

Tensor Graph Regularized Bootstrap for High-Dimensional Bond Yield Reconstructions: Applications in Green Bond Markets

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Related Publications

Graph Signals

Product Graph Structures

Graph Signal Reconstruction

Is GSR Appropriate?

Application: US Municipal Green Bond Markets

Conclusions

Thank You and References

1. Antonian, E. B., Peters, G. W., Chantler, M. J. (2024). Kernel Generalized Least Squares Regression for Network-Structured Data. *Plos One*. <https://doi.org/10.1371/journal.pone.0324087>
2. Antonian, E. B., Peters, G. W., Chantler, M. J. (2024). Bayesian Reconstruction of Cartesian Product Graph Signals with General Patterns of Missing Data. *Journal of the Franklin Institute*, 361.9 (2024): 106805.
3. **Campi M., Peters G.W., Antonian E.. Multiway Graph Signal Reconstruction: A Statistical Framework for Modeling Green Bond Yield Structures. Preprint.**

Software library for highly efficient large factorised graph computations.

1. Antonian, E. B., Peters, G. W., Chantler, M. J. (2023). PyKronecker: A Python Library for the Efficient Manipulation of Kronecker Products and Related Structures. In *The Journal of Open Source Software*, 8(81).

Ph.D. of Dr. Edward Antonian: Supervised by Prof. Peters (UCSB-HW) and Prof. Chantler (HW)

GitHub for Thesis and Code: <https://github.com/nickelnine37>

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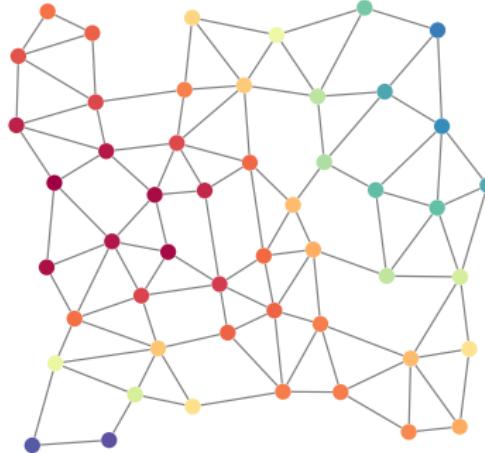
Conclusions

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A graph signal is a vector $\mathbf{y} \in \mathbb{R}^N$ where each element is understood as being measured on a node of the graph ($N = |\mathcal{V}|$).

An example could be temperature over a network of monitoring stations, or user taste preferences over a social network.

A graphical depiction of a smooth graph signal where the value of signal at each node is displayed in colour (at one time instant).



Formally: given an undirected weighted graph $G = (\mathcal{V}, \mathcal{E})$, with $|\mathcal{V}| = N$, then a graph signal

$$f : \mathcal{V} \rightarrow \mathbb{R}$$

is a function defined on the vertices of the graph that maps every vertex $\{v_i\}_{i=1,\dots,N}$ to a real number $y_i := f(i) \in \mathbb{R}$.

Intuitively: we often expect graph signals ($y_i := f(i)$) to be “smooth”, i.e. neighbouring nodes are likely to be similar.

Distance $d(y_i, y_j)$ is small when $v_i \sim v_j$ i.e. when graph vertices have a connecting edge association.

Can measure similarity $d(y_i, y_j)$ via squared Total Variation (Dirichlet energy):

$$\text{TV}_2(\mathbf{y}) = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \mathbf{A}_{ij} (\mathbf{y}_i - \mathbf{y}_j)^2 = \mathbf{y}^\top (\mathbf{D} - \mathbf{A}) \mathbf{y} = \mathbf{y}^\top \mathbf{L} \mathbf{y}$$

The graph Laplacian \mathbf{L} gives a natural basis in which to analyse the frequency content of a graph signal.

$$\mathbf{L} = \mathbf{U} \Lambda \mathbf{U}^\top$$

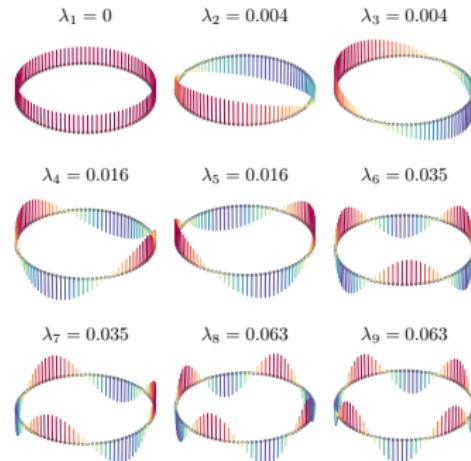
This provides a direct generalisation of classical Fourier analysis to signals residing on an irregular domain.

$$\mathbf{u}_1 = \underset{|\mathbf{u}|^2=1}{\operatorname{argmin}} \quad \text{TV}_2(\mathbf{u})$$

$$\mathbf{u}_2 = \underset{|\mathbf{u}|^2=1, \perp \mathbf{u}_1}{\operatorname{argmin}} \quad \text{TV}_2(\mathbf{u})$$

$$\mathbf{u}_3 = \underset{|\mathbf{u}|^2=1, \perp \mathbf{u}_1, \mathbf{u}_2}{\operatorname{argmin}} \quad \text{TV}_2(\mathbf{u})$$

$$\mathbf{u}_4 = \dots$$



The eigenvectors of the graph Laplacian can be understood as sequentially less smooth with respect to the topology of the graph.

