Distributions.jl: Definition and Modeling of Probability Distributions in the JuliaStats Ecosystem

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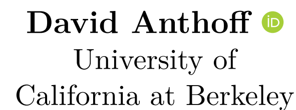
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Abstract

Random variables and their distributions are a central part in many areas of statistical methods. The **Distributions.jl** package provides Julia users and developers tools for working with probability distributions, leveraging Julia features for their intuitive and flexible manipulation, while remaining highly efficient through zero-cost abstractions.

Keywords: Julia, distributions, modeling, interface, mixture, KDE, sampling, probabilistic programming, inference.

1. Introduction

The **Distributions.jl** package (JuliaStats 2019) defines interfaces for representing probability distributions and other mathematical objects describing the generation of random samples. It is part of the JuliaStats open-source organization hosting packages for core mathematical and statistical functions (**StatsFuns.jl**, **PDMats.jl**), model fitting (**GLM.jl** for generalized linear models, **HypothesisTests.jl**, **MixedModels.jl**, **KernelDensity.jl**, **Survival.jl**) and utilities (**Distances.jl**, **Rmath.jl**).

Distributions.jl defines generic and specific behavior required for distributions and other "sample-able" objects. The package implements a large number of distributions to be directly usable for probabilistic modeling, estimation and simulation problems. It leverages idiomatic features of Julia including multiple dispatch and the type system, both presented in more detail in Bezanson, Edelman, Karpinski, and Shah (2017) and Bezanson *et al.* (2018).

In many applications, including but not limited to physical simulation, mathematical optimization or data analysis, computer programs need to generate random numbers from sample spaces or more specifically from a probability distribution or to infer a probability distribution given prior knowledge and observed samples. **Distributions.jl** unifies these use cases under one set of modeling tools.

A core idea of the package is to build an equivalence between mathematical objects and corresponding Julia types. A probability distribution is therefore represented by a type with a given behavior provided through the implementation of a set of methods. This equivalence makes the syntax of programs fit the semantics of the mathematical objects.

Related software

In the `scipy.stats`[1] module of the **SciPy** project (Virtanen *et al.* 2020), distributions are created and manipulated as objects in the object-oriented programming sense. Methods are defined for a distribution class, then specialized for continuous and discrete distribution classes inheriting from the generic distribution, from which inherit classes representing actual distribution families.

Representations of probability distributions have also been implemented in statically-typed functional programming languages, in Haskell in the **Probabilistic Functional Programming** package (Erwig and Kollmansberger 2006), and in OCaml (Kiselyov and Shan 2009), supporting only discrete distributions as an association between collection elements and probabilities. The work in Ścibior, Ghahramani, and Gordon (2015) presents a generic monad-based representation of probability distributions allowing for both continuous and discrete distributions.

The **stats** package, which is distributed as part of the R language, includes functions related to probability distributions which use a prefix naming convention: `r`*`dist`* for random sampling, `d`*`dist`* for computing the probability density, `p`*`dist`* for computing the cumulative distribution function, and `q`*`dist`* for computing the quantiles. The **distr** package (Ruckdeschel, Kohl, Stabla, and Camphausen 2006) also allows R users to define their own distribution as a class of the S4 object-oriented system, with four functions `r, d, p, q` stored by the object. Only one of the four functions has to be provided by the user when creating a distribution object, the other functions are computed in a suitable way. This approach increases flexibility but implies a runtime cost depending on which function has been provided to define a given distribution object. For instance, when only the random generation function is provided, the `RtoDPQ` function empirically constructs an estimation for the others, which requires drawing samples instead of directly evaluating an analytical density.

In C++, the **boost** library (**Boost** Developers 2018), the `maths` component includes common distributions and computations upon them. As in **Distributions.jl**, probability distributions are represented by types (classes), as opposed to functions. The underlying numeric types are rendered generic by the use of templates. The parameters of each distribution are accessed through exposed methods, while common operations are defined as non-member functions, thus sharing a similar syntax with single dispatch.[2] Design and implementation proposals for a multiple dispatch mechanism in C++ have been investigated in Pirkelbauer, Solodkyy, and Stroustrup (2010) and described as a library in Le Goc and Donzé (2015), which would allow for more sophisticated dispatch rules in the **Boost** distribution interface.

This paper is organized as follows. Section 2 presents the main types defined in the package and their hierarchy. In Section 3, the `Sampleable` type and the associated sampling interface are presented. Section 4 presents the distribution interface, which is the central part of the package. Section 5 presents the available tools for fitting and estimation of distributions

[1] https://docs.scipy.org/doc/scipy/reference/stats.html
[2] https://www.boost.org/doc/libs/1_69_0/libs/math/doc/html/math_toolkit/stat_tut/overview/generic.html

from data using parametric and non-parametric techniques. Section 6 presents modeling tools and algorithms for mixtures of distributions. Section 7 highlights two applications of **Distributions.jl** in related packages for kernel density estimation and the implementation of Probabilistic Programming Languages in pure Julia. Section 8 concludes on the work presented and on future development of the ecosystem for probability distributions in Julia.

2. Type hierarchy

The Julia language allows the definition of new types and their use for specifying function arguments using the multiple dispatch mechanism (Zappa Nardelli, Belyakova, Pelenitsyn, Chung, Bezanson, and Vitek 2018).

Most common probability distributions can be broadly classified along two facets:

- the dimensionality of the values (e.g., univariate, multivariate, matrix variate)
- whether it has *discrete* or *continuous* support, corresponding to a density with respect to a counting measure or a Lebesgue measure

In the Julia type system semantics, these properties can be captured by adding type parameters characterizing the random variable to the distribution type which represents it. Parametric typing makes these pieces of information on the sample space available to the Julia compiler, allowing dispatch to be performed at compile-time, making the operation a zero-cost abstraction.

`Distribution` is an abstract type that takes two parameters: a `VariateForm` type which describes the dimensionality, and `ValueSupport` type which describes the discreteness or continuity of the support. These "property types" have singleton subtypes which enumerate these properties:

```
julia> abstract type VariateForm end
julia> struct Univariate    <: VariateForm end
julia> struct Multivariate  <: VariateForm end
julia> struct MatrixVariate <: VariateForm end
julia> abstract type ValueSupport end
julia> struct Discrete   <: ValueSupport end
julia> struct Continuous <: ValueSupport end
```

Various type aliases are then defined for user convenience:

```
julia> DiscreteUnivariateDistribution     = Distribution{Univariate, Discrete}
julia> ContinuousUnivariateDistribution   = Distribution{Univariate, Continuous}
julia> DiscreteMultivariateDistribution   = Distribution{Multivariate, Discrete}
julia> ContinuousMultivariateDistribution = Distribution{Multivariate, Continuous}
```

The Julia `<:` operator in the definition of a new type specifies the direct supertype. Specific distribution families are then implemented as sub-types of `Distribution`: typically these are defined as composite types ("`struct`") with fields capturing the parameters of the distribution. Further information on the type system can be found in Appendix B. For example, the univariate uniform distribution on (a, b) is defined as:

```
julia> struct Uniform{T<:Real} <: ContinuousUnivariateDistribution
```

```
    a::T
    b::T
end
```

Note in this case the `Uniform` distribution is itself a parametric type, this allows it to make use of different numeric types. By default these are `Float64`, but they can also be `Float32`, `BigFloat`, `Rational`, the `Dual` type from **ForwardDiff.jl** in order to support features like automatic differentiation (Revels, Lubin, and Papamarkou 2016), or user defined number types.

