production cross-section predicted by xsec as a function of the stop mass, which is by far the dominant parameter in determining the cross-section. We also show the predicted scale
Fig. 15 The relative error (left) and residual (right) distributions for first and second-generation squark–squark pair-production cross-sections for the test sets $D_{\text{int}}$ (solid) and $D_{\text{MSSM-24}}$ (dashed).
and PDF uncertainties, and compare to values taken directly from Prospino. In generating the plot, we have set all stop and sbottom masses degenerate, $\cos \theta_t = 1$, and all other masses to 1 TeV. At low stop masses we can see that the scale error dominates, while at high masses it is the PDF error, as expected. Throughout the validation range the regression error is subdominant.

The gluino mass can be important for contributions that appear at NLO. In Fig. 17 we show the dependence of the $\tilde{t}_1\tilde{t}_1^*$ cross-section on the gluino mass, adopting a stop mass of $m_{\tilde{t}_1} = 800$ GeV, and 1 TeV for all other masses. Clearly, xsec fully captures the variation in the cross-section due to the gluino contribution at low gluino masses, although this dependence is rather small compared to the scale, PDF, and even $\alpha_s$ uncertainties, which we also show. The Prospino result seems to have some numerical jitter at high gluino masses, although the effect lies well within the regression uncertainty band.

In Fig. 18, we show the stop pair-production cross-section for $m_{\tilde{t}_1} = m_{\tilde{g}} = 800$ GeV as function of the average of the first and second-generation squark masses. To maximize the potential effect from squark loops, the sbottom masses are fixed to the same value as the first and second-generation squarks. We fix the mixing angle to $\cos \theta_t = 1$, while the gluino is decoupled at 3 TeV to remove the more dominant NLO contributions from gluino exchange. We see that the dependence of the cross-section on the other squark masses is so weak that the DGP is relatively insensitive to it. However, we again observe that the Prospino results have some jitter at high squark masses. After some investigation of the sampling, we found that this jitter increases as the gluino mass is increased, and we tentatively interpret this as a numerical problem in the gluino-decoupling regime in Prospino.

We present $\tilde{t}_1\tilde{t}_1^*$ and $\tilde{t}_2\tilde{t}_2^*$ production cross-sections as a function of the mixing angle $\theta_t$ in Fig. 19, for $m_{\tilde{t}_1} = m_{\tilde{t}_2} = 800$ GeV and all other sparticle masses set to 1 TeV. We can see that the dependence on the mixing angle is so small — of the order of 2% — that the limited resolution of the regression means that the DGPs cannot currently capture this behaviour. The error is nonetheless well within that reported by xsec.

Looking at the stop and sbottom residual distributions in $D_{\text{test-tb}}$ and $D_{\text{MSSM-24}}$ (right panel of Fig. 20), we see that they have somewhat longer tails than other process types. The most notable feature is at large negative $z$, indicating a slight tendency to overestimate the cross-section reported by Prospino. This is driven by points with large ($> 2\text{ TeV}$) gluino masses, where we earlier observed the jitter in the training data. Overall, however, the regression errors returned by xsec for the stop and sbottom processes are conservative. The corresponding relative errors are below 10% for the vast majority of test points, with some tails.
Fig. 18 Stop pair-production cross-sections as a function of the average of the first and second-generation squark masses, for $m_{\tilde{t}} = 800\text{GeV}$. The xsec prediction and 1σ regression error is in light green, the scale error in pink, the PDF error in violet, and the $\alpha_s$ error in yellow. The Prospino values are shown as dots, and below we show the residual between the xsec regression result and Prospino.

Fig. 19 Stop pair-production cross-sections as a function of the stop mixing angle $\cos \theta_t$. The central-value xsec prediction and the regression error band is shown in orange ($\tilde{t}_1\tilde{t}_1$) and red ($\tilde{t}_2\tilde{t}_2$). Superimposed on the prediction are the Prospino values (dots).

