Machine Learning Journal Club: Open Learning for Open Science

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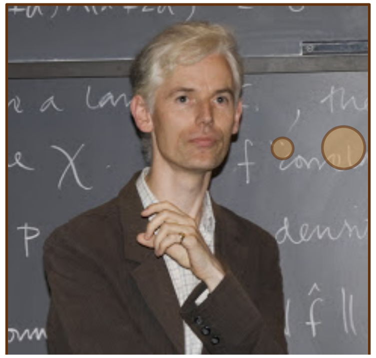
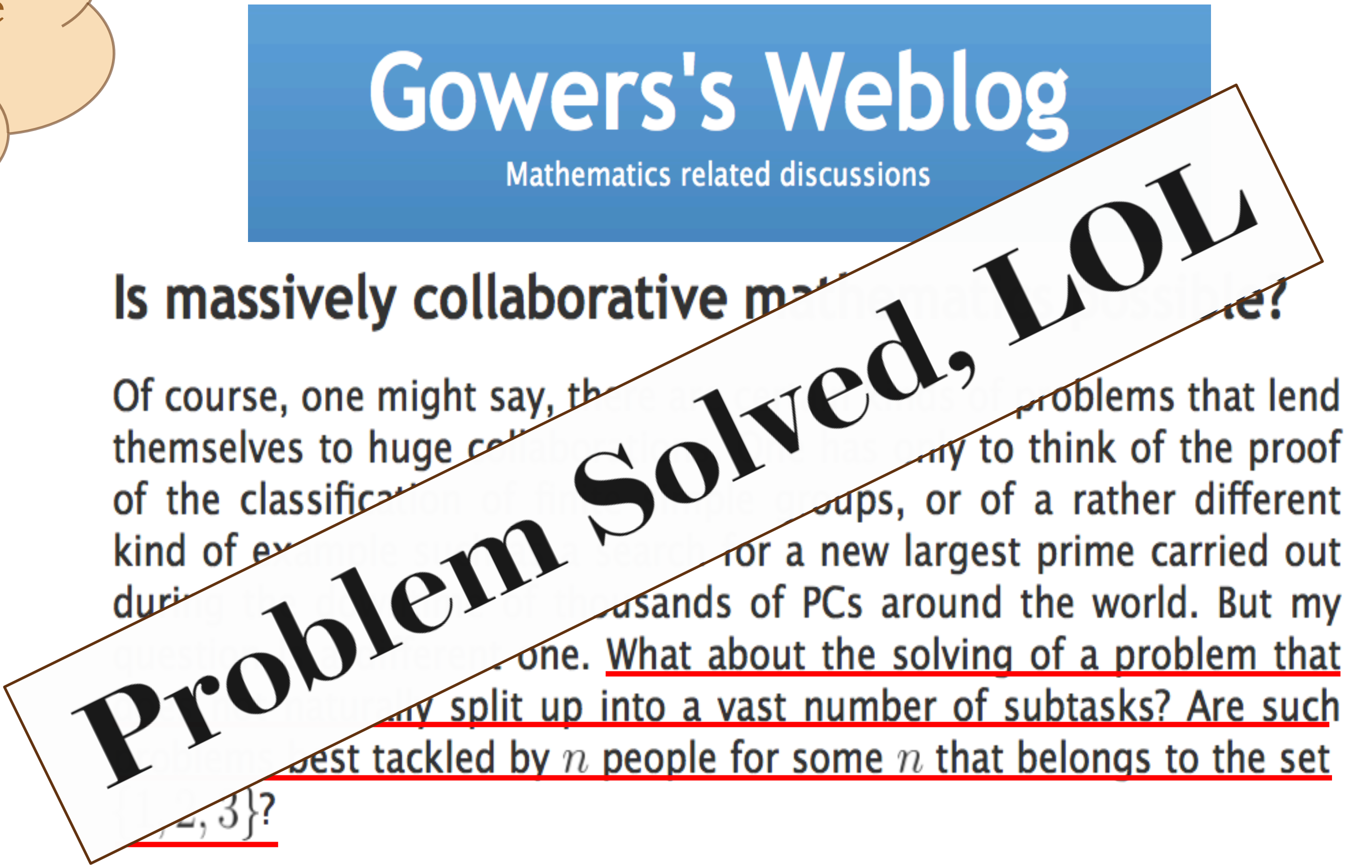
Open Science: is Polymath Project a New Paradigm?