Probabilities are assigned to subsets in a sample space, probabilistic types are qualified based on this sample space from a `VariateForm` corresponding to ranks of the samples (scalar, vector, matrix, tensor) and a `ValueSupport` corresponding to the set from which each scalar element is restricted.

Other types of sample spaces can be defined for different use cases by implementing new sub-types. We provide two examples below, one for `ValueSupport` and one for `VariateForm`.

There are different possibilities to represent stochastic processes using the tools from **Distributions.jl**. One possibility is to define them as a new `ValueSupport` type.

```
julia> using Distributions
julia> abstract type StochasticProcess <: ValueSupport end
julia> struct ContinuousStochasticProcess <: StochasticProcess end
julia> abstract type ContinuousStochasticSampler{F<:VariateForm}
<: Sampleable{F,ContinuousStochasticProcess}
end
```

More complete examples of representations of stochastic processes can be found in **Bridge.jl** (Schauer 2018). **Distributions.jl** can also be extended to support tensor-variate random variables in a similar fashion:

```
julia> using Distributions
julia> struct TensorVariate <: VariateForm end
julia> abstract type TensorSampleable{S<:ValueSupport}
<: Sampleable{TensorVariate,S}
end
```

This allows other developers to define their own models on top of **Distributions.jl** without requiring the modification of the package, while end-users benefit from the same interface and conventions, regardless of whether one type was defined in **Distributions.jl** or in an external package.

The types describing a probabilistic sampling process then depend on two type parameters inheriting from `VariateForm` and `ValueSupport`. The most generic form of such a construct is represented by the `Sampleable` type, defining something from which random samples can be drawn:

```
julia> abstract type Sampleable{F<:VariateForm,S<:ValueSupport}
end
```

A `Distribution` is a sub-type of `Sampleable`, carrying the same type parameter capturing the sample space:

```
julia> abstract type Distribution{F<:VariateForm,S<:ValueSupport} <: Sampleable{F,S}
end
```

A `Distribution` is more specific than a `Sampleable`, it describes the probability law mapping elements of a σ-algebra (subsets of the sample space) to corresponding probabilities of occurrence and is associated with corresponding probability distribution functions (CDF, PDF). As such, it extends the required interface as detailed in Section 4. In **Distributions.jl**, distribution families are represented as types and particular distributions as instances of these types. One advantage of this structure is the ease of defining a new distribution family by creating a sub-type of `Distribution` respecting the interface. The behavior of distributions can also be extended by defining new functions over all sub-types of `Distribution` and using the interface.

3. Sampling interface

Some programs require the generation of random values in a certain fashion without requiring the analytical closed-form probability distribution. The `Sampleable` type and interface serve these use cases.

A random quantity drawn from a sample space with given probability distribution requires a way to sample values. Such construct from which values can be sampled is programmatically defined as an abstract type `Sampleable` parameterized by `F` and `S`. The first type parameter `F` classifies sampling objects and distribution by their dimension, univariate distributions associated with scalar random variables, multivariate distributions associated with vector random variables and matrix-variate distributions associated with random matrices. The second type parameter `S` specifies the support, discrete or continuous. New value support and variate form types can also be defined, subtyped from `ValueSupport` or `VariateForm`.

Furthermore, probability distributions are mathematical functions to consider as immutable. A `Sampleable` on the other hand can be a mutable object as shown below.

Example 3.1. Consider the following implementation of a discrete N-state Markov chain as a `Sampleable`.

```
julia> using Distributions
julia> mutable struct MarkovChain <: Sampleable{Univariate,Discrete}
    s::Int
    m::Matrix{Float64}
end
```

A type implementation can only be a subtype of an abstract type as `Sampleable`. With the structure defined, we can implement the required method for a `Sampleable`, namely `rand` which is defined in `Base` Julia.

```
julia> import Base: rand
julia> import Random
julia> function rand(rng, mc::MarkovChain)
    r = rand(rng)
    v = cumsum(mc.m[mc.s,:])
    idx = findfirst(x -> x >= r, v)
    mc.s = idx
    return idx
end
julia> rand(mc::MarkovChain) = rand(Random.GLOBAL_RNG, mc)
```

`rng` is a random number generator (RNG) object, passing it as an argument makes the `rand` implementation predictable. If reproducibility is not important to the use case, `rand` can be called as `rand(mc)` as implemented in the second method, using the global random number generator `Random.GLOBAL_RNG`.

Note that the Markov chain implementation could have been defined in an immutable way. This implementations however highlights one possible definition of a `Sampleable` different from a probability distribution. This flexibility of implementation comes with a homogeneous interface, any item from which random samples can be generated is called in the same fashion. From the user perspective, where a sampler is defined has no impact on its use thanks to Julia multiple dispatch mechanism: the correct method (function implementation) is called depending on the input type.

The `rand` function is the only required element for defining the sampling with a particular process. Different methods are defined for this function, specifying the pseudo-random number generator (PRNG) to be used. The default RNG uses the Mersenne-Twister algorithm (Matsumoto and Nishimura 1998). The sampling state is kept in a global variable used by default when no RNG is provided. New random number generators can be defined by users, sub-typed from the `Random.AbstractRNG` type.

4. Distribution interface and types

The core of the package are probability distributions, defined as an abstract type as presented in 2. Any distribution must implement the `rand` method, which means random values following the distribution can be generated. The two other essential methods to implement are `pdf` giving the probability density function at one point for continuous distributions or the probability mass function at one point for discrete distributions and `cdf` evaluating the Cumulated Density Function at one point. The `quantile` method from the standard library **Statistics** module can be implemented for a `Distribution` type, with the form `quantile(d::Distribution,p::Number)` and returning the value corresponding to the corresponding cumulative probability `p`. Given that the method `rand()` without any argument follows a uniform pseudo-random number in the interval $[0, 1]$, a default fall-back method for random number generation can be defined by inverse transform sampling for a univariate distribution as:

```
julia> rand(d::UnivariateDistribution) = quantile(d, rand())
```

The equivalent R functions for the normal distribution can be matched to the **Distributions.jl** way of expressing them as follows:

```
julia> using Distributions
julia> rnorm(n, mu, sig) = rand(Normal(mu, sig), n)
julia> dnorm(x, mu, sig) = pdf(Normal(mu, sig), x)
julia> pnorm(x, mu, sig) = cdf(Normal(mu, sig), x)
julia> qnorm(p, mu, sig) = quantile(Normal(mu, sig), p)
```

The advantage of using multiple dispatch is that supporting a new distribution only requires the package API to grow by one element which is the new distribution type, instead of four new functions. Most common probability distributions are defined by a mathematical form and a set of parameters. All distributions must implement the `params` method from the

StatsBase.jl, allowing the following example to always work for any given distribution type `Dist` and `d` an instance of the distribution:

```
julia> p = params(d)
julia> new_dist = Dist(p...)
```

Depending on the distribution, sampling a batch of data can be done in a more efficient manner than multiple individual samples. Specialized samplers can be provided for distributions, letting user sample batches of values. Sampling from the Kolmogorov distribution for instance is done by pulling atomic samples using an alternating series method (Devroye 1986, IV.5), while the Poisson distribution lets users use either a counting sampler or Ahrens-Dieter sampler (Ahrens and Dieter 1982).

We will not expand explanations on most trivial functions of the distribution interface, such as `minimum`, `maximum` which can be defined in terms of `support`. Other values are optional to define for distributions, such as `mean`, `median`, `variance`. Not defining these methods as mandatory allows for instance for the Cauchy-Lorentz distribution to be defined.

5. Distribution fitting and estimation

Given a collection of samples and a distribution dependent on a vector of parameters, the distribution fitting task consists in finding an estimation of the distribution parameters $\hat{\theta}$.