Fig. 20 Distributions for the relative error (left) and residual (right) for the stop and sbottom pair-production cross-sections for the test sets $D_{\text{test-ab}}$ (solid) and $D_{\text{MSSM-24}}$ (dashed).

Fig. 21 The relative error between the predicted stop pair-production cross-section in xsec and the Prospino value as a function of the stop mass versus gluino mass (left) and stop mass versus mixing angle (right).
Finally, in Fig. 21, we show the relative error between the \textit{xsec}-predicted \( \tilde{t}_1 \tilde{t}_1 \) production cross-section and the \textit{Prospino} value, in the planes of common stop mass and gluino mass (left), and stop mass and mixing angle (right). In these plots we set all the other masses to 1 TeV, and in the left-hand plot we fix \( \cos \theta_{\tilde{t}} = 1 \).

We find that \textit{xsec} predicts the values with better than 10\% accuracy in the majority of this space. However, the left-hand panel shows again the problem with numerical jitter from \textit{Prospino} at large gluino (and stop) masses. We also observe a small localised area of underestimated cross-sections (positive relative error) for \( m_{\tilde{t}_1} \sim 1100 \text{ GeV} \) and \( m_{\tilde{g}} \sim 1000 \text{ GeV} \), seen in both plots. This region can also be found in Fig. 16 as a single point where the residual is at the 2\( \sigma \) level.

5 Code structure and usage

5.1 Speeding up cross-section evaluation

To achieve fast cross-section predictions the \textit{xsec} code comes with fully trained GP models. These contain all relevant information about the training points, such as their inverse covariance matrix and the optimised kernel hyperparameter values. The main program, written in \textit{Python}, provides a simple user interface for predicting cross-sections and their uncertainties at a given set of input parameters.

With the time-consuming processes of sampling and training carried out beforehand, two important steps remain in order to obtain predictions for a new parameter point:

1. Performing the matrix-vector multiplications given in Eqs. (21) and (22) to compute predictions from each individual GP expert;
2. Weighting and combining the individual predictions according to the GRBCM prescription, leading to Eq. (31).

As the aggregation step requires no matrix algebra, the first step dominates the computational cost of prediction. It scales in complexity as the square of the number of training points of the GP expert.

The code relies on \texttt{NumPy} [35] functionality for these matrix operations. Significant speed gains are therefore possible if \texttt{NumPy} is properly linked to optimised numerical algebra libraries, like \texttt{BLAS} and \texttt{LAPACK}. Large performance differences exist between different BLAS implementations. Popular ones like \texttt{Intel MKL}, \texttt{OpenBLAS} and \texttt{ATLAS} support multi-threaded calculations, enabling \texttt{NumPy} to take advantage of multi-core machines and \textit{xsec} to achieve the highest evaluation speeds. The \texttt{NumPy} package provides a function \texttt{show_config()} to list the numerical libraries it detected in the system it was built on.

The \textit{xsec} code is compatible with \textit{Python} 2 and 3. While the main program consists of the six independent modules shown in Fig. 22, the intended usage requires no explicit knowledge of this underlying structure. All high-level functions of relevance to the user are immediately accessible upon installing and importing the \textit{xsec} package, as detailed in the following sections.

5.2 Installation

The \textit{xsec} program is available from the Python Package Index (PyPI) and can be installed immediately with the \texttt{pip} package manager, by executing

```
$ pip install xsec
```

in a terminal. Alternatively, the user may wish to access the code directly from its GitHub repository\(^6\) and install a local copy:

```
$ git clone https://github.com/jeriek/xsec.git
$ pip install ./xsec
```

Due to the size of the trained GP datafiles, these are not contained in the repository, nor provided directly by \texttt{pip}. Instead, they are available as separate binaries in the GitHub release. We provide a script for their automatic download and extraction into a directory of choice, called by running

```
xsec-download-gprocs -g gp_dir -t process_type
```

\(^6\)https://github.com/jeriek/xsec
on the command line. Here, \texttt{gp\_dir} is the chosen target directory; a new directory \texttt{gprocs} is created in the current working directory if this argument is omitted. The other optional argument, \texttt{process\_type}, specifies the final-state type for which data will be downloaded: \texttt{gg} (gluino pair production), \texttt{sg} (1st/2nd gen. squark–gluino pair production), \texttt{as} (1st/2nd gen. squark pair production), \texttt{ab} (1st/2nd gen. squark–anti-squark pair production), or \texttt{all} (default).

