
**SciPy 2024**

July 8 - July 14, 2024

Proceedings of the 23rd
Python in Science Conference
ISSN: 2575-9752

multinterp

A Unified Interface for Multivariate Interpolation in the Scientific Python Ecosystem

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Abstract

Multivariate interpolation is a fundamental tool in scientific computing used to approximate the values of a function between known data points in multiple dimensions. Despite its importance, the Python ecosystem offers a fragmented landscape of specialized tools for this task. This fragmentation hinders code reusability, experimentation, and efficient deployment across diverse hardware. The `multinterp` package was developed to address this challenge. It provides a unified interface for various grids used for interpolation (regular, irregular, and curvilinear), supports multiple backends (CPU, parallel, and GPU), and includes tools for multivalued interpolation and interpolation of derivatives. This paper introduces `multinterp`, demonstrates its capabilities, and invites the community to contribute to its development.

Keywords multivariate, interpolation, gpu, rectilinear, curvilinear, scattered

1. INTRODUCTION

In scientific computing, interpolation is a fundamental method used to approximate new data points within a range of known functional data points. When this concept is applied to functions with multiple variables, it is known as multivariate interpolation. This technique is crucial for various scientific applications, including data analysis, numerical modeling, and visualizing complex datasets.

Over time, the scientific Python ecosystem has developed various specialized tools for multivariate interpolation. These powerful tools are spread across different packages, each designed for specific purposes and for distinct data types. This scattering of tools across multiple packages creates challenges for researchers and practitioners.

One major issue is the inconsistency of interfaces across different packages. The varying syntax and usage patterns make it difficult for users to switch between interpolation methods or compare their performance effectively. Additionally, many existing tools are designed for CPU-only execution, lacking GPU acceleration or parallel processing support. This limitation can significantly impact performance, especially when dealing with large datasets or complex interpolation tasks.

Another challenge stems from the restricted functionality of some packages. Certain tools focus solely on specific types of interpolation, such as those for structured data, while lacking support for advanced features like multivalued interpolation or derivative calculations. This specialization often forces researchers to use multiple packages to cover all their interpolation needs, leading to an inefficient workflow. The need to learn and integrate various packages increases development time and introduces potential inconsistencies in the codebase.

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The `multinterp` package was developed to address these challenges to provide a comprehensive framework for multivariate interpolation in python with several key features. It offers a unified interface for various interpolation grids, including regular (rectilinear), irregular (unstructured), and curvilinear grids, allowing users to easily switch between different grid types without changing their code structure.

Furthermore, `multinterp` supports multiple backends, including CPU (using `numpy` and `scipy`), parallel processing (using `numba`), and GPU acceleration (using `cupy`, `pytorch`, and `jax`). This flexibility enables users to optimize performance based on their available computational resources. The package also includes tools for multivalued interpolation and interpolation of derivatives, expanding its utility for a wide range of scientific applications.

Perhaps most importantly, `multinterp` provides a consistent API that allows easy switching between different interpolation methods and backends. This feature simplifies code development and facilitates experimentation with various interpolation techniques and performance optimization strategies.

In the following sections, we will introduce the main concepts of grid interpolation, demonstrate the capabilities of `multinterp` for different types of grids, and compare its performance with existing tools. We will conclude by discussing the project's current state and inviting community contributions to further development.

2. BACKGROUND AND CONCEPTS

Before diving into the specifics of `multinterp`, it is crucial to understand some fundamental concepts in multivariate interpolation and the challenges they present.

2.1. Interpolation Basics

At its core, interpolation is about approximating functional values between known data points. This might involve drawing a line or curve between points in one dimension. The process becomes more complex in multiple dimensions, involving surfaces or hypersurfaces.

2.2. Grid Types

The arrangement of known data points, called the grid, significantly influences the choice of interpolation method and its computational efficiency. In `multinterp`, we consider three main types of grids:

1. **Rectilinear Grids:** These are the simplest and most common. Data points form a regular pattern along each dimension, though the spacing between points may vary. Moreover, these grids can be represented by the cross product of 1-dimensional vectors, making them easy to work with.
2. **Curvilinear Grids:** These maintain a structured relationship between neighboring points, but the grid lines may be curved or warped. Their main advantage is that these grids are monotonic in each coordinate dimension, allowing for an easy and efficient transformation into a rectilinear grid.
3. **Unstructured Grids:** These have irregularly spaced data points with no inherent structure. They are often encountered in experimental data collection or adaptive numerical methods. Interpolation on unstructured grids is more challenging and requires more sophisticated algorithms.

2.3. Existing Interpolation Methods

Various methods exist for interpolation, each with its strengths and limitations:

Table 1. *Grids and structures implemented in “multinterp”.*

Grid	Structure	Geometry
Rectilinear	Regular	Rectangular mesh
Curvilinear	Regular	Quadrilateral mesh
Unstructured	Irregular	Random

- **Nearest Neighbor:** Assigns the value of the nearest known point or a weighted average of the nearest few points. Simple but can be inaccurate.
- **Linear/Multilinear:** Assumes a linear relationship between points. Fast but can miss complex patterns.
- **Polynomial:** Higher-order polynomials are used to fit the data. It can capture more complex relationships but may oscillate between points.
- **Spline:** Uses piecewise polynomials. Offers a balance between smoothness and accuracy.
- **Radial Basis Function (RBF):** Uses a sum of radially symmetric functions. Useful for scattered data.

Each of these methods may be implemented differently for different grid types, leading to the fragmentation in the Python ecosystem that `multinterp` aims to address. `multinterp` currently mainly implements multilinear interpolation and aims to add more methods and grid types in the future.

3. THE `multinterp` PACKAGE

The `multinterp` package is a unified framework for multivariate interpolation in python, designed to address the challenges outlined in the previous sections. It offers several key features:

1. **Unified Interface:** A consistent API for interpolation, regardless of data structure or desired backend, reducing the learning curve and promoting code reusability. This consistency extends across different grid types (rectilinear, curvilinear, and unstructured), allowing users to switch between grid types with minimal code changes.
2. **Hardware Adaptability:** Seamless support for CPU (`numpy`, `scipy`), parallel (`numba`), and GPU (`cupy`, `pytorch`, `jax`) backends, empowering users to optimize performance based on their computational resources.
3. **Broad Functionality:** Tools for regular/rectilinear interpolation, multivalued interpolation, and derivative calculations, addressing a wide range of scientific problems.