The corresponding eigenvalue, **referred to as the frequency**, gives a value specifying how “rough” each eigenvector is relative to the others, as measured by TV_2 .

Undirected graph: first Laplacian eigenvector will always be constant with an eigenvalue of zero ($\lambda_1 = 0$).

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Consider two undirected graphs $\mathcal{G}_A = (\mathcal{V}_A, \mathcal{E}_A)$ and $\mathcal{G}_B = (\mathcal{V}_B, \mathcal{E}_B)$ with vertex sets given by $\mathcal{V}_A = \{a \in \mathbb{N} \mid a \leq N_A\}$ and $\mathcal{V}_B = \{b \in \mathbb{N} \mid b \leq N_B\}$ respectively.

Graph Product: A new graph \mathcal{G} can be constructed by taking the product between factor graphs \mathcal{G}_A and \mathcal{G}_B .

$$\mathcal{G} = \mathcal{G}_A \diamond \mathcal{G}_B = (\mathcal{V}, \mathcal{E})$$

Definitions of graph product \diamond : \mathcal{G} has vertex set \mathcal{V} from factor graphs

$$\mathcal{V} = \mathcal{V}_A \times \mathcal{V}_B = \{(a, b) \in \mathbb{N}^2 \mid a \leq N_A \text{ and } b \leq N_B\}$$

Typically, vertices are arranged in lexicographic order: i.e.
 $(a, b) \leq (a', b')$ iff $a < a'$ or $(a = a' \text{ and } b \leq b')$.

Then a specific graph product is defined by a consistent rule for constructing \mathcal{E} from the factor edge sets \mathcal{E}_A and \mathcal{E}_B .

One can define $2^8 = 256$ possible graph product rules.

Adjacency & Laplacians of the product graph in terms of factor graph matrices:

	Adjacency matrix	Laplacian
Cartesian	$\mathbf{A}_A \oplus \mathbf{A}_B$	$\mathbf{L}_A \oplus \mathbf{L}_B$
Direct	$\mathbf{A}_A \otimes \mathbf{A}_B$	$\mathbf{D}_A \otimes \mathbf{L}_B + \mathbf{L}_A \otimes \mathbf{D}_B - \mathbf{L}_A \otimes \mathbf{L}_B$
Strong	$\mathbf{A}_A \otimes \mathbf{A}_B + \mathbf{A}_A \oplus \mathbf{A}_B$	$\mathbf{D}_A \otimes \mathbf{L}_B + \mathbf{L}_A \otimes \mathbf{D}_B - \mathbf{L}_A \otimes \mathbf{L}_B + \mathbf{L}_A \oplus \mathbf{L}_B$
Lexicographic	$\mathbf{I}_A \otimes \mathbf{A}_B + \mathbf{A}_A \otimes \mathbf{O}_A$	$\mathbf{I}_A \otimes \mathbf{L}_B + \mathbf{L}_A \otimes \mathbf{O}_B + \mathbf{D}_A \otimes (N_B \mathbf{I}_B - \mathbf{O}_B)$

\mathbf{D}_A and \mathbf{D}_B are the diagonal degree matrices, i.e $\mathbf{D}_A = \text{diag } \mathbf{A}_A \mathbf{1}$. \mathbf{I}_A and \mathbf{O}_A are the $(N_A \times N_A)$ identity matrix and matrix of ones respectively.

Graph Products

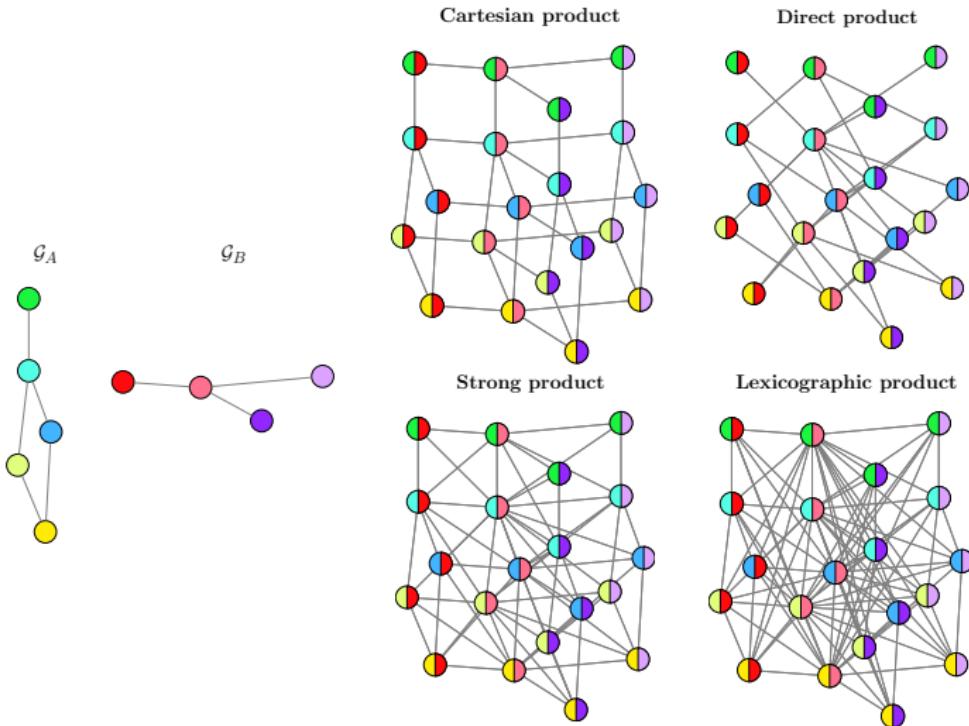


Figure: Depiction of the four standard graph products

Laplacian of a Cartesian product graph satisfies:

