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SparseGridsKit.jl: Adaptive single- and multi-fidelity sparse grid approximation in Julia

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Summary

Approximation of functions with high dimensional domains is important for modern scientific and engineering problems. An example of this is constructing surrogate models for quantities of interest for high dimensional parametrised PDE problems. These surrogate models are constructed to give computationally cheap yet accurate approximations that can be used in applications such as uncertainty quantification, optimisation, parameter estimation (Ghanem et al., 2017). Surrogates may be constructed with global polynomial approximation on the parameter space and a common approach is the use of *sparse grid* approximation techniques. In particular, sparse grid polynomial interpolation techniques allow a practitioner to approximate solutions to parametric problems in a non-intrusive way using existing numerical solvers.

`SparseGridsKit.jl` provides a Julia toolbox to manually and adaptively construct sparse grid polynomial approximations (Bezanson et al., 2017). Interpolation and quadrature routines allow evaluation and integration of the surrogate models. Multi-fidelity approximation via the multi-index stochastic collocation algorithm is also possible (Haji-Ali et al., 2016) (John D. Jakeman et al., 2019) (Piazzola et al., 2022). Approximations can be represented either in a basis of Lagrange interpolation polynomials or in a basis of spectral-type polynomials.

Statement of need

Sparse grid approximation is a well developed methodology and is featured in many survey articles and textbook chapters, e.g. (Bungartz & Griebel, 2004),(Le Maître & Knio, 2010),(Schwab & Gittelson, 2011),(Cohen & DeVore, 2015),(Sullivan, 2015). The need for sparse grid surrogate modelling is demonstrated by its use in many applications, from simpler elliptic and parabolic PDEs to complex practical engineering problems e.g. (Piazzola et al., 2021),(Piazzola et al., 2022),(Li et al., 2024). The `SparseGridsKit.jl` implementation offers a rich set of features to enable this.

Specifically, `SparseGridsKit.jl` is a Julia implementation of sparse grid approximation methods. This offers

- native Julia implementation of adaptive sparse grid approximation functionality,
- dynamical typing, allowing surrogate models to map input parameters to any Julia type offering vector space operations.

Existing sparse grid approximation packages in Julia include `Tasmanian.jl`, wrapping the Tasmanian library, `AdaptiveSparseGrids.jl` and `DistributedSparseGrids.jl`. `SparseGridsKit.jl` offers a more complete set of functionality, with close resemblance to the popular `Sparse Grids MATLAB Kit` (Piazzola & Tamellini, 2024).

Other popular software packages implementing sparse grid approximation include:

- `Sparse Grids MATLAB Kit`: A MATLAB package on which the `SparseGridsKit.jl` is loosely based (Piazzola & Tamellini, 2024).
- `spinterp`: A MATLAB toolbox for sparse grid interpolation (Klimke & Wohlmuth, 2005) (no longer maintained).
- `UQLab`: A broad MATLAB uncertainty quantification toolkit (Marelli & Sudret, 2014).
- `PyApprox`: A Python package for high-dimensional approximation (J. D. Jakeman, 2023).
- `Dakota`: A C++ library for optimisation and surrogate modelling (Adams et al., 2024).
- `UQTk`: A collection of C++/Python uncertianty quantification tools including sparse grid quadrature (Debusschere et al., 2015).
- `Tasmanian`,`SG++`,: C++ sparse grid approximation implementations with wrappers for many popular software languages (Stoyanov, 2015) (Pflüger, 2010).

`SparseGridsKit.jl` offers specific Julia toolkit with minimal complexity for fast algorithm development and prototyping.

`SparseGridsKit.jl` Features

The main features are outlined below:

- One dimensional knots and quadrature rules.
- Multi-index set construction and manipulation.
- Combination technique sparse grid approximations including evaluation and quadrature routines.
- Adaptive sparse grid approximation construction based on the ubiquitous Gerstner-Griebel dimensional adaptive algorithm (Gerstner & Griebel, 2003).
- Adaptive multi-fidelity approximation via the Multi-Index Stochastic Collocation (MISC) algorithm (Haji-Ali et al., 2016) (John D. Jakeman et al., 2019) (Piazzola et al., 2022).
- Conversion to and from Polynomial Chaos / spectral polynomial series representation.
- Limited support for surrogate model differentiation via automatic differentiation.

The functionality described above is tested and documented with examples included in the repository.