The `multinterp` package offers several advantages over existing tools:

1. **Flexibility:** Unlike specialized packages that focus on specific grid types or interpolation methods, `multinterp` provides a unified framework that can handle various grid types and interpolation scenarios.
2. **Performance:** By supporting multiple backends, including GPU acceleration, `multinterp` can offer significant performance improvements over CPU-only implementations, especially for large datasets. Our benchmarks show up to 10x speedup for large 3D grids when using GPU backends.
3. **Ease of Use:** The consistent API across different grid types and backends simplifies the learning curve and makes it easier for users to experiment with different approaches. For instance, switching from CPU to GPU interpolation often requires changing a single parameter.

Currently, `multinterp` primarily implements multilinear interpolation, which balances simplicity, speed, and accuracy for many applications. This method is particularly efficient for

rectilinear grids. The core implementation uses efficient `numpy` operations for fast computation.

However, we recognize the limitations of multilinear interpolation, such as its inability to capture complex, non-linear relationships in the data. Future development plans include implementing additional interpolation methods such as polynomial, spline, and radial basis function interpolation. These methods can offer improved accuracy for certain types of data, albeit at the cost of increased computational complexity.

The `multinterp` package is currently in its beta stage, but it offers a strong foundation and welcomes community contributions to reach its full potential. We invite collaboration to improve documentation, expand the test suite, and ensure the codebase aligns with the highest standards of Python package development.

4. RECTILINEAR INTERPOLATION

Rectilinear grids are the foundation of many scientific computing applications. They are simple yet powerful, allowing for efficient data representation and manipulation. In a rectilinear grid, data points form a regular pattern along each dimension, though the spacing between points may vary.

4.1. The Basics of Rectilinear Grids

A rectilinear grid in 2D can be thought of as a sheet of graph paper where the lines might not be evenly spaced. In 3D, you can imagine a stack of these sheets, again with potentially varying spacing between them. Mathematically, we can represent a 2D rectilinear grid using two 1D arrays of increasing values:

$$\begin{aligned} x &= [x_0, x_1, x_2, \dots, x_n] \\ y &= [y_0, y_1, y_2, \dots, y_m] \end{aligned} \tag{1}$$

where $x_i < x_j$ and $y_i < y_j$ for all $i < j$. The full grid is then represented by the tensor product $x \times y$, resulting in dimensions $n \times m$.

This structure allows for efficient interpolation algorithms, as we can quickly locate the nearest known values to predict the function's behavior in unknown spaces. This is because we only need to search each dimension once and independently of the other.

4.2. Multilinear Interpolation with `multinterp`

The `multinterp` package provides a straightforward yet powerful implementation of multilinear interpolation. It supports various backends, including `numpy`, `scipy`, `numba`, `cupy`, `pytorch`, and `jax`, allowing users to choose the most suitable option for their computational environment.

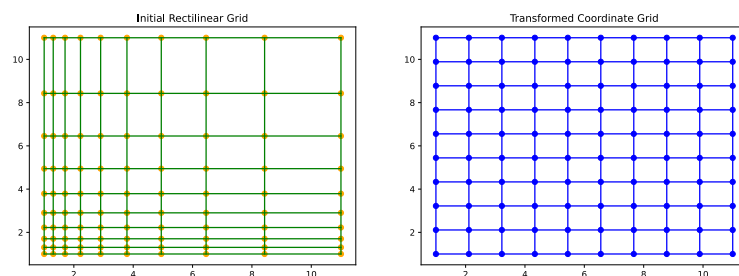


Figure 1. Transformation between non-uniform and uniform rectilinear grids. This process is critical to efficient interpolation on rectilinear grids.

At the heart of `multinterp`'s rectilinear interpolation is the `map_coordinates` function from `scipy.ndimage`. This function is versatile, taking an array of input values and an array of coordinates and returning interpolated values at those coordinates. Here is how it works:

- The input array contains known values on a coordinate (index) grid. For example, `input[i,j,k]` is the known value at coordinate (i,j,k) .
- The coordinates array contains fractional coordinates where we want to interpolate. For instance, `coordinates[0] = (1.5, 2.3, 3.1)` indicates we want to interpolate at a point between integer grid coordinates.

However, real-world functions are often not defined on a simple coordinate grid. This is where `multinterp`'s `get_coordinates` function comes in. It maps the functional input grid (defined on real numbers) and the coordinate grid (defined on non-negative integers).

Let us look at a practical example to see how this works:

```
import `numpy` as np
from multinterp import MultivariateInterp

# Define a function to interpolate
def squared_coords(x, y):
    return x**2 + y**2

# Create a non-uniform rectilinear grid
x_grid = np.geomspace(1, 11, 11) - 1
y_grid = np.geomspace(1, 11, 11) - 1
x_mat, y_mat = np.meshgrid(x_grid, y_grid, indexing="ij")

# Evaluate the function on this grid
z_mat = squared_coords(x_mat, y_mat)

# Create the interpolator
interp = MultivariateInterp(z_mat, [x_grid, y_grid])

# Define points for interpolation
x_new, y_new = np.meshgrid(
    np.linspace(0, 10, 11),
    np.linspace(0, 10, 11),
    indexing="ij",
)

# Perform interpolation
z_interp = interp(x_new, y_new)
```

In this example, we use a squared coordinates function (x^2+y^2) as our test case. This function is chosen because it produces a simple curved surface in 3D, making it easy to verify the interpolation results visually. We create a non-uniform grid using `geomspace`, which gives us more points near the origin and fewer points farther out. This non-uniform grid demonstrates `multinterp`'s ability to handle varying grid spacings effectively.

The `MultivariateInterp` class encapsulates the interpolation process, making it easy to create an interpolator and apply it to new points. This object-oriented approach allows for easy reuse and chaining of operations, as seen in the next section on derivatives.