$$\begin{aligned}\mathbf{L} &= \mathbf{L}_A \oplus \mathbf{L}_B \\ &= \mathbf{L}_A \otimes \mathbf{I}_B + \mathbf{I}_A \otimes \mathbf{L}_B\end{aligned}$$

Can perform eigen decomposition one each graph product component

$$\begin{aligned}\mathbf{L} &= (\mathbf{U}_A \otimes \mathbf{U}_B)(\Lambda_A \oplus \Lambda_B)(\mathbf{U}_A^\top \otimes \mathbf{U}_B^\top) \\ &= \mathbf{U}\Lambda\mathbf{U}^\top\end{aligned}$$

Can develop a definition of filtering in two dimensions.

$$\begin{aligned}\mathbf{H} &= (\mathbf{U}_A \otimes \mathbf{U}_B) g(\Lambda_A \oplus \Lambda_B) (\mathbf{U}_A^\top \otimes \mathbf{U}_B^\top) \\ &= (\mathbf{U}_A \otimes \mathbf{U}_B) \text{ diag vec}(\mathbf{G}) (\mathbf{U}_A^\top \otimes \mathbf{U}_B^\top) \\ &= \mathbf{U}\mathbf{D}_G\mathbf{U}^\top\end{aligned}$$

The matrix $\mathbf{G} \in \mathbb{R}^{N_B \times N_A}$ holds the value of the filter function applied to the sum of pairs of eigenvalues.

$$\mathbf{G}_{ba} = g\left(\lambda_a^{(A)}, \lambda_b^{(B)}; \beta_a, \beta_b\right)$$

Cartesian Product Graph Filters

$$\beta_T = 0.01$$

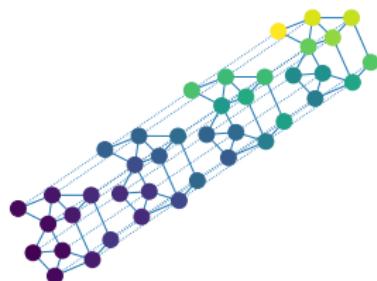
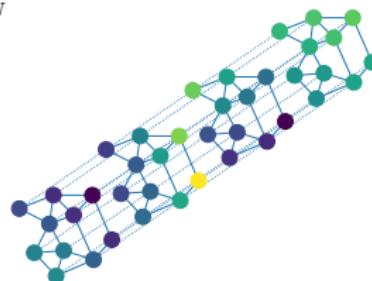
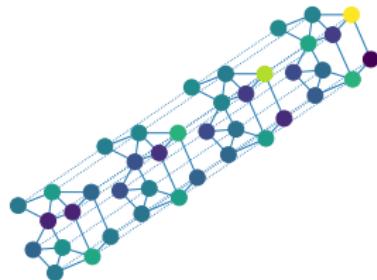
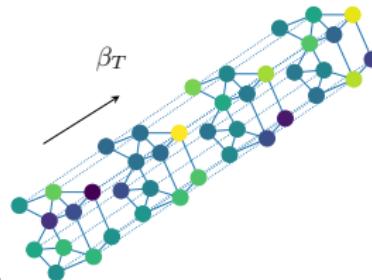
$$\beta_T = 1$$