5.3 Python interface

The primary envisaged use of \texttt{xsec} is as a component in a parameter scan code, where the user chooses the desired particle production processes and varies the input parameters. Appendix A contains a simple example script in Python where these parameters are set by hand. Examples of SLHA file input and usage within a loop over sparticle masses are available in the GitHub repository.

To ensure that any time-consuming computations are only run when strictly necessary, the prediction process is split into four steps:

1. Initialisation
   During the installation (see 5.2), GP model files for all included processes are downloaded to a local directory \texttt{gp\_dir} of choice. At the start of a Python script, \texttt{xsec} must first be pointed to that directory:
   
   ```python
   import xsec
   xsec.init(data_dir="gp\_dir")
   ```

2. Process selection
   Subsequently, the centre-of-mass energy must be set (in GeV) through
   
   ```python
   xsec.set_energy(13000)
   ```

   Currently, only the 13 TeV dataset is available. We expect to add further energies in the near future. Then, one or more sparticle production processes can be specified. A single process is identified by a tuple
   
   ```python
   process = (pid1, pid2)
   ```

   containing the PDG codes of its final-state particles. A list of such tuples is required as the argument to the loading function:
   
   ```python
   xsec.load_processes([process1, process2, ...])
   ```

   This function call decompresses the GP model files (serialised into Python pickles to save space) for the specified processes, and loads them into memory.

   This step only needs to happen once per process. It may take some time, as it involves a matrix multiplication to reconstruct the inverse covariance matrix of the training points from its Cholesky decomposition.

   To show a list of all available trained processes, one can use
   
   ```python
   xsec.list_all_xsec_processes()
   ```

3. Parameter input
   The next step is to set the values of all relevant parameters for the selected processes. The relevant parameters are shown in Table 1. There are three ways to enter the parameters: manually setting their values one by one, setting multiple values at once with a dictionary, or reading all parameters from an SLHA file describing the supersymmetric spectrum.

   ```python
   xsec.set_parameter("name", value)
   xsec.set_parameters(
       {
           "name1": value1,
           "name2": value2,
           ...
       }
   )
   xsec.import_slha("ffilepath")
   ```

   The example script in Appendix A lists all available parameters. The SLHA interface is based on the PySLHA package [53], which is a dependency of \texttt{xsec}. The program currently works with the SLHA1 standard, because we give the decomposition of cross-sections with squarks in terms of their flavour eigenstates (with the exception of the third generation).

   Checking and clearing the current value of one or more parameters is possible with

   ```python
   xsec.get_parameter("name")
   xsec.get_parameters(["name1", "name2", ...])
   xsec.clear_parameter("name")
   xsec.clear_parameters(["name1", "name2", ...])
   ```

   The last line resets all parameter values.

4. Cross-section prediction
   At this point, the cross-section can be evaluated by simply calling
   
   ```python
   xsec.eval_xsection()
   ```

   This function has two optional keywords: \texttt{verbose} (default 2) and \texttt{check\_consistency} (default True). Setting \texttt{verbose=0} makes sure nothing is printed to the screen; \texttt{verbose=1} prints a single line per process that lists, in order: the PDG codes of the two final-state particles, the central cross-section value, and the regression, scale, PDF and $\alpha_s$ error bands (two values

\footnote{To avoid confusing conventions regarding the third-generation mixing angles $\theta_f$ and $\theta_b$, we use the (1, 1) components of the relevant mixing matrices (STOPMIX and SBOTMIX in SLHA files) as parameters.}
each); \texttt{verbose=2} prints a full description of the results. The consistency check will stop the evaluation if the features are outside the range of validity, discussed in Sec. 4, or have not been set.

