# xagg: A Python package to aggregate gridded data onto polygons

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Summary

Scientific data (e.g. gridded weather observations, pollution data, night-time lights, or other remote sensing products) are often interpolated to or created on grids or raster pixels to approximate the continuous real world for ease of calculation, standardization, or due to technical limiations. However, the geospatial or administrative boundaries that occur in the real world rarely approximate a grid. For example, birds fly along complex migratory corridors, rain- and watersheds follow valleys and mountains, and many types of data, such as demographics or agricultural information, are often collected on the county, city, or census tract levels. Often, the geospatial and administrative boundaries that occur in the real world can be represented with polygons.

When these raster and polygon worlds collide, as they often do in social or natural science research, data must be aggregated between them (e.g., Auffhammer et al. (2013)). This aggregation must, however, be done with care to preserve the integrity of the data and subsequent analysis. Consider a researcher working on population and mortality statistics for Los Angeles County. Using gridded temperature data in their work may require aggregating the gridded data onto a polygon representing Los Angeles County (Figure 1). The simplest way to aggregate the data would be to average across every grid cell that overlaps with the county polygon, implicitly weighting each equally. However, some grid cells may only slightly overlap with the county and instead primarily cover areas with different climate characteristics (for example, grid cells primarily covering oceans in Figure 1); giving them equal weight to grid cells fully inside the county may produce a temperature time series that does not reflect what the county actually experiences. Additionally, some grid cells may cover sparsely populated areas of the county; since few people experience temperature in those areas, including those grid cells with equal weight in the aggregated result may be unhelpful when studying the relationship between temperature and mortality.
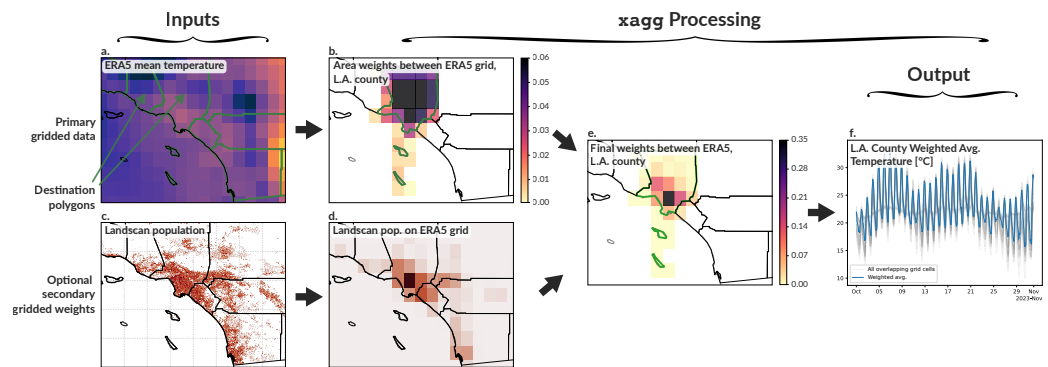
Figure 1: Illustration of xagg workflow. Variables stored on a geographic grid (in this case 2-meter daily temperature from ERA5 reanalysis; Hersbach et al. (2020)), a set of geographic polygons (in this case US county borders, focusing on Los Angeles County as an example), and an optional second weight on a geographic grid (in this case LandScan Day Population; Rose et al. (2017)) are inputted (panels a., c.). xagg calculates the relative overlap between each ERA5 grid cell and each county (panel b.). xagg regrids the population grid to the ERA5 grid (panel d.), and produces a set of final grid cell weights composed of both the area overlap and the population density (panel e.). For each county, these weights are used to calculate weighted averages of daily temperature (panel f.), which can be then be outputted in multiple formats for further analysis.

Therefore, an ideal aggregation would weight not only by the area of overlap between grid cells and polygons, but also optionally by other densities of relevant variables - population, area planted, etc. (Auffhammer et al., 2013).

xagg fulfills this need, by providing a simple interface for aggregating raster data stored in rectangular grids in xarray (Hoyer & Hamman, 2017) Datasets or DataArrays onto polygons stored in geopandas (Bossche et al., 2024) geodataframes, weighted by the fractional area overlap between the raster grid and the polygon, and optionally additionally weighted by a secondary gridded variable (see Figure 1 for a sample workflow). Fractional area weights are generated by constructing polygons for each grid cell and using geopandas' gpd.overlay() function to calculate the overlaps between input polygons and grid cells. Aggregated data is then returned as an xarray Dataset, a pandas DataFrame, or a geopandas GeoDataFrame, depending on the user's needs.

Statement of need

Aggregating gridded data onto polygons is a fundamental aspect of much social and natural science research (e.g., Auffhammer et al. (2013); Hsiang et al. (2017); Carleton et al. (2022); Mastrantonas et al. (2022)). Historically, this process has been conducted on an ad hoc basis by individual research groups, often using simplifications such as averaging over all grid cells that overlap with a county, regardless of the size of that overlap (e.g,. Schlenker & Roberts (2009)).

xagg fills a need for an easy, standardized, and accurate workflow for this aggregation. Accepting and outputting data in xarray and pandas/geopandas formats (including keeping by default relevant metadata and attributes from the inputted polygons) means xagg can be plugged into a wide array of existing workflows in natural and social sciences, and can easily export aggregated results in formats read by other languages often used in research, including R, QGIS, or STATA.

Though other Python packages facilitate the aggregation of raster data, to the authors' knowledge, none provide the same depth of functionality or conduct the final aggregation internally. The mask_3D_frac_approx function from the regionmask package (Hauser et al., 2023) also creates weights from relative overlaps between grid cells and regions, for example;

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this however only works for regular rectangular grids (while xagg works with any rectangular grid), and results in more approximate overlaps than those calculated using xagg. In addition, none allow easy weighting by a secondary raster variable (e.g., population density or yield), or keep polygon metadata intact (which is often needed to merge in other datasets after aggregation).

xagg has already been used in peer-reviewed (e.g., Pulla et al. (2023); Mastrantonas et al. (2022); Schwarzwald & Lenssen (2022)) and upcoming (e.g., Sichone (2024); Peard & Hall (2023)) scientific publications, has reached over 15,000 cumulative downloads across versions, and is a key component of a how-to guide for climate econometrics (Rising et al., 2024).

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