5.1. Maximum likelihood estimation

Maximum Likelihood is a common technique for estimating the parameters θ of a distribution given observations (Wilks 1938; Aldrich 1997), with numerous applications in statistics but also in signal processing (Pham and Garat 1997). The **Distributions.jl** interface is defined as one `fit_mle` function with two methods:

```
Distributions.fit_mle(D, x)
Distributions.fit_mle(D, x, w)
```

With `D` a distribution type to fit, `x` being either a vector of observations if `D` is univariate, a matrix of individuals/attributes if `D` is multivariate, and `w` weights for the individual data points. The function call returns an instance of `D` with the parameter adjusted to the observations from `x`.

Example 5.1. Fitting a normal distribution by maximum likelihood.

```
julia> using Distributions
julia> import Random
julia> Random.seed!(33)
julia> xs = rand(Normal(50.0, 10.0), 1000)
julia> fit_mle(Normal, xs)
Distributions.Normal{Float64}(μ=49.781, σ=10.002)
```

Additional partial information can be provided with distribution-specific keywords. `fit_mle(Normal, x)` accepts for instance the keyword arguments `mu` and `sigma` to specify either a fixed mean or standard deviation.

The maximum likelihood estimation (MLE) function is implemented for specific distribution types, corresponding to the fact that there is no default and efficient MLE algorithm for a generic distribution. The implementations present in **Distributions.jl** only require the computation of sufficient statistics. For a more advanced use cases, section D.3 presents the maximization of the likelihood for a custom distribution over a real dataset with a Cartesian product of univariate distributions. The behavior can be extended to a new distribution type `D` by implementing `fit_mle` for it:

```
julia> using Distributions
julia> struct D <: ContinuousUnivariateDistribution end
julia> function Distributions.fit_mle(::Type{D}, xs::AbstractVector)
    # implementation
end
```

5.2. Non-parametric estimation

Some distribution estimation tasks have to be carried out without the knowledge of the distribution form or family for various reasons. Non-parametric estimation generally comprises the estimation of the Cumulative Density Function and of the Probability Density Function. **StatsBase.jl** provides the `ecdf` function, a higher order function returning the empirical CDF at any new point. Since the empirical CDF is built as a weighted sum of Heaviside functions, it is discontinuous.

StatsBase.jl also provides a generic `fit` function, used to build density histograms. `Histogram` is a type storing the bins and heights, other functions from **Base** Julia are defined on `Histogram` for convenience. `fit` for histogram is defined with the following signature:

```
StatsBase.fit(Histogram, data[, weight][, edges]; closed=:right, nbins)
```

6. Modeling mixtures of distributions

Mixture models are used for modeling populations which consists of multiple sub-populations; mixture models are often applied to clustering or noise separation tasks.

A mixture distribution consists of several *component distributions*, each of which has a relative *component weight* or *component prior probability*. For a mixture of n components, then the densities can be written as a weighted sum:

$$f_{\text{mix}}(x; \pi, \theta) = \sum_{i=1}^{n} \pi_i \, f(x, \theta_i)$$

where the parameters are the component weights $\pi = (\pi_1, \ldots, \pi_n)$, taking values on the unit simplex, and each θ_i parameterizes the ith component distribution.

Sampling from a mixture model consists of first selecting the component according to the relative weight, then sampling from the corresponding component distribution. Therefore a mixture model can also be interpreted as a hierarchical model.

Mixtures are defined as an abstract sub-type of `Distribution`, parameterized by the same type information on the variate form and value support:

```
julia> abstract type AbstractMixtureModel{VF<:VariateForm,VS<:ValueSupport}
<: Distribution{VF, VS}
end
```

Any `AbstractMixtureModel` is therefore a `Distribution` and therefore implements specialized the mandatory methods `insupport`, `mean`, `var`, etc. Mixture models also need to implement the following behavior:

- `ncomponents(d::AbstractMixtureModel)`: returns the number of components in the mixture
- `component(d::AbstractMixtureModel, k)`: returns the k-th component
- `probs(d)`: returns the vector of prior probabilities over components

A concrete generic implementation is then defined as:

```
julia> struct MixtureModel{VF<:VariateForm,VS<:ValueSupport,Component<:Distribution}
<: AbstractMixtureModel{VF,VS}
    components::Vector{Component}
    prior::Categorical
end
```

Once constructed, it can be manipulated as any distribution with the different methods of the interface.

Example 6.1. Figure 1 shows the plot resulting from the following construction of a univariate Gaussian mixture model.

```
julia> using Distributions
julia> import Plots
julia> gmm = MixtureModel(
    Normal.([-1.0, 0.0, 3.0],
            [0.3, 0.5, 1.0]),
    [0.25, 0.25, 0.5],
)
julia> xs = -2.0:0.01:6.0
julia> Plots.plot(xs, pdf.(gmm, xs), legend=nothing)
julia> Plots.ylabel!("\$f_X(x)\$")
julia> Plots.xlabel!("\$x\$")
julia> Plots.title!("Gaussian mixture PDF")
```

The `MixtureModel` constructor is taking as argument a vector of `Normal` distributions, defined here from a vector of mean values and a vector of standard deviation values.

Mixture models remain an active area of research and of development within **Distributions.jl**, estimation methods, and improved multivariate and matrix-variate support are planned for future releases. A more advanced example of estimation of a Gaussian mixture by a generic EM algorithm is presented in section D.4.

7. Applications of Distributions.jl

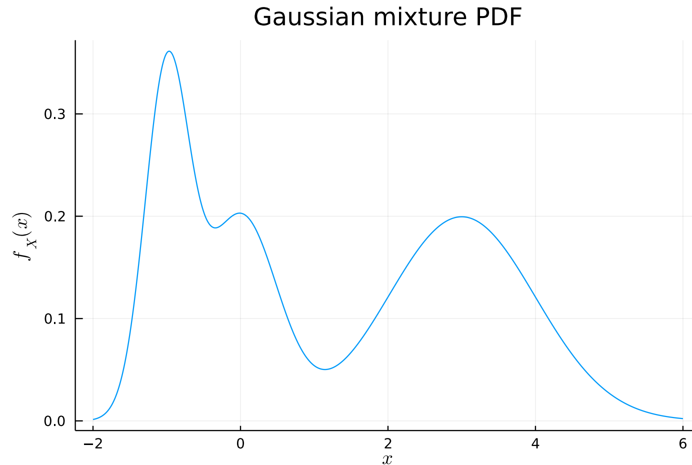

Figure 1: Example PDF of a univariate Gaussian mixture

Distributions.jl has become a foundation for statistical programming in Julia, notably used for economic modeling (Federal Reserve Bank Of New York 2019; Lyon, Sargent, and Stachurski 2017), Markov chain Monte Carlo simulations (Smith 2018) or randomized black-box optimization Feldt (2017) [3]. We present below two applications of the package for non-parametric continuous density estimation and probabilistic programming.

7.1. Kernel density estimation

Probability density functions can be estimated in a non-parametric fashion using kernel density estimation (KDE, Rosenblatt 1956; Parzen 1962). This is supported through the **KernelDensity.jl** package, defining the `kde` function to infer an estimate density from data. Both univariate and bivariate density estimates are supported. Most of the algorithms and parameter selection heuristics developed in **KernelDensity.jl** are based on Silverman (2018). **KernelDensity.jl** supports multiple distributions as base kernels, and can be extended to other families. The default kernel used is Gaussian.