The returned errors are always relative to the central cross-section, and a minus sign in the print-out makes it easy to distinguish the lower from the upper error bounds. Note that currently in \texttt{xsec} the PDF and $\alpha_s$ errors are symmetric by definition, following the PDF4LHC recommendations [48], whereas the regression and scale errors are not. In order to return a symmetric $\alpha_s$ error, we average the outputs from our two GPs trained separately on the upper and lower errors. This can be changed in the code by more advanced users if desired (for example, to allow $\alpha_s$ to be treated more accurately as a nuisance parameter to be scanned over). The regression error is asymmetric because it comes from a log-normal distribution, while the lower (upper) scale error derives from the minimum (maximum) cross-section value obtained by doubling and halving the renormalisation/factorisation scale.

The results from an evaluation for a given parameter point can be added to an existing SLHA file in the \textsc{xsection} block:

```python
results = xsec.eval_xsection()
xsec.write_slha("slha_path", results)
```

The \textsc{xsection} structure does not allow for storing the regression error, so this is omitted. Furthermore, we do not predict individual cross-section values for all the different members of the PDF set used. Thus, in order to provide the PDF error, we follow the PDF4LHC guidelines [48] and give the lower (upper) bound of the 68% confidence interval by incrementing the central PDF set index by 1 (2) in the \textsc{xsection} block.

Finally, it is recommended to run

```python
xsec.finalise()
```

after all evaluations have been completed. This creates a \texttt{BibTeX} file in the current working directory, listing references to all original work that has been used to provide the requested results.

For advanced users, we include an option to write the decompressed GP files to disk and memory-map them for quicker access. This can reduce the memory load when many processes are requested simultaneously. The cache option can be activated by specifying in the initialisation step. The keyword specifying the cache directory is optional; by default a temporary directory with a random name will be created. The cache directory is removed when \texttt{finalise()} is called.

Another option to decrease the memory load when using \texttt{xsec} for many final states is to load the data for only a few processes at a time, make predictions, and clean the memory before loading new processes. The latter can be done by

```python
xsec.unload_processes([process1, process2, ...])
```

If called without arguments, the data for all previously loaded processes will be cleared from memory.

5.4 Command-line interface

We also provide a command-line interface, where the user can supply a set of two final-state PDG codes and the values for the relevant features (parameters and averaged first and second-generation squark mass) involved in the corresponding cross-section. This is invoked as

```bash
xsec 13000 1000021 1000001 -p 1000 500 500 -g gp_dir
```

This example calculates the cross-section for $\tilde{g}\tilde{u}_L$ production at $\sqrt{s} = 13$ TeV, using the GP data directory \texttt{gp_dir} (see 5.2). The features in the call and their order (in this case $m_{\tilde{g}}$, $m_{\tilde{q}_i}$, and $\bar{m}_{\tilde{q}_i}$, all in GeV) can be gleaned from

```bash
xsec 13000 1000021 1000001 --show-input
```

Alternatively, the parameters can be read from an SLHA file located at \texttt{slha_path}:

```bash
xsec 13000 1000021 1000001 -r slha_path -g gp_dir
```

Executing \texttt{xsec --help} in a terminal provides more details on all possible inputs. We do not recommend using the command-line interface in time-sensitive applications requiring multiple cross-section evaluations for the same process. Every evaluation from the command line invokes the (inevitably slow) \texttt{load_processes()} step, while a lot of time can be saved by writing a Python script where this function is called only once.

5.5 Code structure

For the interested user we briefly describe the structure of the code and the content of the various modules. Our design objective was to keep the user interface intuitive and simple enough to be readily integrated within a

https://phystev.cnrs.fr/wiki/2013:groups:tools:slha
larger code, even in another programming language via binding libraries.

The **parameters** module manages a global dictionary of parameter values, and has functions that allow for setting, getting and clearing those values. Furthermore, there is a function that checks the internal consistency of the entered values, ensuring that the mean squark mass and the centre-of-mass energy are set correctly. SLHA interface functions are also collected in this module, enabling one to read parameter values from an SLHA1 file and to write the cross-section results to an **XSECTION** block in that file.