4.3. Derivatives

The `multinterp` package also allows calculating derivatives of the interpolated function defined on a rectilinear grid. This is done by using the function `get_grad`, which wraps `numpy`'s `gradient` function to calculate the gradient of the interpolated function at the given coordinates.

Consider the following function along with its analytical derivatives:

```
def trig_func(x, y):
    return y * np.sin(x) + x * np.cos(y)

def trig_func_dx(x, y):
    return y * np.cos(x) + np.cos(y)

def trig_func_dy(x, y):
    return np.sin(x) - x * np.sin(y)
```

First, we create a sample input gradient and evaluate the function at those points. Notice that we are not using the analytical gradients to create the interpolation function. Instead, we will use these to compare the results of the numerical derivatives.

```
x_grid = np.geomspace(1, 11, 1000) - 1
y_grid = np.geomspace(1, 11, 1000) - 1
x_mat, y_mat = np.meshgrid(x_grid, y_grid, indexing="ij")

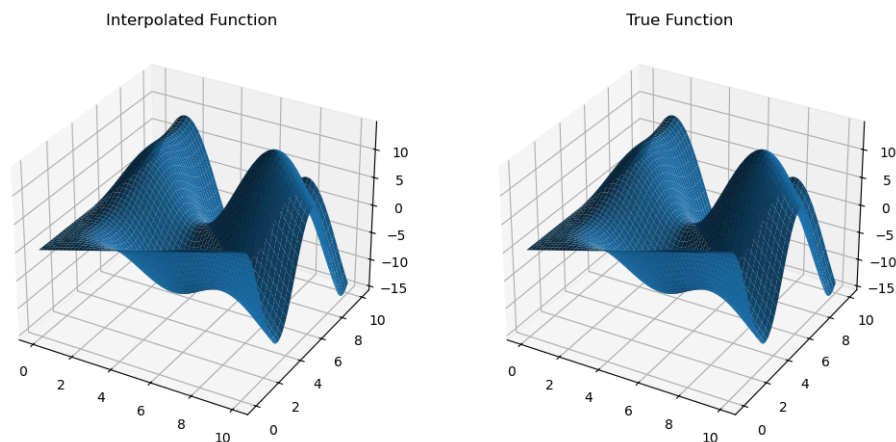
z_mat = trig_func(x_mat, y_mat)
```

Now, we generate a different grid, which will be used as our query points.

```
x_new, y_new = np.meshgrid(
    np.linspace(0, 10, 1000),
    np.linspace(0, 10, 1000),
    indexing="ij",
)
```

Then, we can compare our interpolation function with the analytical function and see that these are very close to each other.

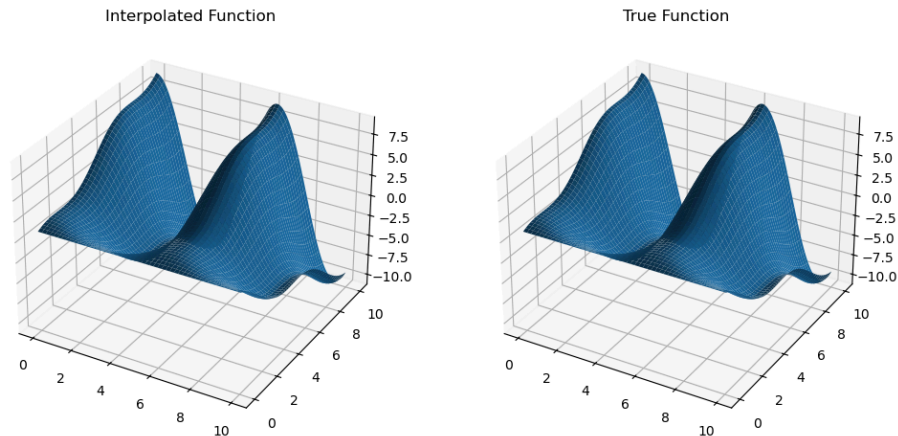
```
mult_interp = MultivariateInterp(z_mat, [x_grid, y_grid], backend="cupy")
z_mult_interp = mult_interp(x_new, y_new).get()
z_true = trig_func(x_new, y_new)
```



We can use the method `.diff(argnum)` of `MultivariateInterp` to evaluate numerical derivatives, which provides an object-oriented way to compute gradients. For example, calling `mult_interp.diff(0)` returns a `MultivariateInterp` object that represents the numerical derivative of the function with respect to the first argument on the same input grid.

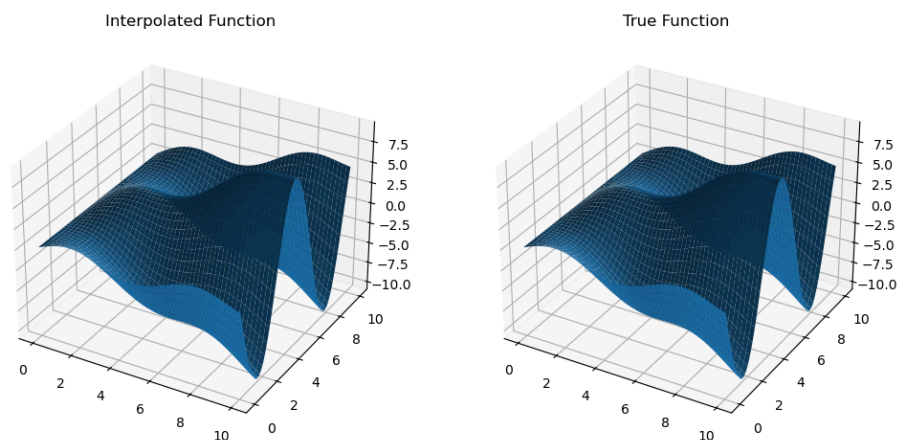
We can now compare the numerical and analytical derivatives and see that these are indeed very close to each other.

```
dfdx = mult_interp.diff(0)
z_dfdx = dfdx(x_new, y_new).get()
dfdx_true = trig_func_dx(x_new, y_new)
```



Similarly, we can compute the derivatives with respect to the second argument and see that they produce an accurate result.

```
dfdy = mult_interp.diff(1)
z_dfdy = dfdy(x_new, y_new).get()
dfdy_true = trig_func_dy(x_new, y_new)
```



The choice of returning object-oriented interpolation functions for the numerical derivatives is beneficial, as it allows for reusability without re-computation and easy chaining of operations. For example, we can compute the function's second derivative with respect to the first argument by calling `mult_interp.diff(0).diff(0)`.

