How can I perform two-dimensional interpolation using scipy?

Asked 6 years, 3 months ago Modified 1 year, 3 months ago Viewed 39k times

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This Q&A is intended as a canonical(-ish) concerning two-dimensional (and multi-dimensional) interpolation using scipy. There are often questions concerning the basic syntax of various multidimensional interpolation methods, I hope to set these straight too.

I have a set of scattered two-dimensional data points, and I would like to plot them as a nice surface, preferably using something like `contourf` or `plot_surface` in `matplotlib.pyplot`. How can I interpolate my two-dimensional or multidimensional data to a mesh using scipy?

I've found the `scipy.interpolate` sub-package, but I keep getting errors when using `interp2d` or `bisplrep` or `griddata` or `RBFInterpolator` (or the older `Rbf`). What is the proper syntax of these methods?

python scipy interpolation

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asked Jun 17, 2016 at 2:27

Andras Deak -- Слава Україні

31.6k 11 75 101

I would also suggest adding other interpolation tasks: input data is scattered or rectangular grid, output data is scattered (i.e. arbitrary coordinates). – Brian D May 12, 2021 at 21:26

@BrianD unless I misunderstood "input data is scattered or rectangular grid" are exactly the two tasks considered in my answer. As for "output data is scattered", I'm not sure that's too interesting: once you have an interpolating function you can query it anywhere. The result shouldn't be qualitatively sensitive to the position of the output points. What do you have in mind? – Andras Deak -- Слава Україні May 12, 2021 at 21:55

That's fair. I suppose I was thinking of 'arbitrary sampling' (as opposed to upsampling or interpolation onto a grid) and was just struggling with `interp2d` and now using the same code with `Rbf` "just works" so... nevermind? – Brian D May 12, 2021 at 21:57

1 @BrianD Hah, yes, that's pretty much my experience from when I put together this Q&A. There's also a new implementation of Rbf in the works which is very close to done. I'll update my answer once that's released because it looks nice (and more future-proof). – Andras Deak -- Слава Україні May 12, 2021 at 22:05

1 @BrianD I'm not sure what functionality you mean (extrapolation, i.e. missing values in the domain, or just clamping the interpolated function values). Sounds like you mean the latter, but that can be done with a

single call to `np.clip` after interpolation. But to answer your question, no, I don't think the new functionality will support this. – Andras Deak -- Слава Україні May 13, 2021 at 20:23

1 Answer

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201

+1000

Disclaimer: I'm mostly writing this post with syntactical considerations and general behaviour in mind. I'm not familiar with the memory and CPU aspect of the methods described, and I aim this answer at those who have reasonably small sets of data, such that the quality of the interpolation can be the main aspect to consider. I am aware that when working with very large data sets, the better-performing methods (namely `griddata` and `RBFInterpolator` without a `neighbors` keyword argument) might not be feasible.

Note that this answer uses the new `RBFInterpolator` class introduced in `SciPy` 1.7.0. For the legacy `Rbf` class see the previous version of this answer.

I'm going to compare three kinds of multi-dimensional interpolation methods (`interp2d` /splines, `griddata` and `RBFInterpolator`). I will subject them to two kinds of interpolation tasks and two kinds of underlying functions (points from which are to be interpolated). The specific examples will demonstrate two-dimensional interpolation, but the viable methods are applicable in arbitrary dimensions. Each method provides various kinds of interpolation; in all cases I will use cubic interpolation (or something close[1]). It's important to note that whenever you use interpolation you introduce bias compared to your raw data, and the specific methods used affect the artifacts that you will end up with. Always be aware of this, and interpolate responsibly.