The **features** module keeps track of the set of parameter values relevant to each specific production process, using a global dictionary and functions that access it.

The **uploader** module contains functions and global variables related to initialisation settings and to loading pre-trained GPs into memory from pickled files. When using the cache option described in Sec. 5.3, this module is responsible for managing the cache directory on the disk.

The implementation of the GP kernels resides within the **kernels** module. These are mostly reproduced from the scikit-learn v0.19.2 [54] source code under the New BSD License, apart from some new kernels and a function that reconstructs kernel function objects from the kernel parameters stored in the pickled GP files.

All functions responsible for GP predictions and combining results from multiple GPs using the GR-BCM prescription are collected in the **evaluation** module. Each production process and cross-section type has its own data directory, containing a **transform** module used by the **evaluation** module, and relevant datafiles. The **transform** module reverses the specific transformations applied to the target values during training.

Internal helper functions are defined in the **utils** module. These are mostly related to the internal naming system for Gaussian process model files, but also include utility functions for outputting results to screen and file, as well as the collection of BibTeX references relevant to the requested processes.

## 6 Conclusions

In this paper, we have presented a new phenomenology code **xsec**, which allows for the fast evaluation of higher-order cross-sections through regression on pre-generated training datasets. The regression in **xsec** is based on Generalised Robust Bayesian Committee Machines, a method that employs distributed Gaussian processes. In addition to the central value and the related regression variance provided by the Gaussian processes, we have trained separate Gaussian processes on the scale, PDF and $\alpha_s$ errors, providing a complete ecosystem for the evaluation of cross-sections and their uncertainties.

The current version of **xsec** 1.0 includes all MSSM strong-production cross-sections at $\sqrt{s} = 13\,\text{TeV}$ at NLO precision in QCD, separated into individual squark flavour final states, and allows for non-degenerate squark masses. We plan to make future updates of **xsec** that will extend the code both in terms of the included energies and processes, as well as with higher-order corrections. The method used here can also be extended to other models, so long as appropriate training sets can be generated. The production of supersymmetric particles in the MSSM serves as a good starting point however, as the absence of s-channel resonances simplifies the training.

We would like to emphasise that the **xsec** code described here is not a new calculation of the included cross-sections. It is a regression estimate based on a pre-generated sample of cross-sections taken from existing results. Thus, users of this code should also reference the original physics results on which the results of **xsec** are based when using them in publications. We provide functionality within the code for easily identifying the relevant references.

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### Appendix A: Code example

Below we show a minimal Python script running the **xsec** program both by specifying masses and other input parameters by hand, and by loading values from an SLHA input file. The script also demonstrates how to store the results in an SLHA file in terms of **XSECTION** blocks.

```python
import xsec

# Set data directory
xsec.init(data_dir='gprocs')
```
# Set centre-of-mass energy (in GeV)
```
xsec.set_energy(13000)
```

# Load GP models for specified process(es)
```
xsec.load_processes([[1000021, 1000021]])
```

# Evaluate cross-section with given inputs
```
xsec.set_parameters({
    'm1000021': 1000.0,
    'm1000001': 500.0,
    'm1000002': 500.0,
    'm1000003': 500.0,
    'm1000004': 500.0,
    'm1000005': 500.0,
    'm1000006': 500.0,
    'm2000001': 500.0,
    'm2000002': 500.0,
    'm2000003': 500.0,
    'm2000004': 500.0,
    'm2000005': 500.0,
    'm2000006': 500.0,
    'sbotmix11': 0.0,
    'stopmix11': 0.0,
    'mean': 500.0,
})
```
```
xsec.eval_xsection()
```

# Evaluate cross-section with SLHA input
```
xsec.import_slha('sps1a.slha')
```
```
results = xsec.eval_xsection()
```
```
xsec.write_slha('sps1a.slha', results)
```

# Create references file
```
xsec.finalise()
```

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