$$\beta_N = 0.01$$

$$\beta_T$$

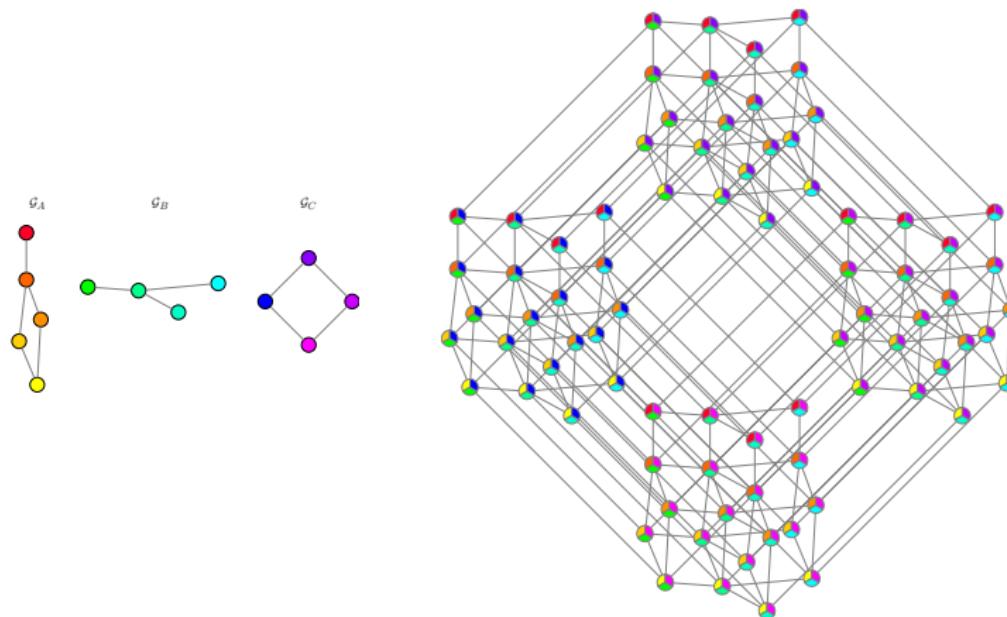
$$\beta_N$$

$$\beta_N = 1$$



We can easily extend the concept of a two-dimensional product to three or more dimensions.

Here, signals become tensors, or multidimensional arrays, and graphs can become extremely large.



Spectral decomposition

Consider a tensor graph signal $\mathcal{Y} \in \mathbb{R}^{N_1 \times N_2 \times \dots \times N_d}$ represented in its multi-dimensional array form.

$$\mathbf{y} = \text{vec}_{\text{RM}}(\mathcal{Y}) \iff \mathcal{Y} = \text{ten}_{\text{RM}}(\mathbf{y})$$

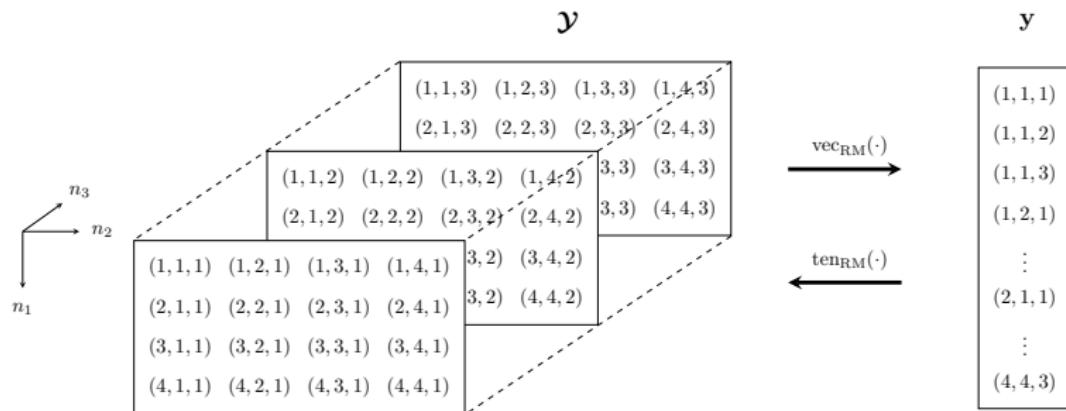


Figure: Depiction of the process of converting an order-3 tensor between its multidimensional array and vector form in **row-major** (RM) order. Note that the elements in the vectorised signal are lexicographically ordered.

Define the Graph Fourier Transform (GFT) and its corresponding inverse (IGFT) of this signal as follows:

$$\text{GFT}(\mathbf{y}) = \text{ten}_{\text{RM}}(\mathbf{U}^T \mathbf{y}) = \text{ten}_{\text{RM}} \left(\left(\bigotimes_{i=1}^d \mathbf{U}^{(i)} \right)^T \text{vec}_{\text{RM}}(\mathbf{y}) \right)$$

$$\text{IGFT}(\mathbf{y}) = \text{ten}_{\text{RM}}(\mathbf{U} \mathbf{y}) = \text{ten}_{\text{RM}} \left(\left(\bigotimes_{i=1}^d \mathbf{U}^{(i)} \right) \text{vec}_{\text{RM}}(\mathbf{y}) \right)$$

Action of a general spectral operator: first apply GFT to signal \mathbf{y} & then apply scaling function to each spectral component. Next transform back into the vertex domain via the IGFT.

$$\mathbf{y}' = \text{IGFT}(\mathcal{G} \circ \text{GFT}(\mathbf{y}))$$

Matrix operator generating this transformation is:

$$\mathbf{H} = \mathbf{U} \text{ diag} \text{vec}_{\text{RM}}(\mathcal{G}) \mathbf{U}^T$$

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Goal of Graph Signal Reconstruction (GSR): is to estimate the value of a partially observed graph signal at nodes where no data was collected.

GSR on a Cartesian product graph where available data is partially observed signal $\mathbf{Y} \in \mathbb{R}^{N \times T}$ where only an arbitrary subset $\mathcal{S} = \{(n_1, t_1), (n_2, t_2), \dots\}$ of the signal elements were recorded.

All other missing elements of \mathbf{Y} are set to zero.