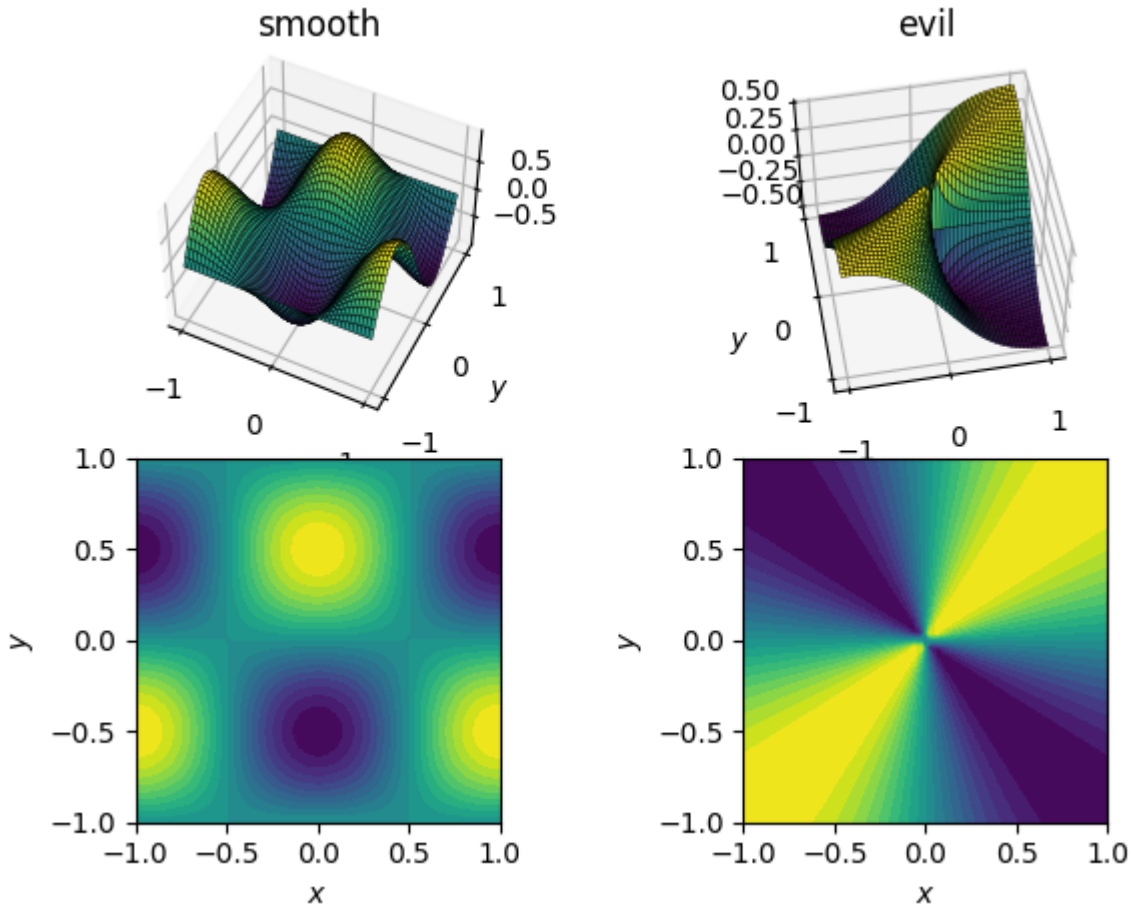
The two interpolation tasks will be

1. upsampling (input data is on a rectangular grid, output data is on a denser grid)
2. interpolation of scattered data onto a regular grid

The two functions (over the domain `[x, y] in [-1, 1]x[-1, 1]`) will be

1. a smooth and friendly function: `cos(pi*x)*sin(pi*y)` ; range in `[-1, 1]`
2. an evil (and in particular, non-continuous) function: `x*y / (x^2 + y^2)` with a value of 0.5 near the origin; range in `[-0.5, 0.5]`

Here's how they look:



I will first demonstrate how the three methods behave under these four tests, then I'll detail the syntax of all three. If you know what you should expect from a method, you might not want to waste your time learning its syntax (looking at you, `interp2d`).

