

A data analysis and publication platform for the web

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What is opendata.fit?

opendata.fit is a cloud-based web platform and execution engine for use by researchers to manage analysis workflows and datasets from development to publication, with a focus on model fitting and optimisation.

Motivation

Model optimisation

Existing analysis platforms (Galaxy, EcoCommons, etc) are domain-specific & largely focused on data processing workflows.

No existing platforms target model fitting and optimisation methods which are used in a multitude of fields (drug discovery, materials science, astronomy), forcing researchers to rely on bespoke solutions.

Reproducibility

Existing analysis workflows vary widely between groups and can be difficult to track and publish in their entirety, resulting in lack of reproducibility.

opendata.fit aims to improve reproducibility by encapsulating entire analysis workflows including history into a single JSON file format. Complete, reproducible workflows can then be included in a publication by citing a single link.

```

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"description": "Example of a datapackage encapsulating a workflow",
"algorithms": [
  {
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    "inputs": [
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        "title": "X input parameter",
        "description": "A parameter to the algorithm (can be input data, an initial parameter value, options for the algorithm, etc.)",
        "type": "resource",
        "resource": "x_data"
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    ],
    "outputs": [...]
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"displays": [
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    "title": "Example workflow display",
    "description": "Defines a display for the example workflow. Describes the user interface components - input fields, output fields, visualisations, etc - to be displayed in the web application.",
    ...
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    "title": "Parameter input view",
    "resources": [
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      "y_data"
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    "specType": "opendatafit-params"
  },
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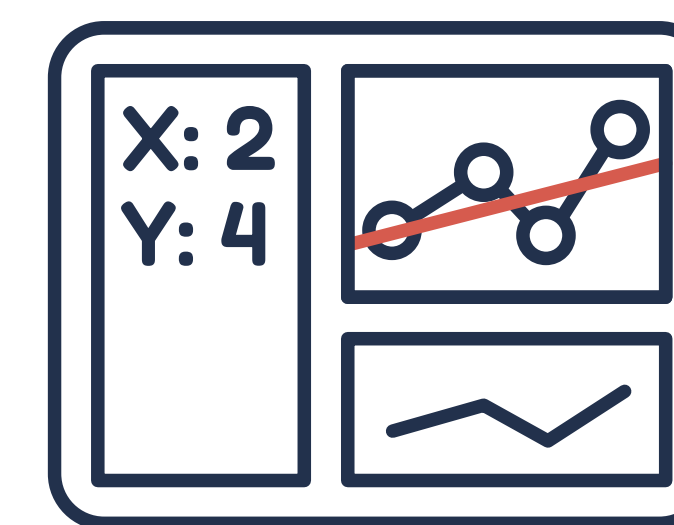
```



Upload instrument data



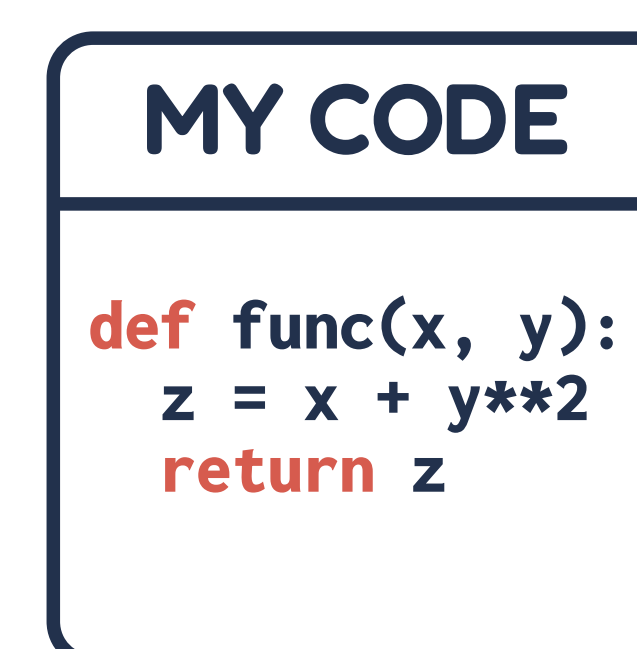
Select from a library of analysis algorithms