Example 7.1. We highlight the estimation of a kernel density on data generated from the mixture of a log-normal and uniform distributions.

```
julia> import Random, Plots, KernelDensity
julia> using Distributions
julia> function generate_point(rng = Random.GLOBAL_RNG)
    thres = rand(rng)
    if thres >= 0.5
        rand(rng, LogNormal())
    else
        rand(rng, Uniform(2.0, 3.0))
    end
end
julia> mt = Random.MersenneTwister(42)
julia> xs = [generate_point(mt) for _ in 1:5000]
```

[3] Other packages depending on **Distributions.jl** can be found on the Julia General registry: `https://github.com/JuliaRegistries/General`

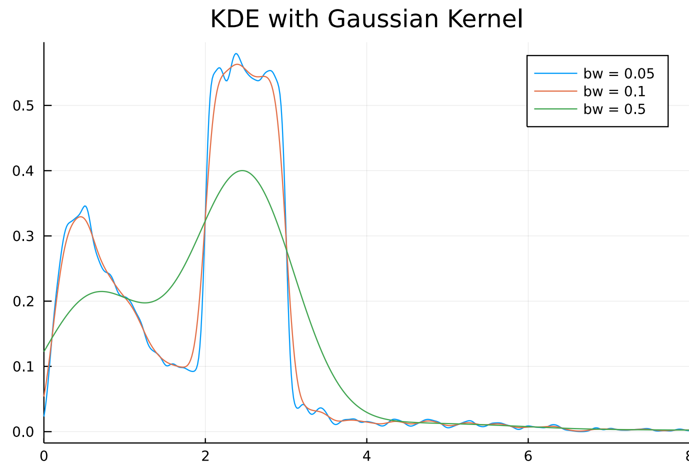

Figure 2: Adjusted KDE with various bandwidths

```
julia> bandwidths = [0.05, 0.1, 0.5]
julia> densities = [KernelDensity.kde(xs, bandwidth = bw) for bw in bandwidths]
julia> p = Plots.plot()
julia> for (b,d) in zip(bandwidths, densities)
    Plots.plot!(p, d.x, d.density, labels = "bw = $b")
end
julia> Plots.xlims!(p, 0.0, 8.0)
julia> Plots.title!("KDE with Gaussian Kernel")
```

The bandwidth $bw = 0.1$ seems not to overfit isolated data points without smoothing out important components. All examples provided use the **Plots.jl** [4] package to plot results, which can be used with various plotting engines as back-end. We can compare the kernel density estimate to the real PDF as done in the following script and illustrated Figure 3.

```
julia> xvals = 0.01:0.01:8.0
julia> yvals = map(xvals) do x
    comp1 = pdf(LogNormal(), x)
    comp2 = pdf(Uniform(2.0, 3.0), x)
    0.5 * comp1 + 0.5 * comp2
end
julia> p = Plots.plot(xvals, yvals, labels = "Real distribution")
julia> kde = KernelDensity.kde(xs, bandwidth = 0.1)
julia> Plots.plot!(p, kde.x, kde.density, labels = "KDE")
julia> Plots.plot!(p, xvals, yvals, labels = "Real distribution")
julia> Plots.xlims!(p, 0.0, 8.0)
```

The kernel density estimation technique relies on a base distribution (the kernel) which is convoluted against the data. The package uses directly the interface presented in section 4 to accept a `Distribution` as second parameter. The following script computes the kernel density estimates with a Gaussian and triangular distributions. The result is illustrated Figure 4.

```
julia> mt = Random.MersenneTwister(42)
```

[4]http://docs.juliaplots.org

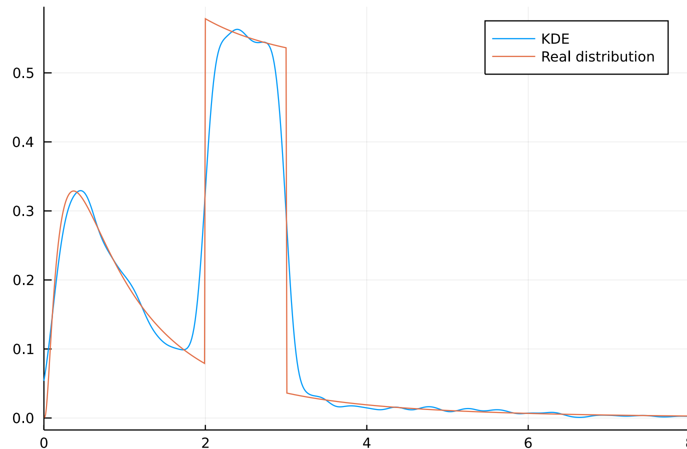

Figure 3: Comparison of the experimental and real PDF

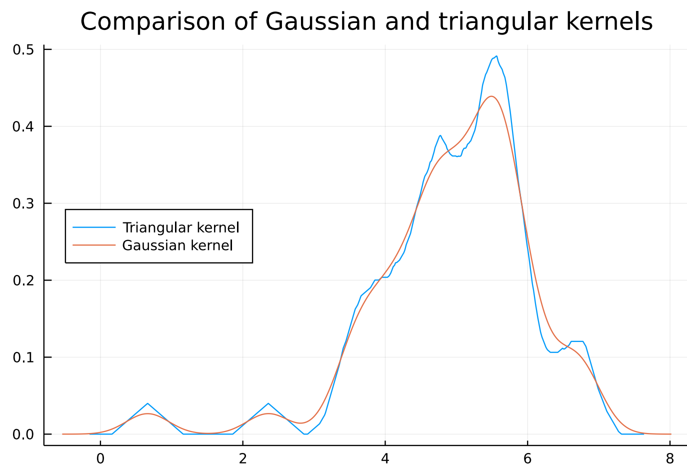

Figure 4: Comparison of different kernels defined as Distribution objects

```
julia> (μ, σ) = (5.0, 1.0)
julia> xs = [rand(mt, Normal(μ, σ)) for _ in 1:50]
julia> ndist = Normal(0.0, 0.3)
julia> gkernel = kde(xs, ndist)
julia> tdist = TriangularDist(-0.5, 0.5)
julia> tkernel = KernelDensity.kde(xs, tdist)
julia> p = Plots.plot(tkernel.x, tkernel.density, labels = "Triangular kernel")
julia> Plots.plot!(p, gkernel.x, gkernel.density,
            labels = "Gaussian kernel", legend = :left)
julia> Plots.title!(p, "Comparison of Gaussian and triangular kernels")
```

The density estimator is computed via the Fourier transform: any distribution with a defined characteristic function (via the `cf` function from **Distributions.jl**) can be used as a kernel. The ability to manipulate distributions as types and objects allows end-users and package developers to compose on top of defined distributions and to define their own to use for kernel density estimations without any additional runtime cost. The kernel estimation of a bi-variate

density is shown in D.2.

7.2. Probabilistic programming languages

Probabilistic programs are computer programs with the added capability of drawing the value of a variable from a probability distribution and conditioning variable values on observations (Gordon, Henzinger, Nori, and Rajamani 2014). They allow for the specification of complex relations between random variables using a set of constructs that go beyond typical graphical models to include flow control (e.g., loops, conditions), recursion, user-defined types and other algorithmic building blocks, differing from explicit graph construction by users, as done for instance in Smith (2018). Probabilistic programming languages (PPL) are programming language or libraries enabling developers to write such a probabilistic program. That is, they are a type of domain-specific language (DSL, Fowler 2010). We refer the interested reader to Van de Meent, Paige, Yang, and Wood (2018) for an overview of PPL design and use, to Ścibior *et al.* (2017) for the analysis of Bayesian inference algorithms as transformations of intermediate representations, and to Vákár, Kammar, and Staton (2019) for representation of recursive types in PPLs. They often fall in two categories.