Test data

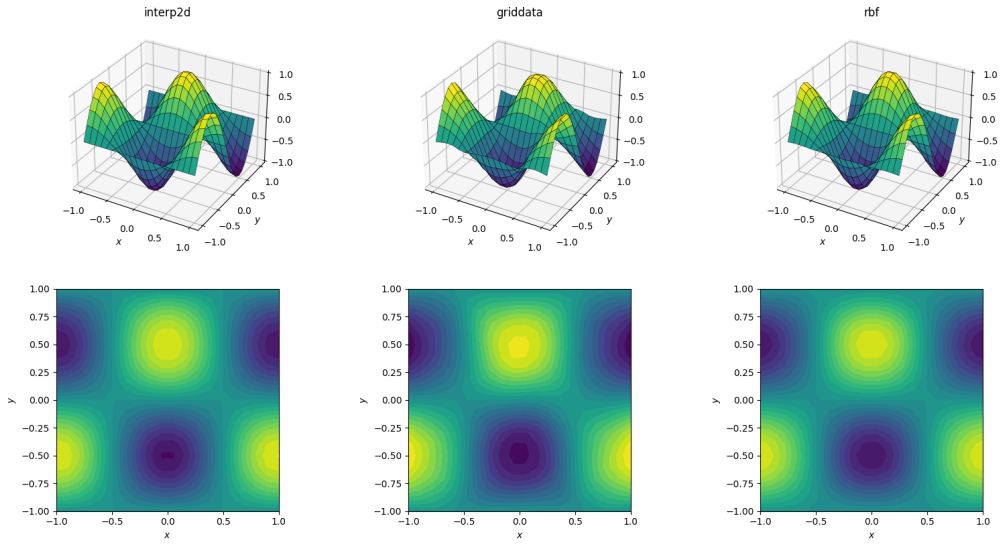
For the sake of explicitness, here is the code with which I generated the input data. While in this specific case I'm obviously aware of the function underlying the data, I will only use this to generate input for the interpolation methods. I use numpy for convenience (and mostly for generating the data), but scipy alone would suffice too.

```
import numpy as np
import scipy.interpolate as interp

# auxiliary function for mesh generation
def gimme_mesh(n):
    minval = -1
    maxval =  1
    # produce an asymmetric shape in order to catch issues with transpositions
    return np.meshgrid(np.linspace(minval, maxval, n),
                       np.linspace(minval, maxval, n + 1))

# set up underlying test functions, vectorized
```

```
# set up underlying test functions, vectorized
def fun_smooth(x, y):

    return np.cos(np.pi*x) * np.sin(np.pi*y)

def fun_evil(x, y):
    # watch out for singular origin; function has no unique limit there
    return np.where(x**2 + y**2 > 1e-10, x*y/(x**2+y**2), 0.5)

# sparse input mesh, 6x7 in shape
N_sparse = 6
x_sparse, y_sparse = gimme_mesh(N_sparse)
z_sparse_smooth = fun_smooth(x_sparse, y_sparse)
z_sparse_evil = fun_evil(x_sparse, y_sparse)

# scattered input points, 10^2 altogether (shape (100,))
N_scattered = 10
rng = np.random.default_rng()
x_scattered, y_scattered = rng.random((2, N_scattered**2))*2 - 1
z_scattered_smooth = fun_smooth(x_scattered, y_scattered)
z_scattered_evil = fun_evil(x_scattered, y_scattered)

# dense output mesh, 20x21 in shape
N_dense = 20
x_dense, y_dense = gimme_mesh(N_dense)
```

Smooth function and upsampling

Let's start with the easiest task. Here's how an upsampling from a mesh of shape `[6, 7]` to one of `[20, 21]` works out for the smooth test function:



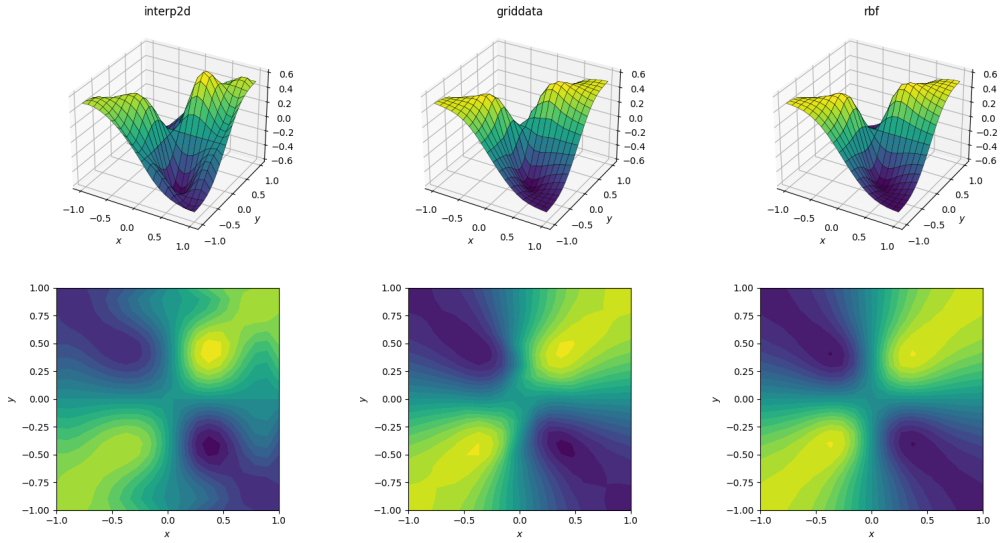
Even though this is a simple task, there are already subtle differences between the outputs. At a first glance all three outputs are reasonable. There are two features to note, based on our prior knowledge of the underlying function: the middle case of `griddata` distorts the data most. Note the `y == -1` boundary of the plot (nearest the `x` label): the function should be strictly zero (since `y == -1` is a nodal line for the smooth function), yet this is not the case for `griddata`. Also note