4.4. Multivalued Interpolation

Finally, the `multinterp` package allows for multivalued interpolation on rectilinear grids via the `MultivaluedInterp` class.

Consider the following multivalued function:

```
def squared_coords(x, y):  
    return x**2 + y**2  
  
def trig_func(x, y):  
    return y * np.sin(x) + x * np.cos(y)  
  
def multivalued_func(x, y):  
    return np.array([squared_coords(x, y), trig_func(x, y)])
```

As before, we can generate values on a sample input grid and create a grid of query points.

```
x_grid = np.geomspace(1, 11, 1000) - 1  
y_grid = np.geomspace(1, 11, 1000) - 1  
x_mat, y_mat = np.meshgrid(x_grid, y_grid, indexing="ij")  
  
z_mat = multivalued_func(x_mat, y_mat)  
  
x_new, y_new = np.meshgrid(  
    np.linspace(0, 10, 1000),  
    np.linspace(0, 10, 1000),  
    indexing="ij",  
)
```

`MultivaluedInterp` can easily interpolate the function at the query points and avoid repeated calculations.

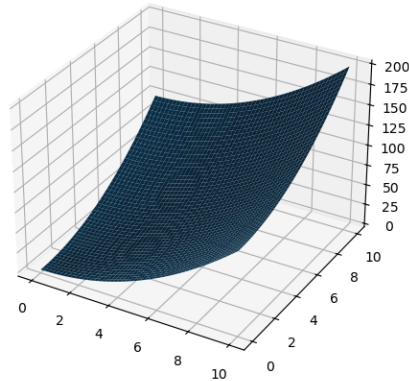

```

from multinterp.rectilinear._multi import MultivaluedInterp

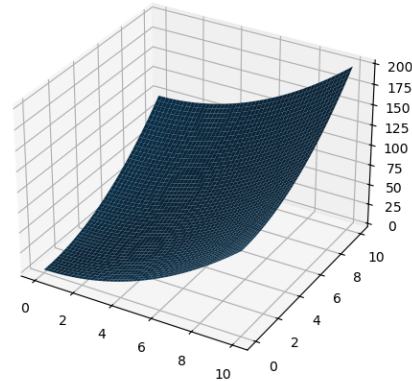
mult_interp = MultivaluedInterp(z_mat, [x_grid, y_grid], backend="cupy")
z_mult_interp = mult_interp(x_new, y_new).get()
z_true = multivalued_func(x_new, y_new)

```

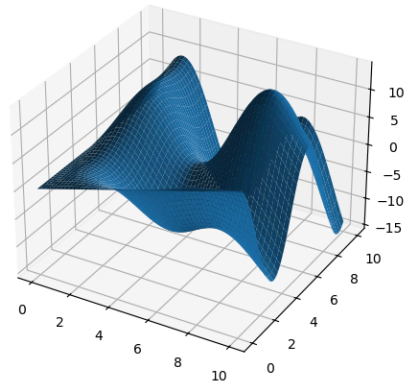
Interpolated Function 1



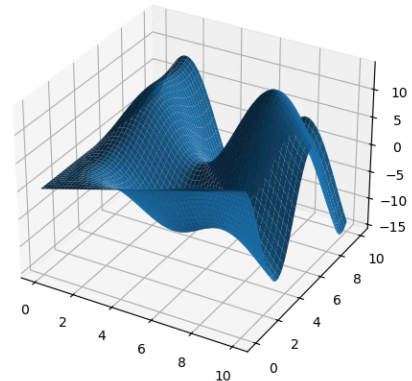
True Function 1



Interpolated Function 2



True Function 2



5. CURVILINEAR INTERPOLATION

A *curvilinear* grid is a regular grid whose input coordinates are *curved* or *warped* in some regular way. However, simple transformations can nevertheless transform it into a regular grid. That is, every quadrangle in the grid can be transformed into a rectangle by remapping its vertices. There are two approaches to curvilinear interpolation in `multinterp`: the first requires a “point location” algorithm to determine which quadrangle the input point lies in, and the second requires a “dimensional reduction” algorithm to generate an interpolated value from the known values in the quadrangle.

Suppose we have a collection of values for an unknown function and their respective coordinate points. For illustration, assume the values come from the following function:

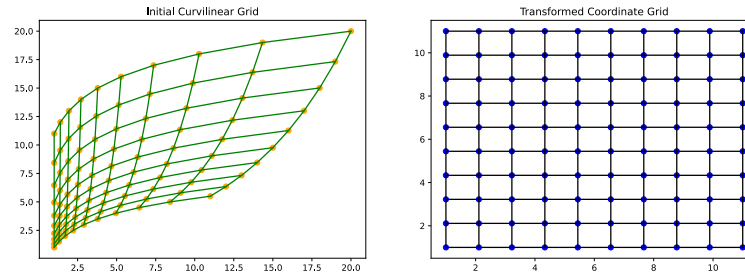


Figure 2. A curvilinear grid can be transformed into a rectilinear grid by simply remapping its vertices.

```
def function_1(x, y):
    return x * (1 - x) * np.cos(4 * np.pi * x) * np.sin(4 * np.pi * y**2) ** 2
```

The points are randomly scattered in the unit square and have no regular structure. This is achieved by randomly shifting a well-structured grid at every point.

```
rng = np.random.default_rng(0)
warp_factor = 0.01
x_list = np.linspace(0, 1, 20)
y_list = np.linspace(0, 1, 20)
x_temp, y_temp = np.meshgrid(x_list, y_list, indexing="ij")
rand_x = x_temp + warp_factor * (rng.random((x_list.size, y_list.size)) - 0.5)
rand_y = y_temp + warp_factor * (rng.random((x_list.size, y_list.size)) - 0.5)
values = function_1(rand_x, rand_y)
```