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References

Adams, B. M., Bohnhoff, W. J., Dalbey, K. R., Ebeida, M. S., Eddy, J. P., Eldred, M. S., Hooper, R. W., Hough, P. D., Hu, K. T., Jakeman, J. D., Khalil, M., Maupin, K. A., Monschke, J. A., Prudencio, E. E., Ridgway, E. M., Robbe, P., Rushdi, A. A., Seidl, D. T., Stephens, J. A., … Winokur, J. G. (2024). *Dakota 6.21.0 documentation. Technical report SAND2024-15492O*. Sandia National Laboratories, Albuquerque, NM. http://snl-dakota.github.io

Bezanson, J., Edelman, A., Karpinski, S., & Shah, V. B. (2017). Julia: A fresh approach to numerical computing. *SIAM Review*, *59*(1), 65–98. https://doi.org/10.1137/141000671

Bungartz, H.-J., & Griebel, M. (2004). Sparse grids. *Acta Numerica*, *13*, 147–269. https://doi.org/10.1017/s0962492904000182

Cohen, A., & DeVore, R. (2015). Approximation of high-dimensional parametric PDEs. *Acta Numerica*, *24*, 1–159. https://doi.org/10.1017/s0962492915000033

Debusschere, B., Sargsyan, K., Safta, C., & Chowdhary, K. (2015). Uncertainty quantification toolkit (UQTk). In *Handbook of uncertainty quantification* (pp. 1–21). Springer International Publishing. https://doi.org/10.1007/978-3-319-11259-6_56-1

Gerstner, T., & Griebel, M. (2003). Dimension–adaptive tensor–product quadrature. *Computing*, *71*(1), 65–87. https://doi.org/10.1007/s00607-003-0015-5

Ghanem, R., Higdon, D., & Owhadi, H. (2017). *Handbook of uncertainty quantification*. Springer International Publishing. https://doi.org/10.1007/978-3-319-12385-1

Haji-Ali, A.-L., Nobile, F., Tamellini, L., & Tempone, R. (2016). Multi-index stochastic collocation for random PDEs. *Computer Methods in Applied Mechanics and Engineering*, *306*, 95–122. https://doi.org/10.1016/j.cma.2016.03.029

Jakeman, J. D. (2023). PyApprox: A software package for sensitivity analysis, bayesian inference, optimal experimental design, and multi-fidelity uncertainty quantification and surrogate modeling. *Environmental Modelling & Software*, *170*, 105825. https://doi.org/10.1016/j.envsoft.2023.105825

Jakeman, John D., Eldred, M. S., Geraci, G., & Gorodetsky, A. (2019). Adaptive multi-index collocation for uncertainty quantification and sensitivity analysis. *International Journal for Numerical Methods in Engineering*, *121*(6), 1314–1343. https://doi.org/10.1002/nme.6268

Klimke, A., & Wohlmuth, B. (2005). Algorithm 847: spinterp: Piecewise multilinear hierarchical sparse grid interpolation in MATLAB. *ACM Transactions on Mathematical Software*, *31*(4), 561–579. https://doi.org/10.1145/1114268.1114275

Le Maître, O. P., & Knio, O. M. (2010). Spectral methods for uncertainty quantification: With applications to computational fluid dynamics. In *Scientific Computation*. Springer Netherlands. https://doi.org/10.1007/978-90-481-3520-2

Li, Y., Zoccarato, C., Piazzola, C., Bru, G., Tamellini, L., Guardiola-Albert, C., & Teatini, P. (2024). *Characterizing aquifer properties through a sparse grid-based bayesian framework and InSAR measurements: A basin-scale application to Alto Guadalentín, Spain*. https://doi.org/10.22541/essoar.172373105.53381390/v1

Marelli, S., & Sudret, B. (2014). UQLab: A framework for uncertainty quantification in Matlab. *Vulnerability, Uncertainty, and Risk*, 2554–2563. https://doi.org/10.1061/9780784413609.257

Pflüger, D. (2010). *Spatially adaptive sparse grids for high-dimensional problems*. Institut für Informatik, Technische Universität München; Verlag Dr. Hut. ISBN: 9783868535556

Piazzola, C., & Tamellini, L. (2024). Algorithm 1040: The sparse grids MATLAB kit - a MATLAB implementation of sparse grids for high-dimensional function approximation and uncertainty quantification. *ACM Transactions on Mathematical Software*, *50*(1), 1–22. https://doi.org/10.1145/3630023

Piazzola, C., Tamellini, L., Pellegrini, R., Broglia, R., Serani, A., & Diez, M. (2022). Comparing multi-index stochastic collocation and multi-fidelity stochastic radial basis functions for forward uncertainty quantification of ship resistance. *Engineering with Computers*, *39*(3), 2209–2237. https://doi.org/10.1007/s00366-021-01588-0

Piazzola, C., Tamellini, L., & Tempone, R. (2021). A note on tools for prediction under uncertainty and identifiability of SIR-like dynamical systems for epidemiology. *Mathematical Biosciences*, *332*, 108514. https://doi.org/10.1016/j.mbs.2020.108514

Schwab, C., & Gittelson, C. J. (2011). Sparse tensor discretizations of high-dimensional parametric and stochastic PDEs. *Acta Numerica*, *20*, 291–467. https://doi.org/10.1017/s0962492911000055

Stoyanov, M. (2015). *User manual: TASMANIAN sparse grids* (ORNL/TM-2015/596). Oak

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Ridge National Laboratory.

Sullivan, T. J. (2015). Introduction to uncertainty quantification. In *Texts in Applied Mathematics*. Springer International Publishing. https://doi.org/10.1007/978-3-319-23395-6

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