In the first type, the PPL is its own independent language, including syntax and parsing, though it may rely on another "host" language for its execution engine. For example, Stan (Carpenter *et al.* 2017), uses its own `.stan` model specification format, though the parser and inference engine are written in C++. This type of approach benefits from defining its own syntax, thus designing it to look similar to the way equivalent statistical models are written. The model is also verified for syntactic correctness at compile-time.[5]

In the second type of PPL, the language is embedded within and makes use of the syntax of the host language, leveraging that language's native constructs. For example, **PyMC** (Patil, Huard, and Fonnesbeck 2010; Kochurov, Carroll, Wiecki, and Lao 2019), Pyro (Bingham *et al.* 2019), and **Edward** (Tran, Kucukelbir, Dieng, Rudolph, Liang, and Blei 2016) all use Python as the host language, leveraging **Theano**, **Torch**, and **TensorFlow**, respectively, to perform many of the underlying inference computations. Here, the key advantage is that these PPLs gain access to the ecosystem of the host language (data structures, libraries, tooling). User documentation and development efforts can also focus on the key aspects of a PPL instead of the full stack.[6]

However, both approaches to PPLs suffer from drawbacks. In the first type of PPLs, users must add new elements to their toolchains for the development and inference of statistical models. That is, they are likely to use a general-purpose programming language for other tasks, then switch to the PPL environment for the sampling and inference task, and then read the result back into the general-purpose programming language. One solution to this problem is to develop APIs in general purpose languages, but full inter-operability between two environments is non-trivial. Developers must then build a whole ecosystem around the PPL, including data structures, input/output, and text editor support, which costs time that might otherwise go toward improving the inference algorithms and optimization procedures.

While the second type of PPL may not require the development of a separate, parallel set of tools, it often runs into "impedance mismatches" of its own. In many cases, the host language has not been designed for a re-use of its constructs for probabilistic programming, resulting

[5] An example model combining **Stan** with R can be found at Gelman (2019).

[6] The same golf putting data were used using **PyMC** as PPL in **PyMC** (2019).

in syntax that aligns poorly with users' mathematical intuitions. Moreover, duplication may still occur at the level of classes or libraries, as, for example, Pyro and Edward depend on Torch and TensorFlow, which replicate much of the linear algebra functionality of NumPy for their own array constructs.

By contrast, the design of **Distributions.jl** has enabled the development of embedded probabilistic programming languages such as **Turing.jl** (Ge, Xu, and Ghahramani 2018), **SOSS.jl** (Scherrer 2019), **Omega.jl** (Tavares 2018) or **Poirot.jl** (Innes 2019) with comparatively less overhead or friction with the host language. These PPLs are able to make use of three elements unique to the Julia ecosystem to challenge the dichotomy between embedded and stand-alone PPLs. First, they make use of Julia's rich type system and multiple dispatch, which more easily support modeling mathematical constructs as types. Second, they all utilize **Distributions.jl**'s types and hierarchy for the sampling of random values and representation of their distributions. Finally, they use manipulations and transformations of the user Julia code to create new syntax that matches domain-specific requirements.

These transformations are either performed through macros (for **Soss.jl** and **Turing.jl**) or modifications of the compilation phases through compiler overdubbing (**Omega.jl** and **Poirot.jl** use **Cassette.jl** and **IRTools.jl** respectively to modify the user code or its intermediate representations). As in the Lisp tradition, Julia's macros are written and manipulable in Julia itself and rewrite code during the lowering phase (Bezanson *et al.* 2018). Macros allow PPL designers to keep programs close to standard Julia while introducing package-specific syntax that more closely mimics statistical conventions, all without compromising on performance. For instance, a simple model definition from the **Turing.jl** documentation illustrates a model that is both readable as Julia code while staying close to statistical conventions:

```
julia> @model coinflip(y) = begin
    p ~ Beta(1, 1)

    N = length(y)
    for n in 1:N
        y[n] ~ Bernoulli(p)
    end
end
```

With these syntax manipulation capabilities, along with compiled language performance, the combination of Julia with **Distributions.jl** provides an excellent foundation for further research and development of PPLs. [7]

8. Conclusion and future work

We presented some of the types, structures and tools for modeling and computing on probability distributions in the **JuliaStats** ecosystem. The **JuliaStats** packages leverage some key constructs of Julia such as definition of new composite types, abstract parametric types and sub-typing, along with multiple dispatch. This allows users to express computations involving random number generation and the manipulation of probability distributions. A clear interface allows package developers to build new distributions from their mathematical definition. New algorithms can be developed, using the Distribution interface and as such extending the

[7] The golf putting model was ported to **Turing.jl** in Duncan (2020).

new features to all sub-types. These two features of Julia, namely extension of behavior to new types and definition of behavior over existing type hierarchy, allow different features built around the Distribution type to inter-operate seamlessly without hard coupling nor additional work from the package developers or end-users. Future work on the package will include the implementation of maximum likelihood estimation for other distributions, including mixtures and matrix-variate distributions.

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A. Installation of the relevant packages

The recommended installation of the relevant packages is done through the **Pkg.jl**[8] tool available within the Julia distribution standard library. The common way to interact with the tool is within the REPL for Julia 1.0 and above. The closing square bracket "]" starts the pkg mode, in which the REPL stays until a return key is stroke.

```
julia> ] add StatsBase
(v1.0) pkg> add Distributions
(v1.0) pkg> add KernelDensity
```

This installation and all code snippets are guaranteed to work on Julia 1.0 and later with the semantic versioning commitment. Once installed, a package can be removed with the command `rm PackageName` or updated. All package modifications are guaranteed to respect version constraints for their direct and transitive dependencies. The packages **StatsBase.jl**, **Distributions.jl**, **KernelDensity.jl** are all open-source under the MIT license.

B. Julia type system

B.1. Functions and methods

In Julia, a function "is an object that maps a tuple of argument values to a return value".[9] A special case is an empty tuple as input, as in `y = f()`, and a function that returns the `nothing` value.

A function definition creates a top-level identifier with the function name. This can be passed around as any other value, for example to other functions. The function `map` takes a function and a collection `map(f, c)`, and applies the function to each element of the collection to return the mapped values.

A function might represent a conceptual computation but different specific implementations might exist for this computation. For instance, the addition of two numbers is a common concept, but how it is implemented depends on the number type. The specific implementation of addition for complex numbers is[10]

```
julia> +(z::Complex, w::Complex) = Complex(real(z) + real(w), imag(z) + imag(w))
```

This specific implementation is a **method** of the `+` function. Users can define their own implementation of existing functions, thus creating a new method for this function. Different methods can be implemented by changing the tuple of arguments, either with a different number of arguments or different types.[11]

Example B.1. In the following example, the function `f` has two methods. The function called depends on the number of arguments.

[8] https://docs.julialang.org/en/v1/stdlib/Pkg/
[9] Julia documentation - Functions: https://docs.julialang.org/en/v1/manual/functions
[10] Julia source code, base/complex.jl
[11] Julia documentation - Methods: https://docs.julialang.org/en/v1/manual/methods

```
julia> function f(x)
    println(x)
end
julia> function f(x, y)
    println("x: $x & y: $y")
end
```

Example B.2. In the following example, the function `g` has two methods. The first one is the most specific method and will be called for any type of the argument `x` that is a `Number`. Otherwise, the second method, which is less specific, will be called.

```
julia> g(x::T) where {T<:Number} = (3*x, x)
julia> g(x) = (x, 3)
```

Note that the order of definitions does not matter here, the least specific could have been defined first, and then the number-specialized implementation.

The method dispatched on by the Julia runtime is always the most specific.