the `x == -1` boundary of the plots (behind, to the left): the underlying function has a local

maximum (implying zero gradient near the boundary) at `[-1, -0.5]`, yet the `griddata` output shows clearly non-zero gradient in this region. The effect is subtle, but it's a bias none the less.

Evil function and upsampling

A bit harder task is to perform upsampling on our evil function:



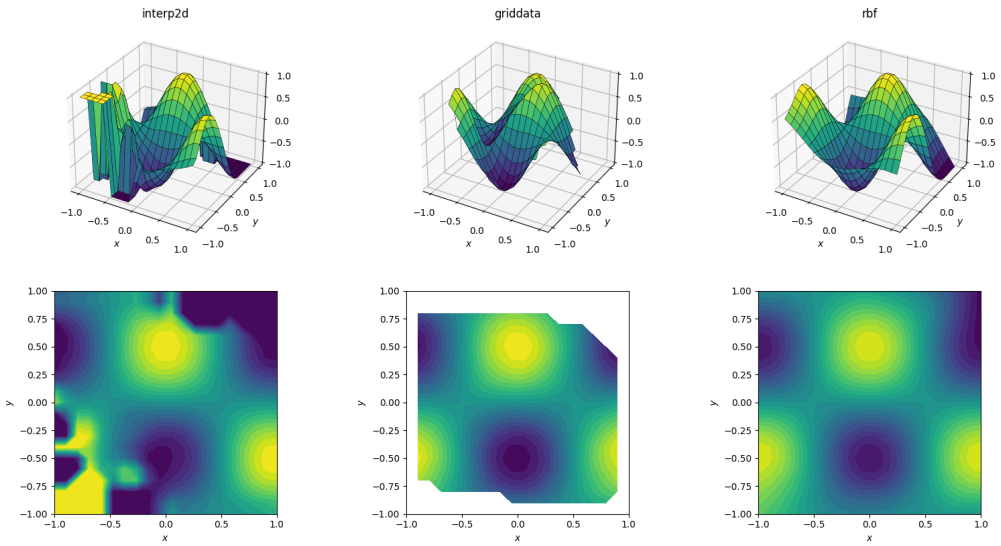
Clear differences are starting to show among the three methods. Looking at the surface plots, there are clear spurious extrema appearing in the output from `interp2d` (note the two humps on the right side of the plotted surface). While `griddata` and `RBFInterpolator` seem to produce similar results at first glance, producing local minima near `[0.4, -0.4]` that is absent from the underlying function.

However, there is one crucial aspect in which `RBFInterpolator` is far superior: it respects the symmetry of the underlying function (which is of course also made possible by the symmetry of the sample mesh). The output from `griddata` breaks the symmetry of the sample points, which is already weakly visible in the smooth case.

Smooth function and scattered data

Most often one wants to perform interpolation on scattered data. For this reason I expect these tests to be more important. As shown above, the sample points were chosen pseudo-uniformly in the domain of interest. In realistic scenarios you might have additional noise with each measurement, and you should consider whether it makes sense to interpolate your raw data to begin with.