Binary Sensing Matrix $\mathbf{S} \in \{0, 1\}^{N \times T}$ tracks missing elements of \mathbf{Y} :

$$\mathbf{S}_{nt} = \begin{cases} 1 & \text{if } (n, t) \in \mathcal{S} \\ 0 & \text{otherwise.} \end{cases}$$

Data input to GSR problem is as follows:

$$\text{input data} = \left\{ \mathbf{Y} \in \mathbb{R}^{N \times T}, \mathbf{S} \in \{0, 1\}^{N \times T}, \mathbf{A} \in \mathbb{R}^{NT \times NT} \right\}$$

Assume \mathbf{Y} is a noisy partial observation of underlying signal $\mathbf{F} \in \mathbb{R}^{N \times T}$, assumed to be smooth w.r.t. the graph topology:

$$\mathbf{Y} = \mathbf{S} \odot (\mathbf{F} + \mathbf{E})$$

Matrix \mathbf{E} represents the model error assumed an independent normal distribution with unit variance.

Distribution of \mathbf{Y} given latent graph signal \mathbf{F} is

$$\text{vec}(\mathbf{Y}) \mid \mathbf{F} \sim \mathcal{N}\left(\text{vec}(\mathbf{S} \odot \mathbf{F}), \text{diag vec}(\mathbf{S})\right)$$

Covariance matrix $\text{diag vec}(\mathbf{S})$ is semi-positive definite by construction and reflects constraint that some elements of \mathbf{Y} are zero with probability 1.

Note: we also extended these methods to exponential family models & categorical and ordinal data settings on graphs!

Bayesian estimation sets a prior on the latent random graph signal \mathbf{F} which is specified as smooth with respect to the topology of the graph:

w.l.o.g. assume the prior mean for \mathbf{F} is zero across all elements.

$$\text{vec}(\mathbf{F}) \sim \mathcal{N}(\mathbf{0}, \gamma^{-1} \mathbf{H}^2)$$

Given observations \mathbf{Y} then Bayes' rule gives posterior over \mathbf{F} :

$$\pi(\text{vec}(\mathbf{F}) | \mathbf{Y}) = \frac{\pi(\text{vec}(\mathbf{Y}) | \mathbf{F}) \pi(\mathbf{F})}{\pi(\mathbf{Y})}.$$

In the Gaussian-Gaussian model this produces the posterior mean:

$$\widehat{\text{vec}(\mathbf{F})} = \mathbb{E}[\text{vec}(\mathbf{F}) | \mathbf{Y}] = \left(\text{diag} \text{vec}(\mathbf{S}) + \gamma \mathbf{H}^{-2} \right)^{-1} \text{vec}(\mathbf{Y})$$

Calculating: $\left(\text{diag vec}(\mathbf{S}) + \gamma \mathbf{H}^{-2} \right)^{-1}$

Coefficient matrix defining the system is size $NT \times NT$

⇒ direct methods e.g. Gaussian elimination infeasible

⇒ direct computational cost of inversion $O(N^3 T^3)$ arithmetic operations.

Alternative solvers include: stationary iterative methods; Krylov methods; or multigrid methods.

In the following work:

Antonian, E. B., Peters, G. W., Chantler, M. J. (2024). Bayesian Reconstruction of Cartesian Product Graph Signals with General Patterns of Missing Data. *Journal of the Franklin Institute*, 361.9 (2024): 106805.

we propose a stationary iterative method and a Krylov method and compare their relative behaviour.

Convergence behaviour of each is derived theoretically and verified numerically.

In both cases, we show that each step of the iterative process can be completed in $O(N^2 T + NT^2)$ operations, making a solution feasible for relatively large graph problems.

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When is Graph Signal Reconstruction effective?

i.e. Is the partially observed signal exhibiting smoothness with respect to the available graph?

Illustrated for single graph setting...

1. Downsample partially observed signal $\mathbf{y} \in \mathbb{R}^N$ into a vector $\tilde{\mathbf{y}} \in \mathbb{R}^{\tilde{N}}$ s.t. only observed elements kept.
2. Adjust adjacency matrix to produce $\tilde{\mathbf{A}} \in \mathbb{R}^{\tilde{N} \times \tilde{N}}$, which represents the connections between the available nodes
3. Create corresponding Laplacian $\tilde{\mathbf{L}} \in \mathbb{R}^{\tilde{N} \times \tilde{N}}$.
4. Pre-whiten $\tilde{\mathbf{y}}$ for mean of zero and unit variance.
5. Compute the total square variation of $\tilde{\mathbf{y}}$ as

$$TV_2(\tilde{\mathbf{y}}) = \tilde{\mathbf{y}}^\top \tilde{\mathbf{L}} \tilde{\mathbf{y}} = \sum_{n=1}^{\tilde{N}} \tilde{\lambda}_n (\tilde{\mathbf{U}}^\top \tilde{\mathbf{y}})_n^2$$

which can be used for a test.

We define the following hypothesis test:

Null hypothesis \mathcal{H}_0 : The vector $\tilde{\mathbf{y}}$ is spherically distributed in the Fourier domain.

Alternative hypothesis \mathcal{H}_1 : $\tilde{\mathbf{y}}$ is biased towards low-frequency Fourier components.

Under \mathcal{H}_0 : $(\tilde{\mathbf{U}}^\top \tilde{\mathbf{y}})_n \sim \mathcal{N}(0, 1)$ and $\text{Cov}((\tilde{\mathbf{U}}^\top \tilde{\mathbf{y}})_i, (\tilde{\mathbf{U}}^\top \tilde{\mathbf{y}})_j) = \delta_{ij}$.