Example B.3. If there is no unique most specific method, Julia will raise a `MethodError`

```
julia> f(x, b::Float64) = x
f (generic function with 1 method)
julia> f(x::Float64, b) = b
f (generic function with 2 methods)
julia> f(3.0, 2.0)
ERROR: MethodError: f(::Float64, ::Float64) is ambiguous. Candidates:
  f(x::Float64, b) in Main at REPL[2]:1
  f(x, b::Float64) in Main at REPL[1]:1
Possible fix, define
  f(::Float64, ::Float64)
```

B.2. Types

Julia enables users to define their own types including abstract types, mutable and immutable composite types or structures and primitive types (composed of bits). Packages often define abstract types to regroup types under one label and provide default implementation for a group of types. For examples, lots of methods require arguments which are identified as `Number`, upon which arithmetic operations can be applied, without having to re-define methods for each of the concrete number types. The most common type definition for end-users is composite types with the keyword `struct` as follows:

```
julia> struct S
    field1::TypeOfField1
    field2::TypeOfField2
    field3 # a field without specified type will take the type 'Any'
end
```

In some cases, a type is defined for the sole purpose of creating a new method and does not require additional data in fields. The following definition is thus valid:

```
julia> struct S end
```

An instance of S is called a **singleton**, there is only one instance of such type.

Example B.4. One use case is the specification of different algorithms for a procedure. The input of the procedure is always the same, so is the expected output, but different ways to compute the result are available.

```
julia> struct Alg1 end
julia> struct Alg2 end
julia> mul(x::Unsigned, y::Unsigned, ::Alg1) = x * y
julia> mul(x::T, y::Unsigned, ::Alg2) where {T<:Unsigned} = T(sum(x for _ in 1:y))
```

Note that in the second example, the information of the concrete type T of x is required to convert the sum expression into a number of type T.

C. Comparison of Distributions.jl, Python/SciPy and R

In this section, we develop several comparative examples of how various computation tasks linked with probability distributions are performed using R, Python with **SciPy/NumPy** and Julia.

C.1. Sampling from various distributions

The following programs draw 100 samples from a Gamma distribution $\Gamma(k = 10, \theta = 2)$, in R:

```
R> set.seed(42)
R> rgamma(100, shape = 10, scale = 2)
```

The following Python version uses the **NumPy** & **SciPy** libraries.

```
>>> import numpy as np
>>> import scipy.stats as stats
>>> np.random.seed(42)
>>> stats.gamma.rvs(10, scale = 2, size = 100)
```

The following Julia version is written to stay close to the previous ones, thus setting the global seed and not passing along a new RNG object.

```
julia> import Random
julia> using Distributions
julia> Random.seed(42)
julia> g = Gamma(10, 2)
julia> rand(g, 100)
```

C.2. Representing a distribution with various scale parameters

The following code examples are in the same order as the previous sub-section:

```
R> x <- seq(-3.0,3.0,0.01)
R> y <- dnorm(x, mean = 0.5, sd = 0.75)
R> plot(x, y)
```

The Python example uses **NumPy**, **SciPy** and **matplotlib**.

```
>>> import numpy as np
>>> from scipy import stats
>>> from matplotlib import pyplot as plt
>>> x = np.arange(-3.0,3.0,0.01)
>>> y = stats.norm.pdf(x, loc = 0.5, scale = 0.75)
>>> plt.plot(x,y)
```

The Julia version uses defines a Gaussian random variable object `n`:

```
julia> using Distributions
julia> using Plots
julia> n = Normal(0.5, 0.75)
julia> x = -3.0:0.01:3.0
julia> y = pdf.(n, x)
julia> plot(x, y)
```

Note that unlike the R and Python examples, x does not need to be represented as an array but as an iterable not storing all intermediate values, saving time and memory. The dot or broadcast operator in `pdf.(n, x)` applies the function to all elements of `x`.

D. Wine data analysis

In this section, we show the example of analyses run on the wine dataset Aeberhard, Coomans, and De Vel (1994) obtained on the UCI machine learning repository. The data can be fetched directly over HTTP from within Julia.

```
julia> using Distributions, DelimitedFiles
julia> import Plots
julia> wine_data_url =
    "https://archive.ics.uci.edu/ml/machine-learning-databases/wine/wine.data"
julia> wine_data_file = download(wine_data_url)
julia> raw_wine_data = readdlm(wine_data_file, ',', Float64)
julia> wine_quant = raw_wine_data[:,2:end]
julia> wine_labels = Int.(raw_wine_data[:,1])
```

D.1. Automatic multivariate fitting

We can then fit a multivariate distribution to some variables and observe the result:

```
julia> alcohol = wine_quant[:,1]
julia> log_malic_acid = log.(wine_quant[:,2])
julia> obs = permutedims([alcohol log_malic_acid])
julia> res_normal = fit_mle(MvNormal, obs)
julia> cont_func(x1, x2) = pdf(res_normal, [x1,x2])
julia> p = Plots.contour(11.0:0.05:15.0, -0.5:0.05:2.5, cont_func)
julia> Plots.scatter!(p, alcohol, log_malic_acid, label="Data points")
julia> Plots.title!(
    p, "Wine scatter plot & Gaussian maximum likelihood estimation")
```

Note that `fit_mle` needs observations as columns, hence the use of `permutedims`.

D.2. Non-parametric density estimation

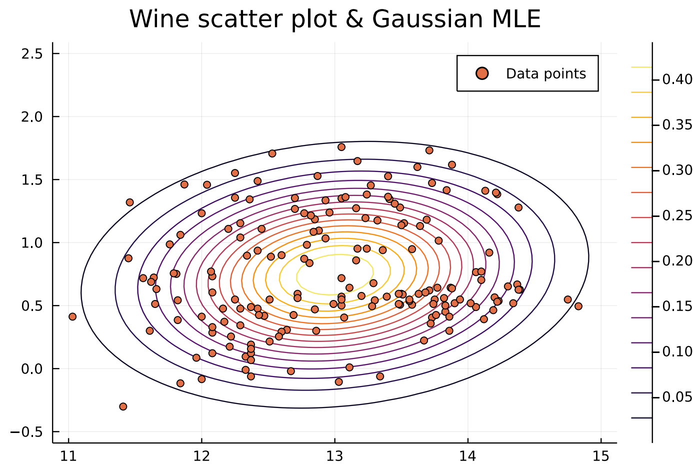

Figure 5: Multivariate Gaussian MLE over (x_1, x_2) of the wine data

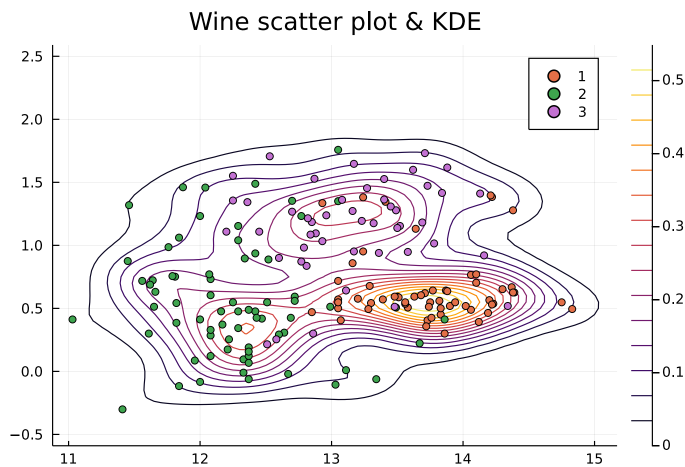

Figure 6: KDE over (x_1, x_2) of the wine data

Assuming a multivariate Gaussian distribution might be considered a too strong assumption, a kernel density estimator can be used on the same data:

```
julia> wine_kde = KernelDensity.kde((alcohol, log_malic_acid))
julia> cont_kde(x1, x2) = pdf(wine_kde, x1, x2)
julia> p = Plots.contour(11.0:0.05:15.0, -0.5:0.05:2.5, cont_kde)
julia> Plots.scatter!(p, alcohol, log_malic_acid, group=wine_labels)
julia> Plots.title!(p, "Wine scatter plot & Kernel Density Estimation")
```

The resulting kernel density estimation is shown Figure 6. The level curves highlight the centers of the three classes of the dataset.