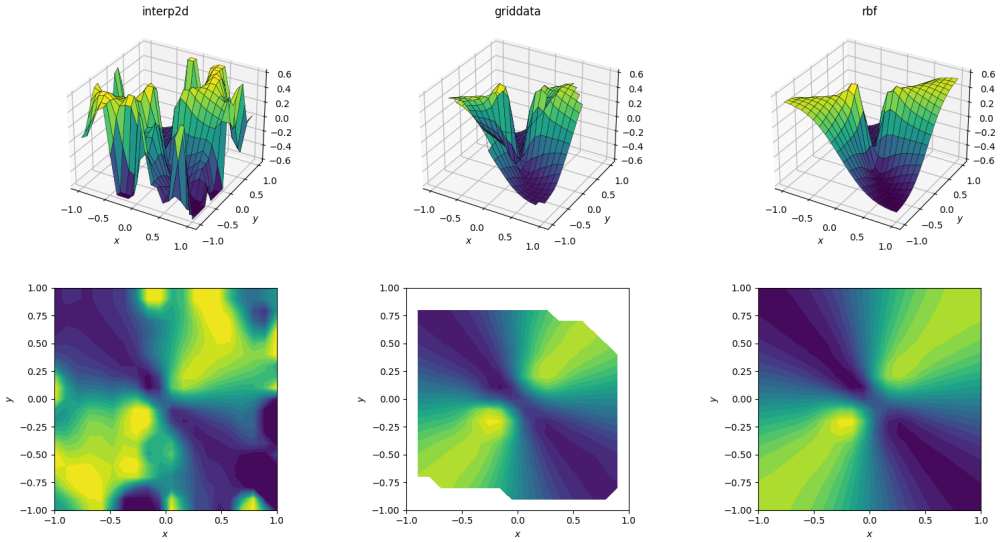
Output for the smooth function:



Now there's already a bit of a horror show going on. I clipped the output from `interp2d` to between `[-1, 1]` exclusively for plotting, in order to preserve at least a minimal amount of information. It's clear that while some of the underlying shape is present, there are huge noisy regions where the method completely breaks down. The second case of `griddata` reproduces the shape fairly nicely, but note the white regions at the border of the contour plot. This is due to the fact that `griddata` only works inside the convex hull of the input data points (in other words, it doesn't perform any *extrapolation*). I kept the default NaN value for output points lying outside the convex hull.[2] Considering these features, `RBFInterpolator` seems to perform best.

Evil function and scattered data

And the moment we've all been waiting for:



It's no huge surprise that `interp2d` gives up. In fact, during the call to `interp2d` you should expect some friendly `RuntimeWarning`s complaining about the impossibility of the spline to be constructed. As for the other two methods, `RBFInterpolator` seems to produce the best output, even near the borders of the domain where the result is extrapolated.

So let me say a few words about the three methods, in decreasing order of preference (so that the worst is the least likely to be read by anybody).

`scipy.interpolate.RBFInterpolator`

The RBF in the name of the `RBFInterpolator` class stands for "radial basis functions". To be honest I've never considered this approach until I started researching for this post, but I'm pretty sure I'll be using these in the future.

Just like the spline-based methods (see later), usage comes in two steps: first one creates a callable `RBFInterpolator` class instance based on the input data, and then calls this object for a given output mesh to obtain the interpolated result. Example from the smooth upsampling test:

```
import scipy.interpolate as interp

sparse_points = np.stack([x_sparse.ravel(), y_sparse.ravel()], -1)  # shape (N, 2) in
2d
dense_points = np.stack([x_dense.ravel(), y_dense.ravel()], -1)  # shape (N, 2) in 2d

zfun_smooth_rbf = interp.RBFInterpolator(sparse_points, z_sparse_smooth.ravel(),
                                         smoothing=0, kernel='cubic')  # explicit
default smoothing=0 for interpolation
z_dense_smooth_rbf = zfun_smooth_rbf(dense_points).reshape(x_dense.shape)  # not really
a function, but a callable class instance

zfun_evil_rbf = interp.RBFInterpolator(sparse_points, z_sparse_evil.ravel(),
                                       smoothing=0, kernel='cubic')  # explicit default
smoothing=0 for interpolation
z_dense_evil_rbf = zfun_evil_rbf(dense_points).reshape(x_dense.shape)  # not really a
function, but a callable class instance
```

Note that we had to do some array building gymnastics to make the API of `RBFInterpolator` happy. Since we have to pass the 2d points as arrays of shape `(N, 2)`, we have to flatten the input grid and stack the two flattened arrays. The constructed interpolator also expects query points in this format, and the result will be a 1d array of shape `(N,)` which we have to reshape back to match our 2d grid for plotting. Since `RBFInterpolator` makes no assumptions about the number of dimensions of the input points, it supports arbitrary dimensions for interpolation.