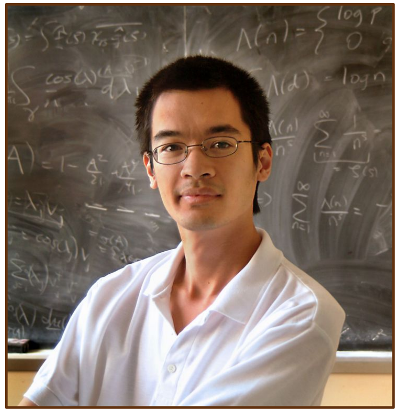
Tim Gowers



Is massively collaborative mathematics possible?



Terence Tao



https://www.scientificamerican.com/article/problem-solved-lol/

MLJC: a Contribution to Open Science

MLJC as a learning experience: **Machine Learners**

- Python for Scientific Computing

NumPy pandas $y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$ matplotlib

- Hands On Machine & Deep Learning

Keras PyTorch TensorFlow 2.0

GitHub

Focusing

Machine Learning Journal Club Unito

MLJCUnito

MLJC: a Contribution to Open Science

MLJC as a research experience: **Social Resistance**

A **"quantitative"** way to understand and explain reality when **Fake** and **Real** seem to be mixed up

DeepFakes

FakeNews

Fake News Detection on Social Media using Geometric Deep Learning

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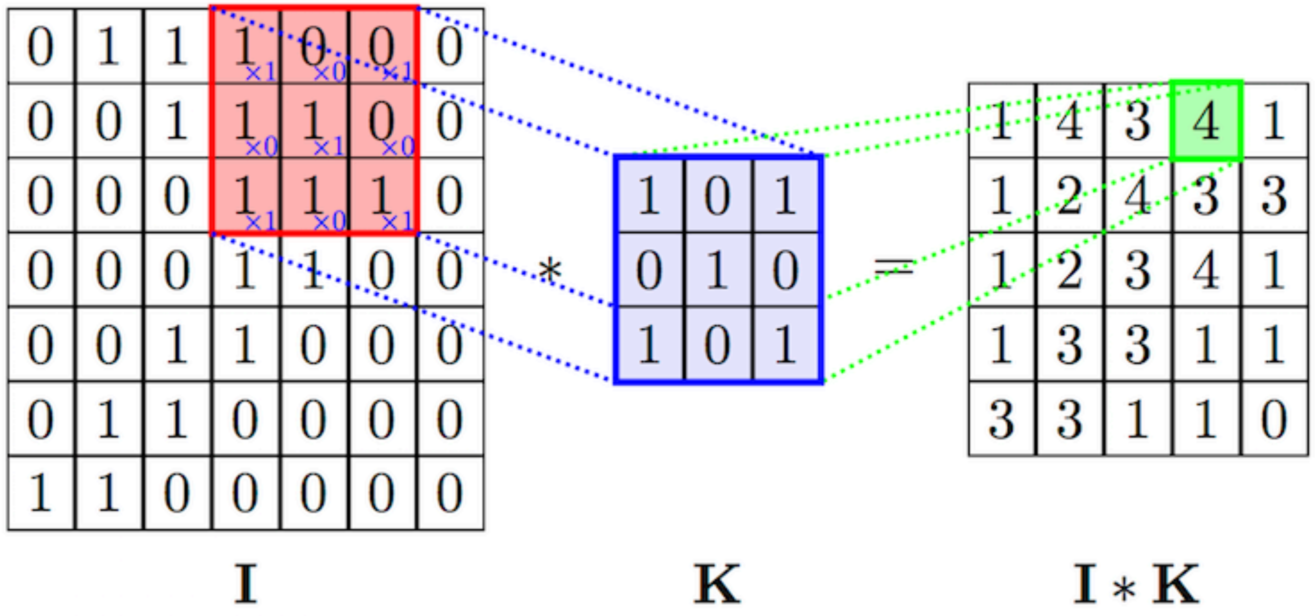
United Kingdom