$\Rightarrow \text{TV}_2(\tilde{\mathbf{y}})$ is the sum of \tilde{N} independent gamma random variables, where

$$\tilde{\lambda}_n (\tilde{\mathbf{U}}^\top \tilde{\mathbf{y}})_n^2 \sim \Gamma(k = \frac{1}{2}, \theta = 2\tilde{\lambda}_n)$$

Hence:

$$\mathbb{E} \left[\tilde{\lambda}_n (\tilde{\mathbf{U}}^\top \tilde{\mathbf{y}})_n^2 \right] = \tilde{\lambda}_n, \quad \text{Var} \left[\tilde{\lambda}_n (\tilde{\mathbf{U}}^\top \tilde{\mathbf{y}})_n^2 \right] = 2\tilde{\lambda}_n^2$$

so by Lyapunov central limit theorem, under the null hypothesis, $\text{TV}_2(\tilde{\mathbf{y}})$ will be approximately distributed as ($\tilde{N} \rightarrow \infty$) by

$$\text{TV}_2(\tilde{\mathbf{y}}) | \mathcal{H}_0 \sim \mathcal{N} \left(\sum_{n=1}^{\tilde{N}} \tilde{\lambda}_n, 2 \sum_{n=1}^{\tilde{N}} \tilde{\lambda}_n^2 \right) = \mathcal{N} \left(\text{Tr}(\tilde{\mathbf{L}}), 2 \text{Tr}(\tilde{\mathbf{L}}^2) \right)$$

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Problem: Pricing securities across multiple dimensions when observations are extremely sparse.

Green bond yields depend on **multiple characteristics simultaneously**:

- Environmental purpose (solar, wind, water, transportation...)
- Credit rating (AAA, AA+, AA, ... BBB+)
- Maturity (1 year to 50 years)
- Tax treatment (federal/state exempt, AMT, taxable...)

Extreme sparsity: 99.27% of characteristic combinations have no observable prices

Market size: \$1.5 trillion globally — accurate pricing matters!

⇒ **Neither traditional econometrics nor standard ML handles this well.**

Dataset: Weekly yield-to-maturity from Bloomberg

829 distinct bonds with sufficient trading history

429 weekly observations (June 2018 – March 2023)

Period includes: COVID-19 disruption, Fed rate hikes

Five-dimensional tensor structure:

Dimension	Size	Graph Structure
Time	429	Chain (weekly)
Environmental purpose	161	Hierarchical tree (IEA/Bloomberg)
Credit rating	8	Ordered chain (AAA → BBB+)
Maturity	8	Chain (0-1y → 40-50y)
Tax status	7	Custom graph (legal provisions)

Theoretical tensor size: $429 \times 161 \times 8 \times 8 \times 7 \approx 31 \text{ million}$ values

Credit Ratings: Ordered chain

AAA \leftrightarrow AA+ \leftrightarrow AA \leftrightarrow ... \leftrightarrow

BBB+

Adjacent ratings = similar
default risk

Maturity: Ordered chain

0-1y \leftrightarrow 1-2y \leftrightarrow ... \leftrightarrow 40-50y

Term structure smoothness

Environmental Purpose: Hierarchy

Solar \sim Wind (both renewable)

Renewable \neq Water
infrastructure

Tax Status: Custom graph

Edges connect statuses sharing
legal provisions

Similar tax \Rightarrow similar investor
base

Key insight: Encode domain knowledge through graphs, don't learn
from sparse data!

Key question: Is the assumed graph structure actually appropriate?

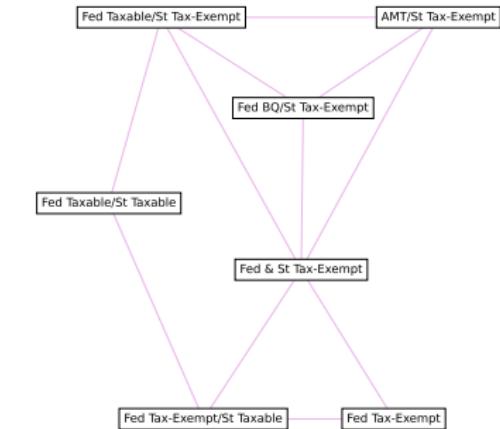
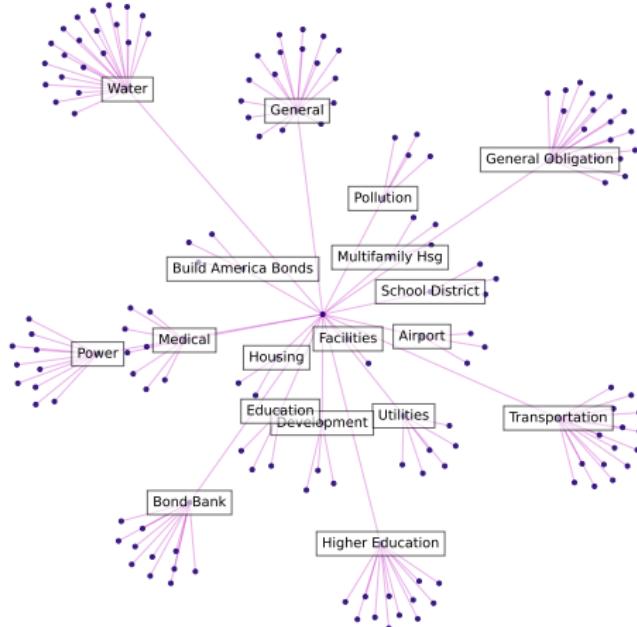
Isotropy test: Compare observed smoothness to random signals

$$Z = \frac{\text{TV}_2(\tilde{\mathbf{y}}) - \mathbb{E}[\text{TV}_2]}{\sqrt{\text{Var}[\text{TV}_2]}}$$