D.3. Product distribution model

Given that a logarithmic transform was used for x_2, a shifted log-normal distribution can be fitted: $X_2 - 0.73 \sim LogNormal(\mu, \sigma)$. The maximum likelihood estimator could be computed

as in section D.1. Instead, we will demonstrate the simplicity of building new constructs and optimize over them. A `Product` distribution is implemented in **Distributions.jl**, defining a Cartesian product of the two variables, thus assuming their independence:

$$X = (X_1, X_2) \tag{1}$$

Assuming X_1 follows a normal distribution, given a vector of 4 parameters $[\mu_1, \sigma_1, \mu_2, \sigma_2]$, the distribution can be constructed:

```
julia> function build_product_distribution(p)
    return product_distribution([
        Normal(p[1], p[2]),
        LogNormal(p[3], p[4]),
    ])
end
```

Computing the log-likelihood of a product distribution boils down to the sum of the individual log-likelihood. The gradient could be computed analytically but automatic differentiation will be leveraged here using **ForwardDiff.jl** (Revels *et al.* 2016):

```
julia> function loglike(p)
    d = build_product_distribution(p)
    return loglikelihood(d.v[1], wine_quant[:,1]) +
           loglikelihood(d.v[2], wine_quant[:,2] .- 0.73)
end
julia> ∇L(p) = ForwardDiff.gradient(loglike, p)
```

Once the gradient obtained, first-order optimization methods can be applied. To keep everything self-contained, a gradient descent with decreasing step will be applied:

$$x_{k+1} = x_k + \rho_k \nabla\mathcal{L}(x_k) \tag{2}$$

$$\rho_{k+1} = \rho_0/(k+m) \tag{3}$$

With (ρ_0, m) constants.

```
julia> p = [10.0 + 3.0 * rand(), rand()+1, 2.0 + 3.0*rand(), rand()+1]
julia> iter = 1
julia> maxiter = 5000
julia> while iter <= maxiter && sum(abs.(∇L(p))) >= 10^-6
    p = p + 0.05 * inv(iter+5) * ∇L(p)
    p[2] = p[2] < 0 ? -p[2] : p[2]
    p[4] = p[4] < 0 ? -p[4] : p[4]
    iter += 1
end
julia> d = build_product_distribution(p)
```

Without further code or method tuning, the optimization takes about $590\mu s$ and few iterations to converge as shown Figure 8. For more complex use cases, users would look at more sophisticated techniques as developed in **JuliaSmoothOptimizers** (Orban and Siqueira 2019) or **Optim.jl** (Mogensen and Riseth 2018). Figure 7 highlights the resulting marginal and joint distributions.

D.4. Implementation of an Expectation-Maximization algorithm

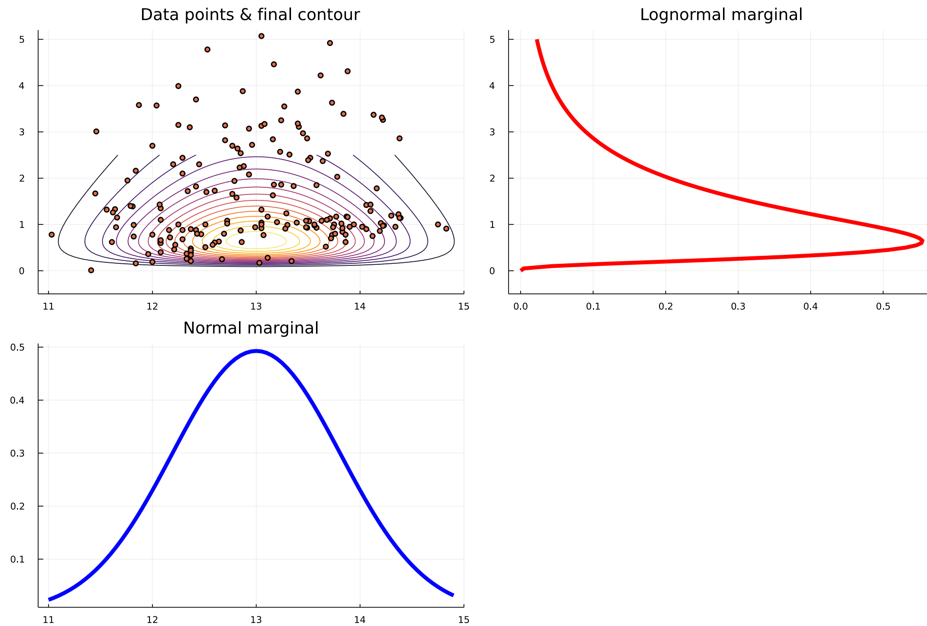

Figure 7: Resulting inferred joint and marginal distribution for (X_1, X_2)

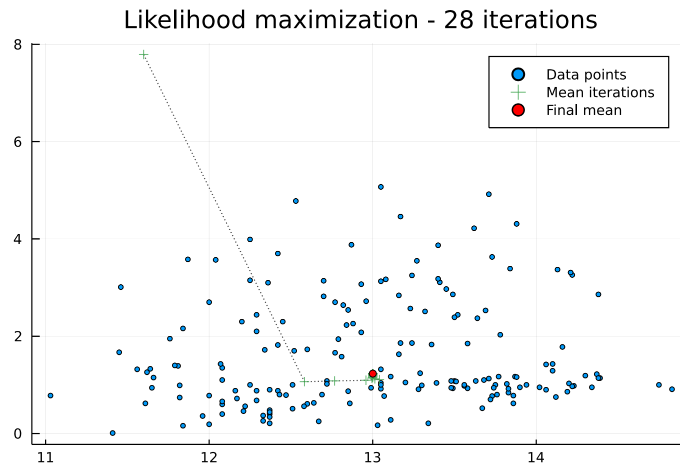

Figure 8: Illustration of the likelihood maximization convergence

In this section, we highlight how Julia dispatch mechanism and **Distributions.jl** type hierarchy can help users define algorithms in a generic fashion, leveraging specific structure but allowing their extension. We know that the observations from the wine data set are split into different classes Z. We will consider only the two first variables, with the second at a log-scale: $X = (x_1, log(x2))$.

The expectation step computes the probability for each observation i to belong to each label k:

```
julia> function expectation_step(X, dists, prior)
    n = size(X, 1)
    Z = Matrix{Float64}(undef, n, length(prior))
```

```
    for k in eachindex(prior)
        for i in 1:n
            Z[i,k] = prior[k] * pdf(dists[k], X[i,:]) /
                     sum(
                        prior[j] * pdf(dists[j], X[i,:])
                        for j in eachindex(prior)
                    )
        end
    end
    return Z
end
```

`dists` is a vector of distributions, note that no assumption is needed on these distributions, other than the standard interface. The only computation applied is indeed the computation of the `pdf` for each of these.