So, `scipy.interpolate.RBFInterpolator`

- produces well-behaved output even for crazy input data

- supports interpolation in higher dimensions
- extrapolates outside the convex hull of the input points (of course extrapolation is always a gamble, and you should generally not rely on it at all)
- creates an interpolator as a first step, so evaluating it in various output points is less additional effort
- can have output point arrays of arbitrary shape (as opposed to being constrained to rectangular meshes, see later)
- more likely to preserving the symmetry of the input data
- supports multiple kinds of radial functions for keyword `kernel`: `multiquadric`, `inverse_multiquadric`, `inverse_quadratic`, `gaussian`, `linear`, `cubic`, `quintic`, `thin_plate_spline` (the default). As of SciPy 1.7.0 the class doesn't allow passing a custom callable due to technical reasons, but this is likely to be added in a future version.
- can give inexact interpolations by increasing the `smoothing` parameter

One drawback of RBF interpolation is that interpolating `N` data points involves inverting an `N x N` matrix. This quadratic complexity very quickly blows up memory need for a large number of data points. However, the new `RBFInterpolator` class also supports a `neighbors` keyword parameter that restricts computation of each radial basis function to `k` nearest neighbours, thereby reducing memory need.

`scipy.interpolate.griddata`

My former favourite, `griddata`, is a general workhorse for interpolation in arbitrary dimensions. It doesn't perform extrapolation beyond setting a single preset value for points outside the convex hull of the nodal points, but since extrapolation is a very fickle and dangerous thing, this is not necessarily a con. Usage example:

```
sparse_points = np.stack([x_sparse.ravel(), y_sparse.ravel()], -1)  # shape (N, 2) in
2d
z_dense_smooth_griddata = interp.griddata(sparse_points, z_sparse_smooth.ravel(),
                                          (x_dense, y_dense), method='cubic')  #
default method is linear
```

Note that the same array transformations were necessary for the input arrays as for `RBFInterpolator`. The input points have to be specified in an array of shape `[N, D]` in `D` dimensions, or alternatively as a tuple of 1d arrays:

```
z_dense_smooth_griddata = interp.griddata((x_sparse.ravel(), y_sparse.ravel()),
                                          z_sparse_smooth.ravel(), (x_dense, y_dense),
method='cubic')
```

The output point arrays can be specified as a tuple of arrays of arbitrary dimensions (as in both

above snippets), which gives us some more flexibility.

In a nutshell, `scipy.interpolate.griddata`

- produces well-behaved output even for crazy input data
- supports interpolation in higher dimensions
- does not perform extrapolation, a single value can be set for the output outside the convex hull of the input points (see `fill_value`)
- computes the interpolated values in a single call, so probing multiple sets of output points starts from scratch
- can have output points of arbitrary shape
- supports nearest-neighbour and linear interpolation in arbitrary dimensions, cubic in 1d and 2d. Nearest-neighbour and linear interpolation use `NearestNDInterpolator` and `LinearNDInterpolator` under the hood, respectively. 1d cubic interpolation uses a spline, 2d cubic interpolation uses `CloughTocher2DInterpolator` to construct a continuously differentiable piecewise-cubic interpolator.
- might violate the symmetry of the input data

`scipy.interpolate.interp2d` / `scipy.interpolate.bisplrep`

The only reason I'm discussing `interp2d` and its relatives is that it has a deceptive name, and people are likely to try using it. Spoiler alert: don't use it (as of scipy version 1.7.0). It's already more special than the previous subjects in that it's specifically used for two-dimensional interpolation, but I suspect this is by far the most common case for multivariate interpolation.

As far as syntax goes, `interp2d` is similar to `RBFInterpolator` in that it first needs constructing an interpolation instance, which can be called to provide the actual interpolated values. There's a catch, however: the output points have to be located on a rectangular mesh, so inputs going into the call to the interpolator have to be 1d vectors which span the output grid, as if from `numpy.meshgrid`:

```
# reminder: x_sparse and y_sparse are of shape [6, 7] from numpy.meshgrid
zfun_smooth_interp2d = interp.interp2d(x_sparse, y_sparse, z_sparse_smooth,
kind='cubic')   # default kind is 'linear'
# reminder: x_dense and y_dense are of shape (20, 21) from numpy.meshgrid
xvec = x_dense[0,:] # 1d array of unique x values, 20 elements
yvec = y_dense[:,0] # 1d array of unique y values, 21 elements
z_dense_smooth_interp2d = zfun_smooth_interp2d(xvec, yvec)   # output is (20, 21)-
shaped array
```

One of the most common mistakes when using `interp2d` is putting your full 2d meshes into the interpolation call, which leads to explosive memory consumption, and hopefully to a hasty `MemoryError`.