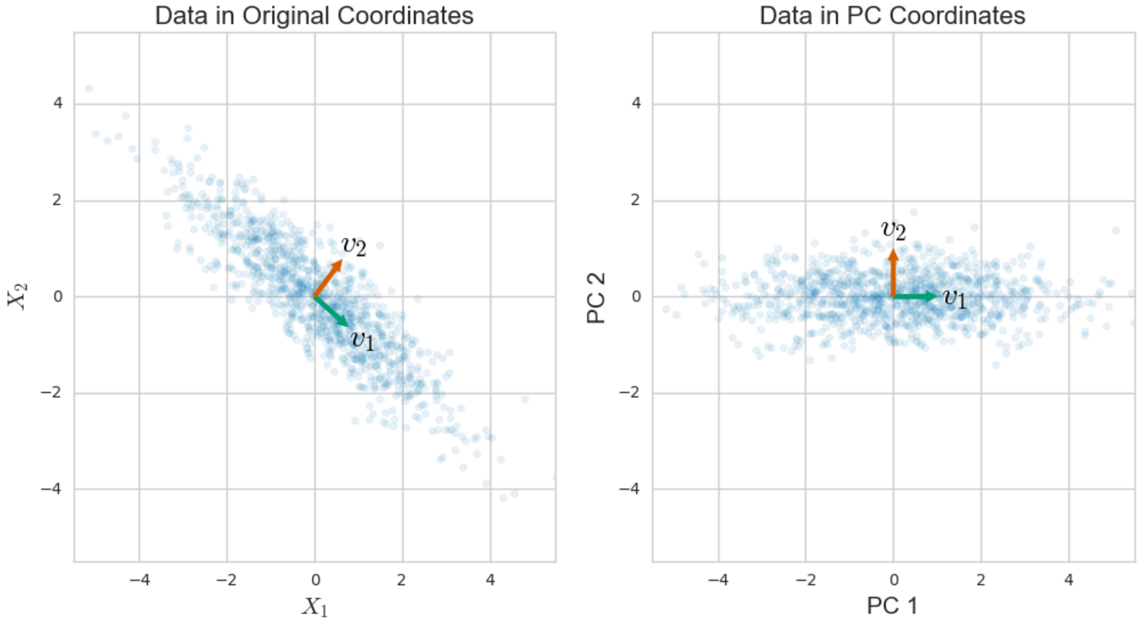
Geometric Priors in ML

In ML there is an ubiquitous **prior** :
data and models are always embedded in a **Euclidean space**

Convolutional **N**eural **N**etworks (**CNN**)



Principal **C**omponent **A**nalysis (**PCA**)



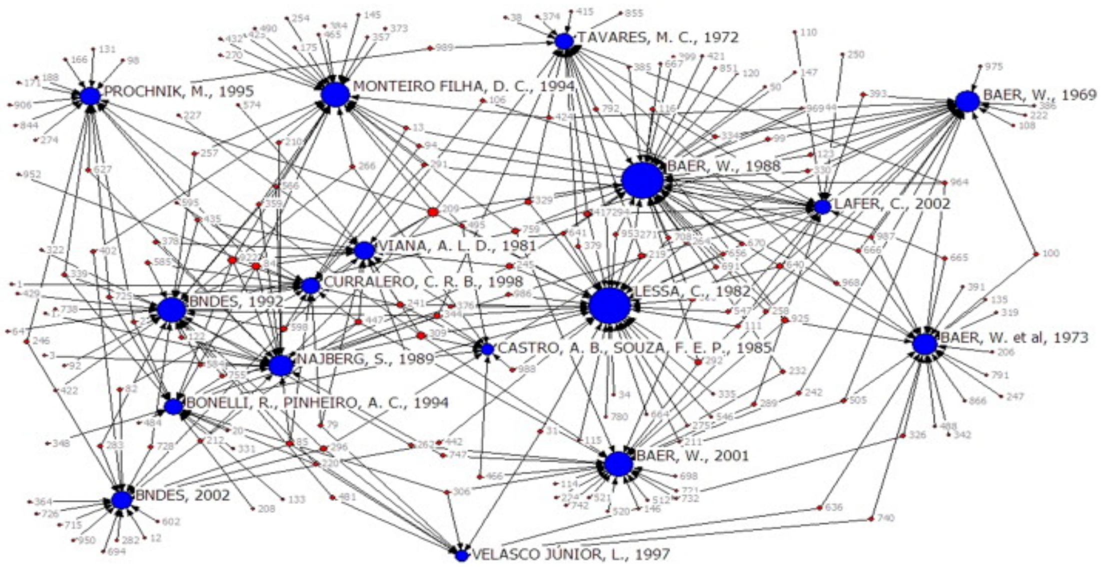
Non Euclidean Data: Graphs

Why?
A lot of real data can be represented or are embedded in structures like **Manifolds** or **Graphs**

$$\mathcal{G} = (\mathcal{V}, \mathcal{E}) \qquad \mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$$

$$|\mathcal{V}| = N \quad |\mathcal{E}| = L \leq N^2$$

Can we define **Convolution** on such objects?