Maturity Bucket	Mean Z -score	Aggregate Z	p -value
5–10 years	−0.16	−2.58	0.005
10–20 years	−0.83	−13.06	< 0.001
20–30 years	−0.77	−12.13	< 0.001
30–40 years	−0.15	−2.25	0.012

Result: All buckets reject H_0 ($p < 0.02$). Yields ARE smoother than random on the rating chain — graph structure is empirically validated!

Graph Structures



Tax status graph (legal provisions)

Environmental purpose hierarchy
(IEA/Bloomberg taxonomy)

Data Sparsity: Bond Distribution

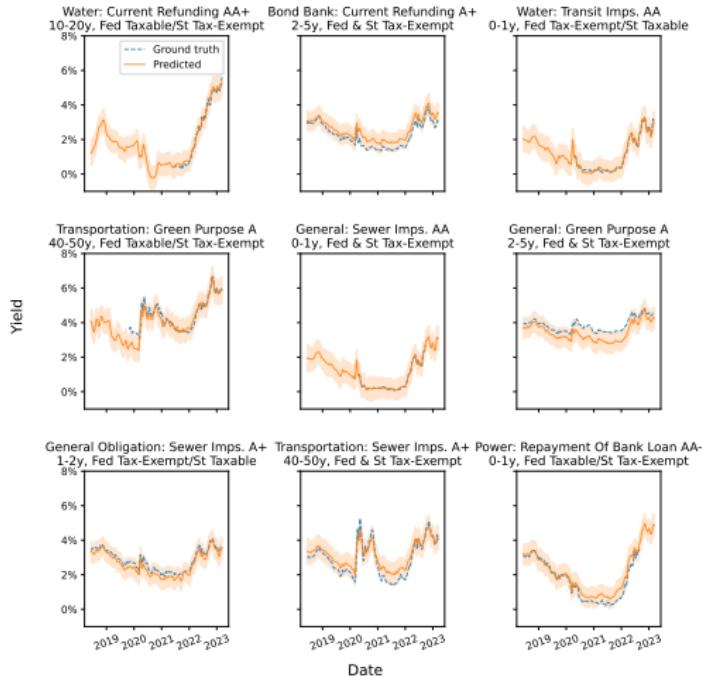


Number of bonds by Credit Rating × Maturity. Note extreme sparsity at short maturities (0–2y) and lower ratings (A-, BBB+). This is why standard methods fail.

Model	Validation		Test	
	MSE	R ²	MSE	R ²
GSR (ours)	0.332	0.819	0.319	0.823
KGR (ours)	0.333	0.820	0.317	0.824
Ridge	0.501	0.729	0.497	0.725
Lasso	0.482	0.739	0.506	0.720

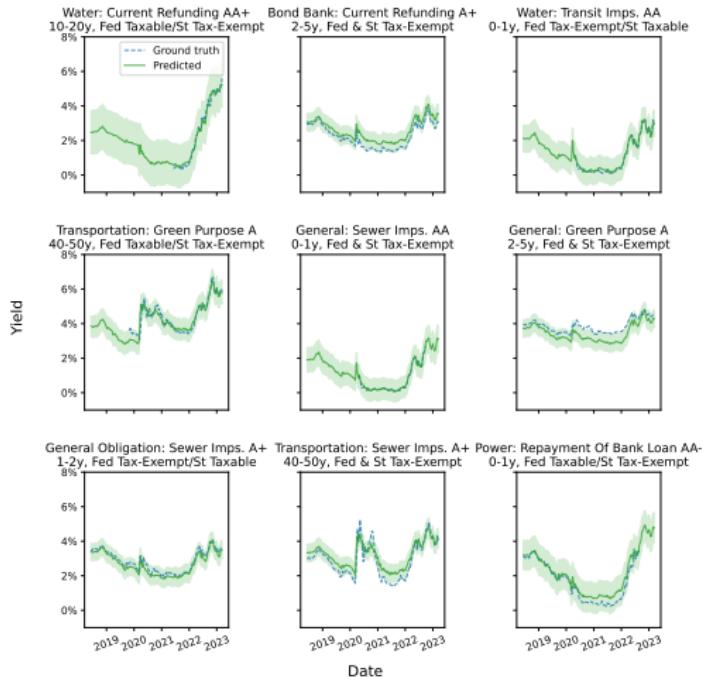
- **36% reduction** in prediction error vs Ridge/Lasso
- Test set: 83 bonds **never seen** during training
- Graph structure prevents overfitting despite 99% missing data
- Learned $\beta_{\text{env}} = 2.0$ (strongest) reveals market fragmentation