Suppose we want to interpolate this function on a rectilinear grid, a process called “regridding.”

```
grid_x, grid_y = np.meshgrid(
    np.linspace(0, 1, 100),
    np.linspace(0, 1, 100),
    indexing="ij",
)
```

We use `multinterp`’s `Warped2DInterp` and `Curvilinear2DInterp` classes to do this. The class takes the following arguments:

- `values`: an ND-array of values for the function at the points
- `grids`: a list of ND-arrays of coordinates for the points
- `backend`: the backend to use for interpolation currently only `scipy` and `numba` are supported for `Warped2DInterp`, and only `scipy` is supported for `Curvilinear2DInterp` for now.

```
from multinterp.curvilinear import Curvilinear2DInterp, Warped2DInterp

warped_interp = Warped2DInterp(values, (rand_x, rand_y), backend="numba")
warped_interp.warmup()
```

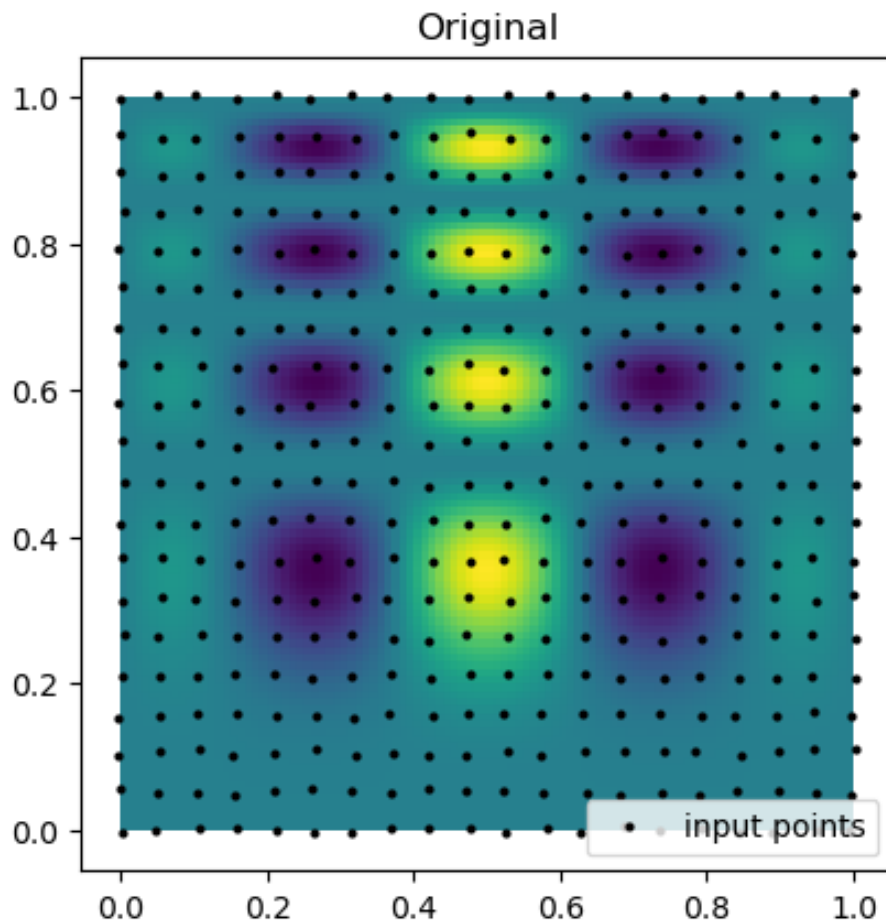
Once we create the interpolator objects, we can evaluate the functions on the query grids and compare their time performance.

```
start = time()
warped_grid = warped_interp(grid_x, grid_y)
print(f"Warped interpolation took {time() - start:.5f} seconds")
```

```
curvilinear_interp = Curvilinear2DInterp(values, (rand_x, rand_y))
start = time()
curvilinear_grid = curvilinear_interp(grid_x, grid_y)
print(f"Curvilinear interpolation took {time() - start:.5f} seconds")
```

Now, we can compare the interpolation results with the original function. Below, we plot the original function and the known sample points. Notice that the points are almost rectilinear but have been randomly shifted to create a more challenging interpolation problem.

```
plt.imshow(function_1(grid_x, grid_y).T, extent=(0, 1, 0, 1), origin="lower")
plt.plot(rand_x.flat, rand_y.flat, "ok", ms=2, label="input points")
plt.title("Original")
plt.legend(loc="lower right")
```



Then, we can look at the result for each interpolation method and compare it to the original function.

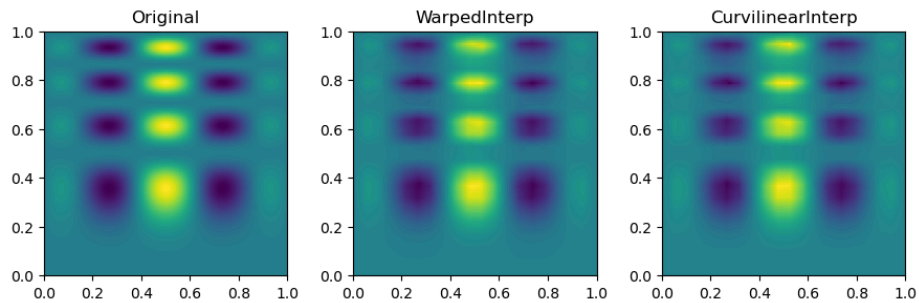
```

fig, axs = plt.subplots(1, 3, figsize=(9, 6))
titles = ["Original", "WarpedInterp", "CurvilinearInterp"]
grids = [function_l(grid_x, grid_y), warped_grid, curvilinear_grid]

for ax, title, grid in zip(axs.flat, titles, grids):
    im = ax.imshow(grid.T, extent=(0, 1, 0, 1), origin="lower")
    ax.set_title(title)

plt.tight_layout()
plt.show()

```



In short, `multinterp`'s `Warped2DInterp` and `Curvilinear2DInterp` classes are helpful for interpolating functions on curvilinear grids with a quadrilateral structure but are not perfectly rectangular.