Nodes state

$$a = (a_1, ..., a_N) \in \mathbb{R}^N$$

Links state

$$W = W^T$$

$$W \in \mathbb{R}^{N \times N}$$

Some Definitions

We can define **Hilbert Spaces** by introducing inner products of Graph functions

$$\langle f, g \rangle_{L^2(\mathcal{V})} = \sum_{i \in \mathcal{V}} a_i f_i g_i$$

$$\langle F, G \rangle_{L^2(\mathcal{E})} = \sum_{(i,j) \in \mathcal{E}} w_{i,j} F_{i,j} G_{i,j}$$

In the same way, **operators** on such spaces

$$\nabla : L^2(\mathcal{V}) \longrightarrow L^2(\mathcal{E}) \quad (\nabla f)_{i,j} = f_i - f_j$$

$$div : L^2(\mathcal{E}) \longrightarrow L^2(\mathcal{V}) \quad (div F)_i = \frac{1}{a_i} \sum_{(i,j) \in \mathcal{E}} w_{i,j} F_{i,j}$$

Some Definitions II

We can write the **Laplace operator** and it's equation in matrix form

$$div \circ \nabla = (\Delta f)_i = \frac{1}{a_i} \sum_{(i,j)\in\mathcal{E}} w_{i,j}(f_i - f_j)$$

$$\Delta f = A^{-1}(D - W)f$$

$$A = diag(a_1, \ldots, a_N) \qquad D = diag(\sum_{j:j\neq i} w_{i,j})$$

Solving Laplace Problem on Graphs

It is possible to solve the **Laplace eigenproblem** as an optimization problem :

$$\Delta \phi_i = \lambda \phi_i$$

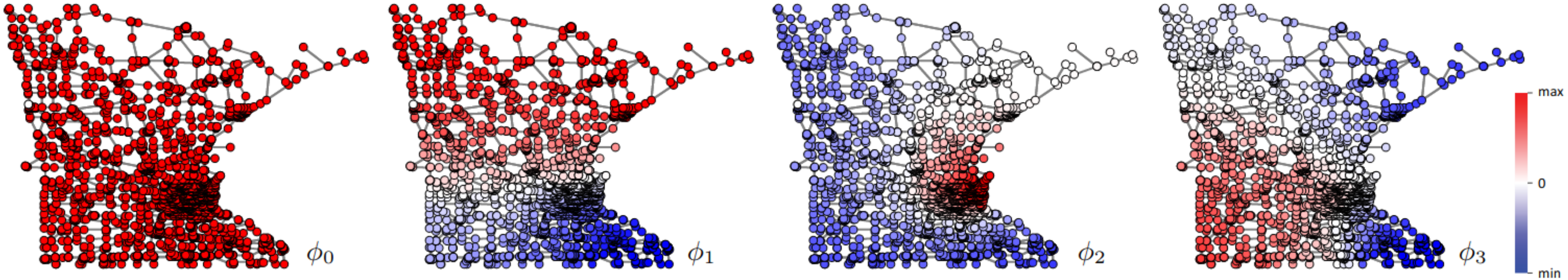
$$\min_{\phi_i :\ \|\phi_i\|=1} \{\mathcal{E}_{Dir}(\phi_i)\}$$

$$\mathcal{E}_{Dir} = \langle \phi, \Delta \phi \rangle_{L^2(\mathcal{V})}$$

$$\phi_i \perp span(\phi_0, ..., \phi_{i-1})$$

M.Bronstein et al, IEEE SIC PROG MAG (2016)

First four Minnesota road graph eigenfunctions



Convolution on Graphs

And use these results to design **CNN**s that work on graphs

$$g_\theta * x = \Phi g_\theta \Phi^T x \approx \sum_{k=0}^{K} \theta'_k T_k(\Delta)$$

Spectral Convolutional Layer (1st order approx.)

$$H^{(l+1)}(g_\theta * H^{(l)}) = \sigma\left(\tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2}H^{(l)}\Theta\right)$$

e.g. Zachary's
Karate Club