Out-of-Sample Predictions: GSR



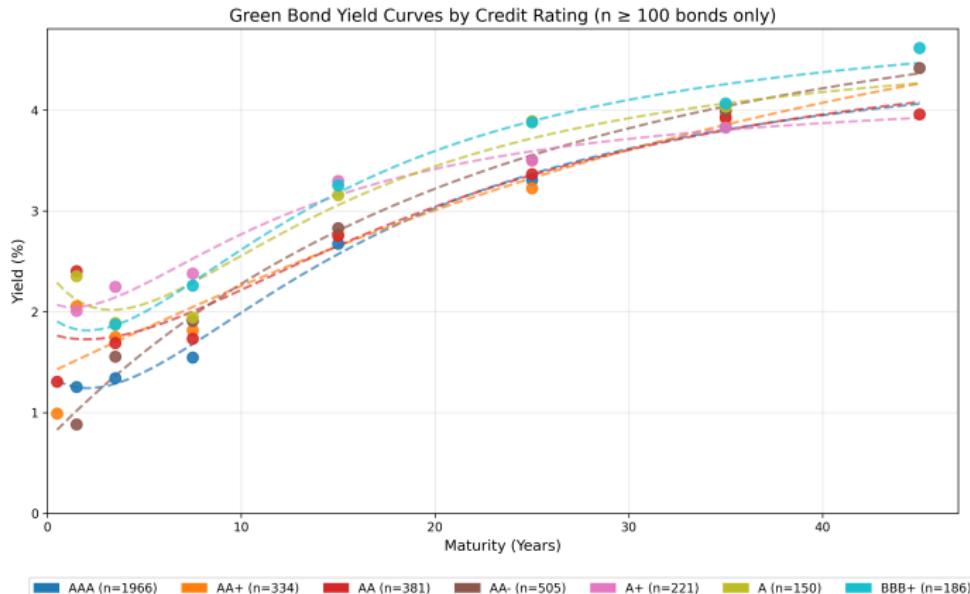
GSR predictions (orange) vs actual yields (blue) for 9 test bonds. Shaded regions show $\pm 2\sigma$ uncertainty. Model captures both levels and dynamics despite never seeing these bonds.

Out-of-Sample Predictions: KGR



KGR predictions (green) incorporate macroeconomic covariates. Better captures sharp market movements (2022 Fed rate hikes). Uncertainty bands adapt to changing conditions.

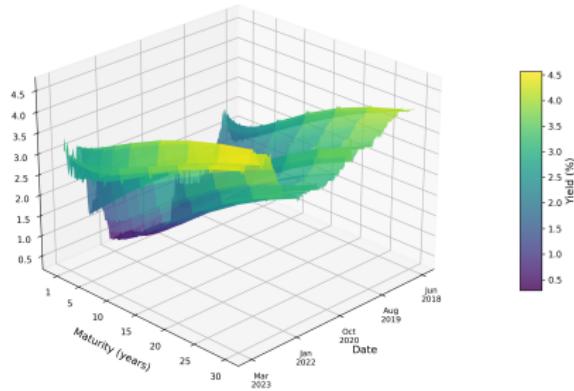
Nelson-Siegel: Fitted Yield Curves



Yield curves by credit rating (ratings with $n \geq 100$ bonds). Dashed lines = NS fit; points = observed averages. Enables yield interpolation at **any** maturity.

Yield Surface Dynamics

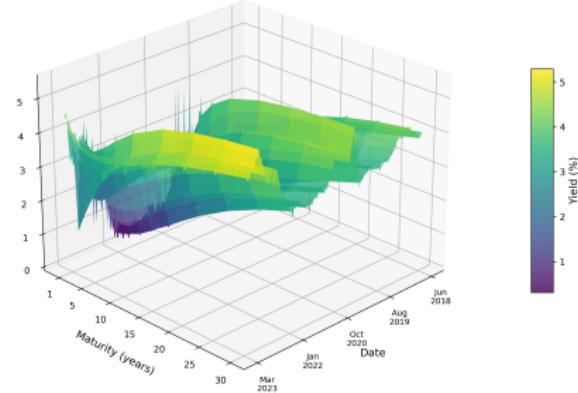
Reconstructed Yield Surface: AAA Rated Bonds
Nelson-Siegel on Fixed Tenor Grid (Jun 2018 - Mar 2023)



AAA-rated bonds

Time evolution of yield curves. COVID decline (March 2020), Fed rate hikes (2022). BBB+ shows higher levels and greater volatility than AAA.

Reconstructed Yield Surface: BBB+ Rated Bonds
Nelson-Siegel on Fixed Tenor Grid (Jun 2018 - Mar 2023)



BBB+ rated bonds

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- **Problem:** 99% missing data in high-dimensional bond market
- **Solution:** Graph-regularized learning with validated structure
 - Isotropy tests confirm smoothness ($p < 0.001$)
 - Credit chains, maturity sequences, environmental hierarchies
- **Results:** $R^2 = 0.82$ vs 0.72 for Ridge/Lasso (**36% error reduction**)
- **Practical workflow:** GSR → Nelson-Siegel → actionable yield curves
- **Extensions:** Corporate bonds, MBS, private equity, real estate

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