The operation for which the specific structure of the distribution is required is the maximization step. For many distributions, a closed-form solution of the maximum-likelihood estimator is known, avoiding expensive optimization schemes as developed in D.3. In the case of the Normal distribution, the maximum likelihood estimator is given by the empirical mean and covariance matrix. We define the function `maximization_step` to take a distribution type, the data `X` and current label estimates Z, computing both the prior probabilities of each of the classes π_k and the corresponding conditional distribution D_k, it returns the pair of vectors (D, π).

```
julia> function maximization_step(::Type{<:MvNormal}, X, Z)
    n = size(X, 1)
    Nk = size(Z, 2)
    μ = map(1:Nk) do k
        num = sum(Z[i,k] .* X[i,:] for i in 1:n)
        den = sum(Z[i,k] for i in 1:n)
        num / den
    end

    Σ = map(1:Nk) do k
        num = zeros(size(X, 2), size(X, 2))
        for i in 1:n
            r = X[i,:] .- μ[k]
            num .= num .+ Z[i,k] .* (r * r')
        end
        den = sum(Z[i,k] for i in 1:n)
        num ./ den
    end
    prior = [inv(n) * sum(Z[i,k] for i in 1:n)
            for k in 1:Nk
        ]
    dists = map(1:Nk) do k
        MvNormal(μ[k], Σ[k] + 10e-7I)
    end
    return (dists, prior)
end
```

The final block is a function alternatively computing Z and (D, π) until convergence:

```
julia> function expectation_maximization(
        D::Type{<:Distribution},
        X, Nk,
        maxiter = 500,
        loglike_diff = 10e-5)
    # initialize classes
    n = size(X,1)
    Z = zeros(n, Nk)
    for i in 1:n
        j0 = mod(i,Nk)+1
        j1 = j0 > 1 ? j0-1 : 2
        Z[i,j0] = 0.75
        Z[i,j1] = 0.25
    end
    (dists, prior) = maximization_step(D, X, Z)
    l = loglike_mixture(X, dists, prior)
    lprev = 0.0
    iter = 0
    # EM iterations
    while iter < maxiter && abs(lprev-l) > loglike_diff
        Z = expectation_step(X, dists, prior)
        (dists, prior) = maximization_step(D, X, Z)
        lprev = l
        l = loglike_mixture(X, dists, prior)
        iter += 1
    end
    return (dists, prior, Z, l, iter)
end
julia> function loglike_mixture(X, dists, prior)
    l = zero(eltype(X))
    n = size(X,1)
    for i in 1:n
        l += log(
            sum(prior[k] * pdf(dists[k], X[i,:]) for k in eachindex(prior))
        )
    end
    return l
end
```

Starting from an alternated affectation of observations to labels, it calls the two methods defined above for the E and M steps.

The strength of this implementation is that extending it to more functions only requires to implement `maximization_step(D, X, Z)` for the new distribution. The rest of the structure will then work as expected.

E. Benchmarks on mixture PDF evaluations

In this section, we evaluate the computation time for the PDF of mixtures of distributions, on mixture of Gaussian univariate distributions, and then on a mixture of heterogeneous distributions including normal and log-normal distributions.

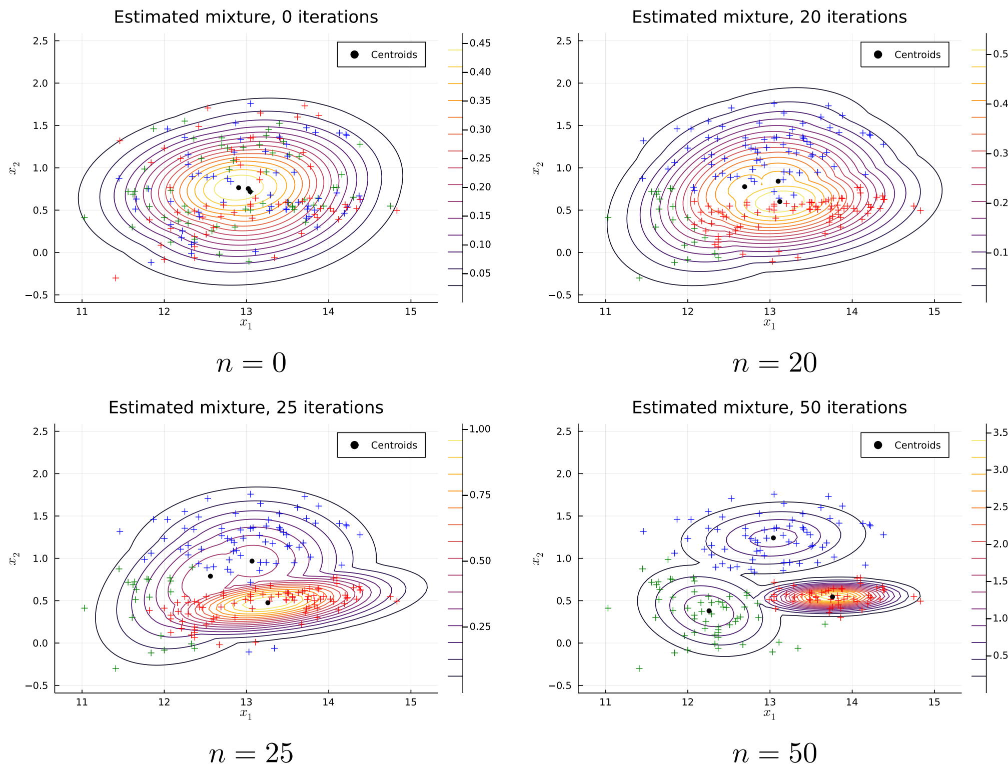

Figure 9: Convergence of the EM algorithm

```
julia> using BenchmarkTools: @btime
julia> distributions = [
    Normal(-1.0, 0.3),
    Normal(0.0, 0.5),
    Normal(3.0, 1.0),
]
julia> priors = [0.25, 0.25, 0.5]
julia> gmm_normal = MixtureModel(distributions, priors)
julia> x = rand()
julia> @btime pdf($gmm_normal, $x)
julia> large_normals = [Normal(rand(), rand()) for _ in 1:1000]
julia> large_probs = [rand() for _ in 1:1000]
julia> large_probs .= large_probs ./ sum(large_probs)
julia> gmm_large = MixtureModel(large_normals, large_probs)

@btime pdf($gmm_large, $x)

julia> large_h = append!(
    ContinuousUnivariateDistribution[Normal(rand(), rand()) for _ in 1:1000],
    ContinuousUnivariateDistribution[LogNormal(rand(), rand()) for _ in 1:1000],
)
julia> large_h_probs = [rand() for _ in 1:2000]
julia> large_h_probs .= large_h_probs ./ sum(large_h_probs)
julia> gmm_h = MixtureModel(large_h, large_h_probs)
julia> @btime pdf($gmm_h, $x)
```

The PDF computation on the small, large and heterogeneous mixture take on average $332ns$, $105\mu s$ and $259\mu s$ respectively. We also compare the computation time with the manual computation of the mixture evaluated as such:

```
julia> function manual_computation(mixture, x)
    v = zero(eltype(mixture))
    p = probs(mixture)
    d = components(mixture)
    for i in 1:ncomponents(mixture)
        if p[i] > 0
            v += p[i] * pdf(d[i], x)
        end
    end
    return v
end
```

The PDF computation currently in the library is faster than the manual one, the sum over weighted PDF of the components being performed without branching. The ratio of manual time over the implementation of **Distributions.jl** being on average 1.24, 5.88 and 1.28 respectively. The greatest acceleration is observed for large mixtures with homogeneous component types. The slow-down for heterogeneous component types is due to the compiler not able to infer the type of each element of the mixture, thus replacing static with dynamic dispatch. The **Distributions.jl** package also contains a `/perf` folder containing experiments on performance to track possible regressions and compare different implementations.

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