6. UNSTRUCTURED INTERPOLATION

Suppose we have a collection of values for an unknown function and their respective coordinate points. For illustration, assume the values come from the following function:

```

def function_l(u, v):
    return u * np.cos(u * v) + v * np.sin(u * v)

```

The points are randomly scattered within a square and have no regular structure.

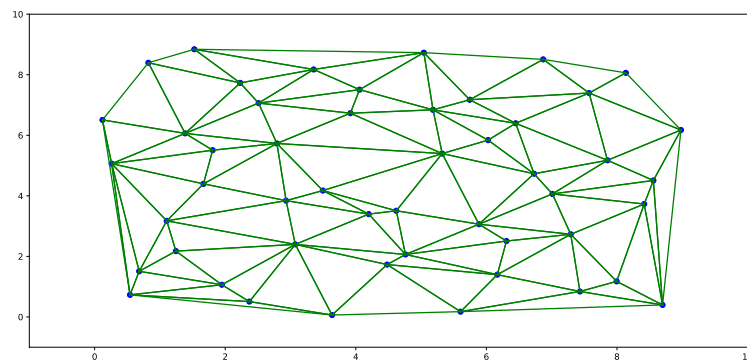


Figure 3. Unstructured grids are irregular and often require a triangulation step, which might be computationally expensive and time-consuming.

```
rng = np.random.default_rng(0)
rand_x, rand_y = rng.random((2, 1000)) * 3
values = function_1(rand_x, rand_y)
```

Suppose we want to interpolate this function on a rectilinear grid.

```
grid_x, grid_y = np.meshgrid(
    np.linspace(0, 3, 100),
    np.linspace(0, 3, 100),
    indexing="ij",
)
```

We use `multinterp`'s `UnstructuredInterp` class to do this. The class takes the following arguments:

- `values`: an ND-array of values for the function at the points
- `grids`: a list of ND-arrays of coordinates for the points
- `method`: the interpolation method to use, with options “nearest”, “linear”, “cubic” (for 2D only), and “rbf”. The default is ‘linear’.

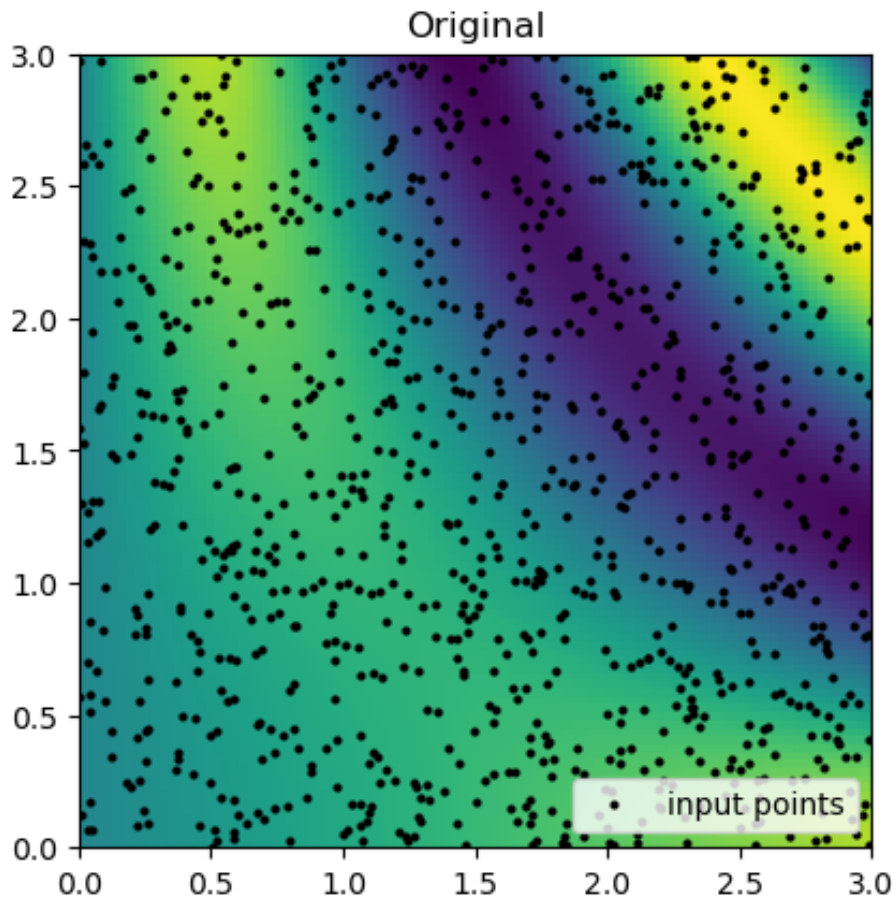
The `UnstructuredInterp` class is an object-oriented wrapper around `scipy.interpolate`'s functions for multivariate interpolation on unstructured data, which are `NearestNDInterpolator`, `LinearNDInterpolator`, `CloughTocher2DInterpolator`, and `RBFInterpolator`. The advantage of using `multinterp`'s `UnstructuredInterp` class is that it provides a consistent interface for all these methods, making it easier to switch between them and other interpolators in the `multinterp` package.

```
nearest_interp = UnstructuredInterp(values, (rand_x, rand_y), method="nearest")
linear_interp = UnstructuredInterp(values, (rand_x, rand_y), method="linear")
cubic_interp = UnstructuredInterp(values, (rand_x, rand_y), method="cubic")
rbf_interp = UnstructuredInterp(values, (rand_x, rand_y), method="rbf")
```

