# Scientific Python

Community developed, community owned

## Usage and needs for sparse data in scikit learn

Sparse Data – Meeting 1
Monday, Sept. 26th
11AM - 12PM Pacific time
Julien Jerphanion (`@jjerphan`)

# Context: sparse data support via SciPy sparse matrices

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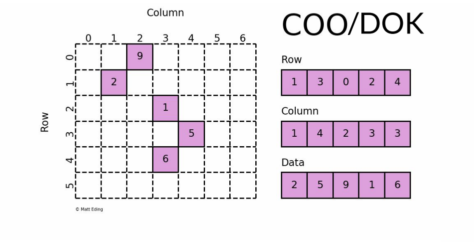


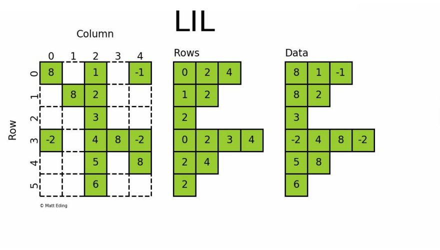


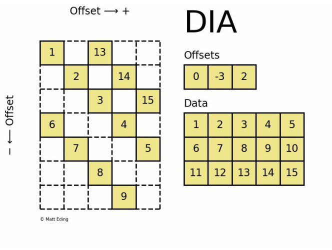


5% of use-cases, *e.g.*:

- Sparse matrices construction
- Generalized Linear Models
- `Spectral{Biclustering,Embedding}`
- `AgglomerativeClustering`

Used via SciPy's Python API.
Use-cases' needs are covered.

*Animations courtesy of [Matt Eding's blog post on Sparse Matrices]*

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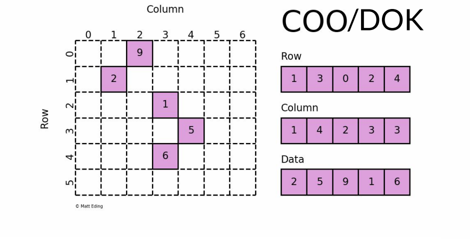


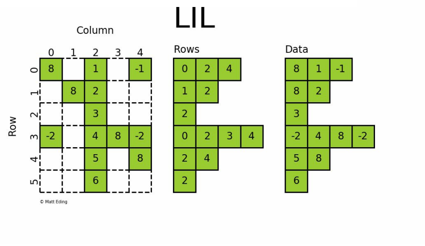


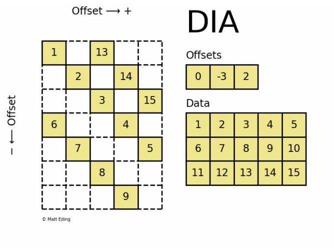


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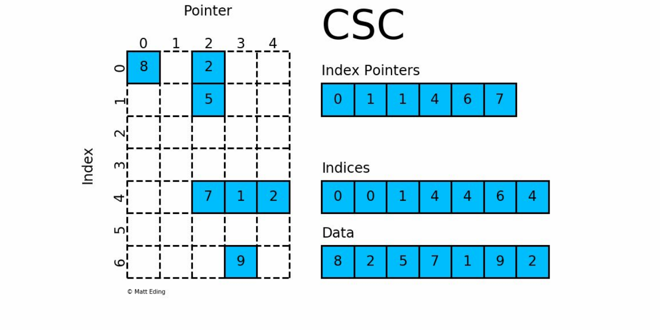


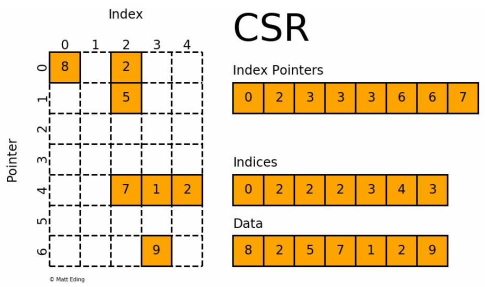


Used for performance:

- CSC: column-wise processing
- CSR: row-wise processing

Used via:

- SciPy's Python API
- Dedicated low-level Cython routines in scikit-learn working on the arrays directly, *e.g.*:
  [`sklearn/utils/sparsefuncs_fast`]()
  [`DistanceMetrics.(r)dist_csr`]()
  [`{Dense,Sparse}²DatasetsPairs`]()

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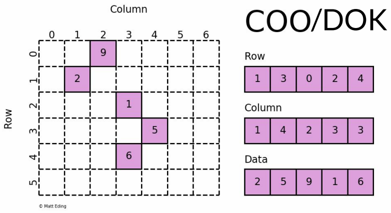


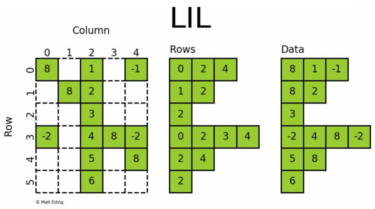


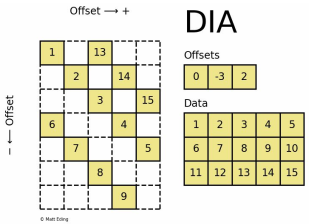


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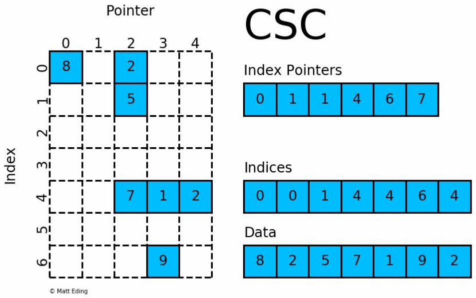


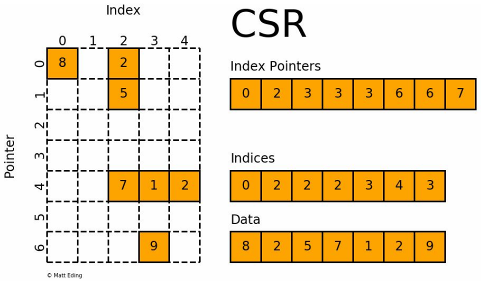


95% of usages: a lot of transformers and machine learning algorithms

Use-cases' needs can better be addressed.

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# Sparse-Dense matrices operations: usage and needs

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[Sandwich product use case in Generalized Linear Models’ solvers]

$$\mathbf{X}^\top \mathrm{diag}(\mathbf{d})\, \mathbf{X}$$

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Generalized Matrix-Matrix Multiplication on dense-sparse matrices' pairs

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**Needs:** efficient low-level implementations for such operations

# Sparse-Dense matrices operations: possible solutions



💡 Recode the needed operations in Cython

- ✅ Pros:
  - full control on those implementations (tailorable to our use-cases)
- ❌ Cons:
  - maintenance complexity:
    - fused-type restrictions on Cython extension types
    - `indptr`, `indices` dtypes runtime dependence (scipy#16774)

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💡 Dependent (optionally) on another library like [tabmat]():

- ✅ Pros:
  - efficient and stable implementations
  - support block-wise sparse and dense structure arrays
- ❌ Cons:
  - would add another dependency
  - no-public C/C++/Cython API
  - potential costly data structures' adaptations

# Proposals for discussions

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🎯 Needs/wishes:

- API UX uniformity across NumPy and SciPy usages
  - output containers' type returning match input containers' type
  - *e.g.*: `np.{h,v}stack` supporting SciPy matrices

- Ideally multi-thread and efficient implementations of the previous operations:
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  - Why have signed integers historical been chosen?
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*Thank you for your attention!*