Now, the greatest problem with `interp2d` is that it often doesn't work. In order to understand this, we have to look under the hood. It turns out that `interp2d` is a wrapper for the lower-level functions `bisplrep` + `bisplev`, which are in turn wrappers for FITPACK routines (written in Fortran). The equivalent call to the previous example would be

```
kind = 'cubic'
if kind == 'linear':
    kx = ky = 1
elif kind == 'cubic':
    kx = ky = 3
elif kind == 'quintic':
    kx = ky = 5
# bisplrep constructs a spline representation, bisplev evaluates the spline at given
points
bisp_smooth = interp.bisplrep(x_sparse.ravel(), y_sparse.ravel(),
                              z_sparse_smooth.ravel(), kx=kx, ky=ky, s=0)
z_dense_smooth_bisplrep = interp.bisplev(xvec, yvec, bisp_smooth).T  # note the
transpose
```

Now, here's the thing about `interp2d`: (in scipy version 1.7.0) there is a nice comment in `interpolate/interpolate.py` for `interp2d`:

```
if not rectangular_grid:
    # TODO: surfit is really not meant for interpolation!
    self.tck = fitpack.bisplrep(x, y, z, kx=kx, ky=ky, s=0.0)
```

and indeed in `interpolate/fitpack.py`, in `bisplrep` there's some setup and ultimately

```
tx, ty, c, o = _fitpack._surfit(x, y, z, w, xb, xe, yb, ye, kx, ky,
                                task, s, eps, tx, ty, nxest, nyest,
                                wrk, lwrk1, lwrk2)
```

And that's it. The routines underlying `interp2d` are not really meant to perform interpolation. They might suffice for sufficiently well-behaved data, but under realistic circumstances you will probably want to use something else.

Just to conclude, `interpolate.interp2d`

- can lead to artifacts even with well-tempered data
- is specifically for bivariate problems (although there's the limited `interpn` for input points defined on a grid)
- performs extrapolation
- creates an interpolator as a first step, so evaluating it in various output points is less additional effort
- can only produce output over a rectangular grid, for scattered output you would have to call

the interpolator in a loop

- supports linear, cubic and quintic interpolation
- might violate the symmetry of the input data

[1]I'm fairly certain that the `cubic` and `linear` kind of basis functions of `RBFInterpolator` do not exactly correspond to the other interpolators of the same name.
[2]These NaNs are also the reason for why the surface plot seems so odd: matplotlib historically has difficulties with plotting complex 3d objects with proper depth information. The NaN values in the data confuse the renderer, so parts of the surface that should be in the back are plotted to be in the front. This is an issue with visualization, and not interpolation.

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edited Jun 21, 2021 at 0:15

answered Jun 17, 2016 at 2:27

Andras Deak -- Слава Україні
31.6k 11 75 101

3 Rbf can consume more memory than griddata depending on the number of data points and number of dimensions. Also griddata has underlying object LinearNDInterpolator that can be used like Rbf in 2 steps. – denfromufa Jun 18, 2016 at 22:33

1 Griddata's cubic interpolation is limited to 2 (?) dimensions. For higher dimensions smolyak sparse grids based on chebfun are worth considering. – denfromufa Jun 19, 2016 at 10:52

4 griddata linear interpolation is local, griddata cubic interpolation is global. Extrapolation is not supported, because I did not have time to figure out how to preserve continuity/differentiability. Rbf is fine for small data sets, but to interpolate n data points it needs to invert n x n matrix, which eventually becomes impossible after n>5000. Rbf can also be sensitive to the distribution of the data and you may need to fine-tune its parameters by hand. It is possible to do Rbf for large datasets, but this is not implemented in scipy. – pv. Jun 20, 2016 at 19:38

2 here is rbf for large datasets: github.com/scipy/scipy/issues/5180 – denfromufa Jun 21, 2016 at 14:40

2 @DavidKong as I noted in my answer, you can also use the interpolator functions used by griddata under the hood when you need to, e.g. `CloughTocher2DInterpolator` . I'm sure `interp2d` has use cases where it makes sense, but yeah, I'd go for some other tool. – Andras Deak -- Слава Україні Dec 20, 2021 at 21:17

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