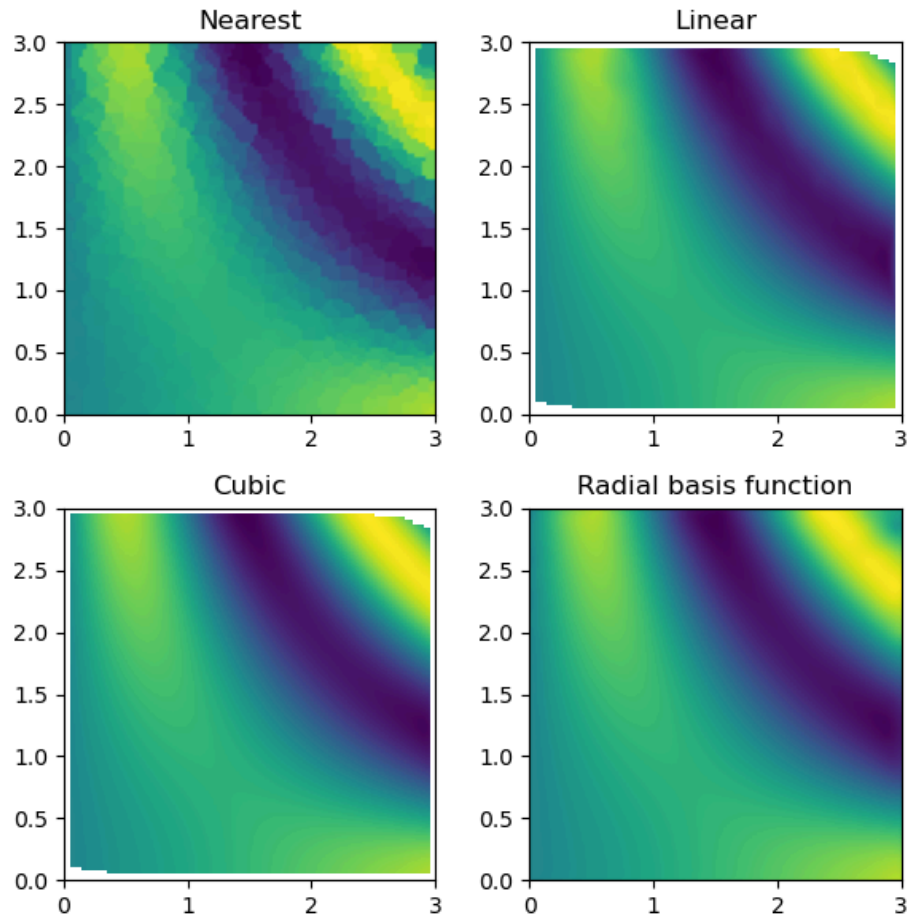
Once we create the interpolator objects, we can use them using the `__call__` method, which takes as many arguments as there are dimensions.

```
nearest_grid = nearest_interp(grid_x, grid_y)
linear_grid = linear_interp(grid_x, grid_y)
cubic_grid = cubic_interp(grid_x, grid_y)
rbf_grid = rbf_interp(grid_x, grid_y)
```

Now, we can compare the interpolation results with the original function. Below, we plot the original function and the known sample points.



Then, we can look at the result for each interpolation method and compare it to the original function.



Finally, `multinterp` also provides a set of interpolators organized around the concept of *regression*. As a demonstration, below, we use a `RegressionUnstructuredInterp` interpolator, which uses a Gaussian Process regression model from `scikit-learn` [1] to interpolate the function defined on the unstructured grid. The `RegressionUnstructuredInterp` class takes the same arguments as the `UnstructuredInterp` class but requires the user to specify the regression model to use.

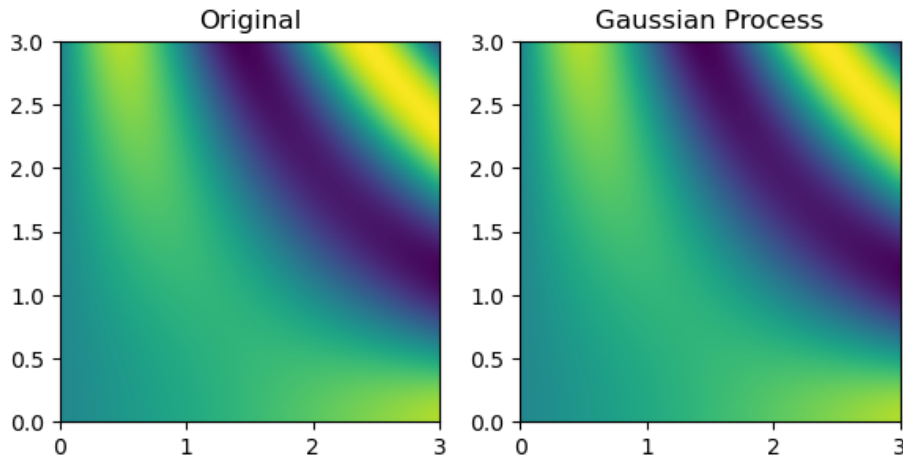
```

from multinterp import RegressionUnstructuredInterp

gaussian_interp = RegressionUnstructuredInterp(
    values,
    (rand_x, rand_y),
    model="gaussian-process",
    std=True,
)

gaussian_grid = gaussian_interp(grid_x, grid_y)

```



7. PERFORMANCE COMPARISONS

We conducted a series of benchmarks to assess the performance of `multinterp` and compare it with existing tools. The benchmarks evaluated the interpolation speed and accuracy of `multinterp` across different grid sizes, dimensions, and backends.

7.1. Benchmark Setup

The benchmarks were conducted using the following setup:

- **Test Function:** A multivariate function with a known analytical solution generated the input data.
- **Grid Sizes:** The input data was generated on grids of varying sizes, ranging from 10x10 to 1000x1000.
- **Dimensions:** The benchmarks were conducted for both 2D and 3D grids.
- **Backends:** The benchmarks were run using different backends, including CPU (`numpy` and `scipy`), parallel (`numba`), and GPU (`cupy`, `pytorch`, and `jax`).

7.2. Comparison with `scipy.interpolate.RegularGridInterpolator`

The first set of benchmarks compares the performance of `multinterp` with `scipy.interpolate.RegularGridInterpolator`, a widely-used interpolation library in the scientific Python ecosystem. The benchmarks were conducted for both 2D and 3D grids, and the results are presented in the following figures.

7.3. Backend Comparison

The second set of benchmarks compares the performance of different backends in `multinterp`. The benchmarks were conducted for both 2D and 3D grids, and the results are presented in the following figures.

7.4. Discussion

The benchmark results demonstrate that `multinterp` outperforms `scipy.interpolate.RegularGridInterpolator` for 2D and 3D grids, especially for larger grid sizes. This is likely due to the efficient implementation of `multinterp`'s core functions, such as `map_coordinates` and `get_coordinates`.