Perform analysis using a simple web interface



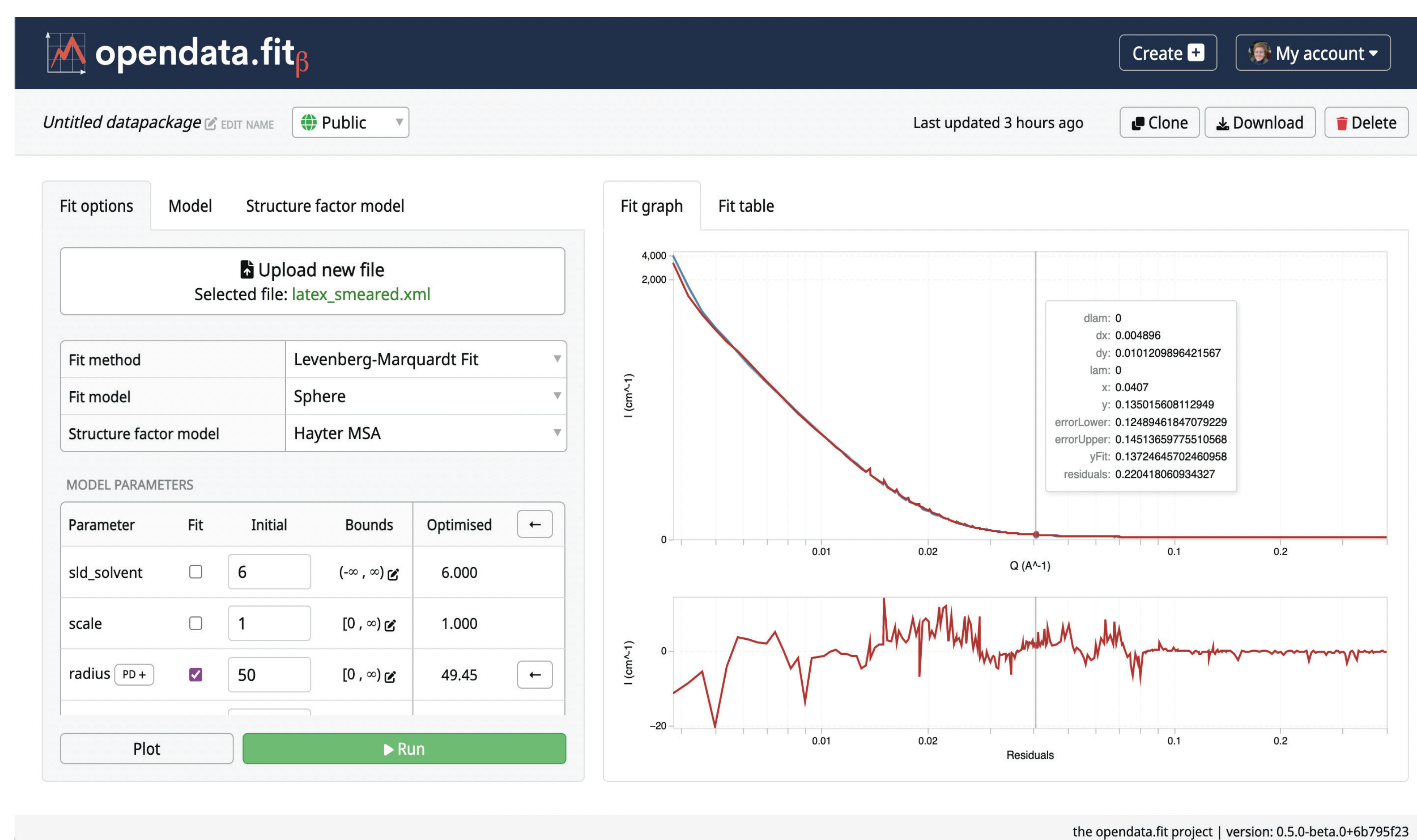
Visualise results



Write and contribute custom analysis algorithms

[42] Jane Smith, *opendata.fit: Example Analysis, Sept 2022.* Available at <https://app.opendata.fit/s/cdf85>

Publish complete workflow with a link



Datapackages

Workflows in opendata.fit are packaged into a single JSON file format called a datapackage, which extends the existing open source Frictionless data standard. Visualisations are defined using the open source Vega visualisation language.

Each datapackage is a complete, portable record of a workflow including datasets, algorithms, analysis process and input and output parameters. Datapackage algorithms are fully containerised through Docker maintaining a consistent execution environment.

Built on FAIR data principles

 Findable

Datapackages and resources are created with a unique and persistent URL

 Accessible

Datapackages can be retrieved via API or downloaded via the web interface

 Interoperable

Datapackages extend the well documented Frictionless data standard

 Reusable

Datapackages contain provenance metadata and full history of the analysis allowing it to be reused