The backend comparison shows that GPU backends (`cupy`, `pytorch`, and `jax`) can provide significant performance improvements for large grid sizes, especially in 3D. However, data transfer overhead between the CPU and GPU can make GPU backends slower for smaller grid sizes. Parallel backends (`numba`) can also provide performance improvements for CPU-bound tasks, but the benefits are less pronounced than those of GPU backends.

Overall, the benchmark results highlight the advantages of `multinterp` regarding performance and flexibility. The package offers a unified interface for various types of interpolation, supports multiple backends, and includes tools for multivalued interpolation and interpolation of derivatives.

8. FUTURE WORK AND CONTRIBUTIONS

The `multinterp` package is currently in its beta stage, and there are several areas where future development and community contributions would be valuable.

8.1. Planned Features

1. **Additional Interpolation Methods:** Implement support for additional interpolation methods, such as spline, polynomial, inverse distance weight, and radial basis function interpolation. This will give users more options to handle various types of data and interpolation requirements.
2. **Optimization and Performance Improvements:** Continue to optimize the core functions of `multinterp` to improve performance and efficiency, particularly for large datasets and high-dimensional interpolation.
3. **Documentation and Examples:** Expand the documentation and provide more examples to demonstrate the capabilities of `multinterp`, including comparisons between different interpolation methods and grid types.
4. **Extended Grid Support:** Enhance support for complex grid types and improve interpolation efficiency on unstructured grids.

8.2. Community Contributions

We welcome contributions from the community to help improve the `multinterp` package. There are several ways to contribute:

1. **Code Contributions:** Submit pull requests to add new features, fix bugs, or improve the documentation.
2. **Issue Reporting:** Report any issues or bugs you encounter using `multinterp`.
3. **Testing:** Help expand the test suite to ensure the package works correctly across various scenarios.
4. **Documentation:** Contribute to the documentation by writing tutorials, examples, or improving the existing documentation.

To get started with contributing, please refer to our [Contribution Guidelines](#) for detailed information on our development process, coding standards, and how to submit pull requests.

8.3. Documentation and Resources

For more information about `multinterp`, please refer to the following resources:

- **Source Code:** The source code is hosted on GitHub at <https://github.com/alanlujan91/multinterp>
- **Issue Tracker:** Report bugs or request features on our [GitHub Issues page](#)
- **Contribution Guidelines:** Learn how to contribute at [CONTRIBUTING.md](#)
- **Examples:** A collection of Jupyter notebooks with usage examples can be found in the [examples directory](#) of our GitHub repository

We encourage users to explore these resources and contact the community through our [GitHub Discussions](#) for any questions or feedback.

9. CONCLUSION

Multivariate interpolation is a cornerstone of scientific computing, yet the Python ecosystem [2] presents a fragmented landscape of tools. While individually powerful, these packages often lack a unified interface. This fragmentation makes it difficult for researchers to experiment with different interpolation methods, optimize performance across diverse hardware, and handle varying data structures (regular, rectilinear, curvilinear, unstructured).

The `multinterp` project seeks to change this. Its goal is to provide a unified, comprehensive, and flexible framework for multivariate interpolation in python. This framework will streamline workflows by offering:

- **Unified Interface:** A consistent API for interpolation, regardless of data structure or desired backend, reducing the learning curve and promoting code reusability.
- **Hardware Adaptability:** Seamless support for CPU (`numpy` C. R. Harris *et al.* [3], `scipy` P. Virtanen *et al.* [4]), parallel (`numba` S. K. Lam, A. Pitrou, and S. Seibert [5]), and GPU (`cupy` R. Okuta, Y. Unno, D. Nishino, S. Hido, and C. Loomis [6], `pytorch` A. Paszke *et al.* [7], `jax` J. Bradbury *et al.* [8]) backends, empowering users to optimize performance based on their computational resources.
- **Broad Functionality:** Tools for regular/rectilinear interpolation, multivalued interpolation, and derivative calculations, addressing a wide range of scientific problems.

The `multinterp` package (<https://github.com/alanlujan91/multinterp>) is currently in its beta stage. It offers a strong foundation but welcomes community contributions to reach its full potential. We invite collaboration to improve documentation, expand the test suite, and ensure the codebase aligns with the highest standards of Python package development.

REFERENCES

- [1] F. Pedregosa *et al.*, “Scikit-learn: Machine Learning in Python,” *Journal of machine learning research: JMLR*, pp. 2825–2830, Feb. 2011.
- [2] T. E. Oliphant, “Python for Scientific Computing,” *Computing in science & engineering*, vol. 9, no. 3, pp. 10–20, 2007, doi: [10.1109/MCSE.2007.58](https://doi.org/10.1109/MCSE.2007.58).
- [3] C. R. Harris *et al.*, “Array programming with NumPy,” *Nature*, vol. 585, no. 7825, pp. 357–362, Sep. 2020, doi: [10.1038/s41586-020-2649-2](https://doi.org/10.1038/s41586-020-2649-2).
- [4] P. Virtanen *et al.*, “SciPy 1.0: fundamental algorithms for scientific computing in Python,” *Nature methods*, vol. 17, no. 3, pp. 261–272, 2020, doi: [10.1038/s41592-019-0686-2](https://doi.org/10.1038/s41592-019-0686-2).

- [5] S. K. Lam, A. Pitrou, and S. Seibert, “Numba: a LLVM-based Python JIT compiler,” in *Proceedings of the Second Workshop on the LLVM Compiler Infrastructure in HPC*, in LLVM '15. New York, NY, USA, Nov. 2015, pp. 1–6. doi: [10.1145/2833157.2833162](https://doi.org/10.1145/2833157.2833162).
- [6] R. Okuta, Y. Unno, D. Nishino, S. Hido, and C. Loomis, “CuPy: A NumPy-Compatible Library for NVIDIA GPU Calculations.” 2017.
- [7] A. Paszke *et al.*, “PyTorch: An imperative style, high-performance deep learning library,” *arXiv [cs. LG]*, pp. 8026–8037, Dec. 2019.
- [8] J. Bradbury *et al.*, “JAX: composable transformations of Python+NumPy programs.” 2018.