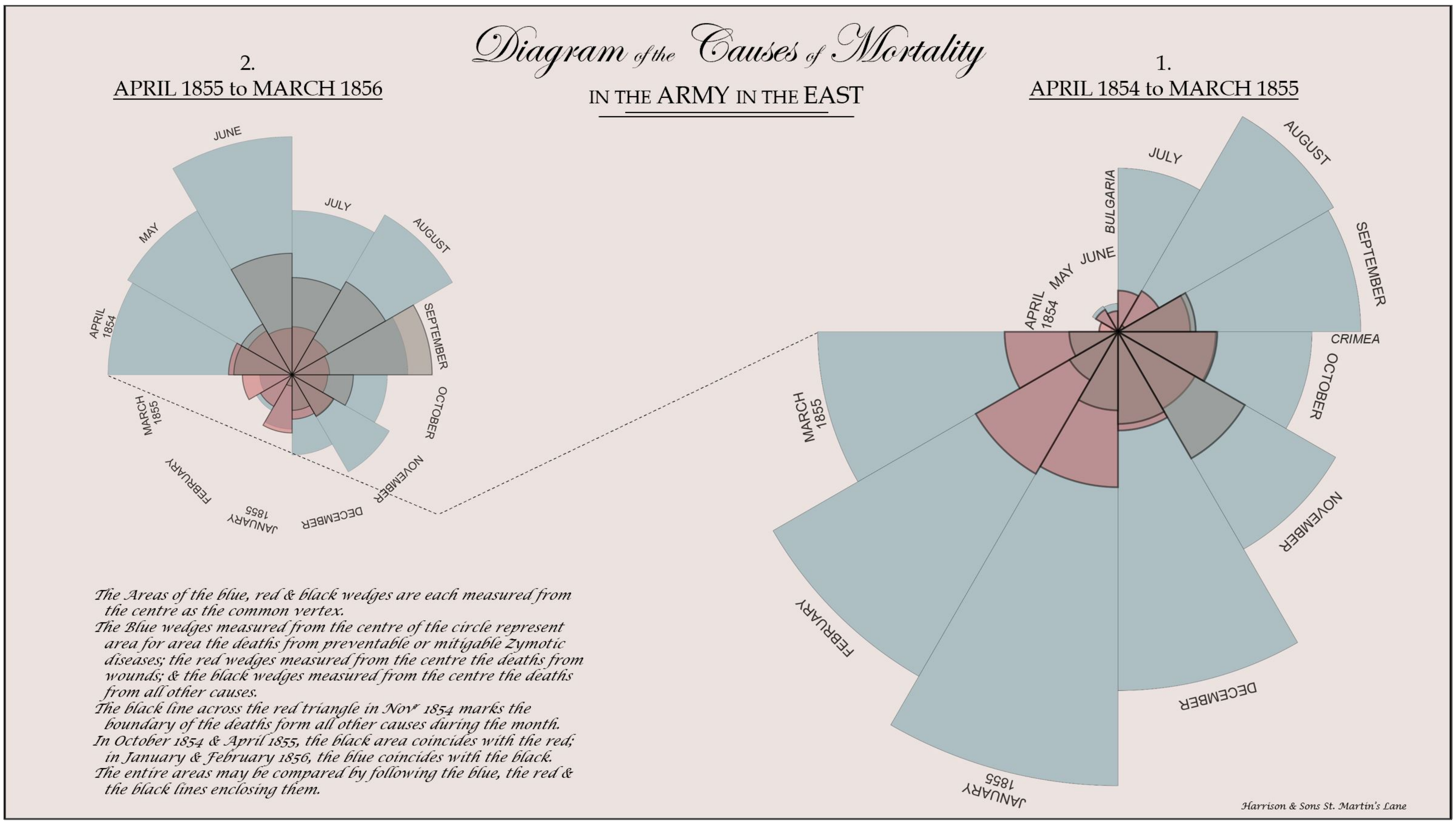
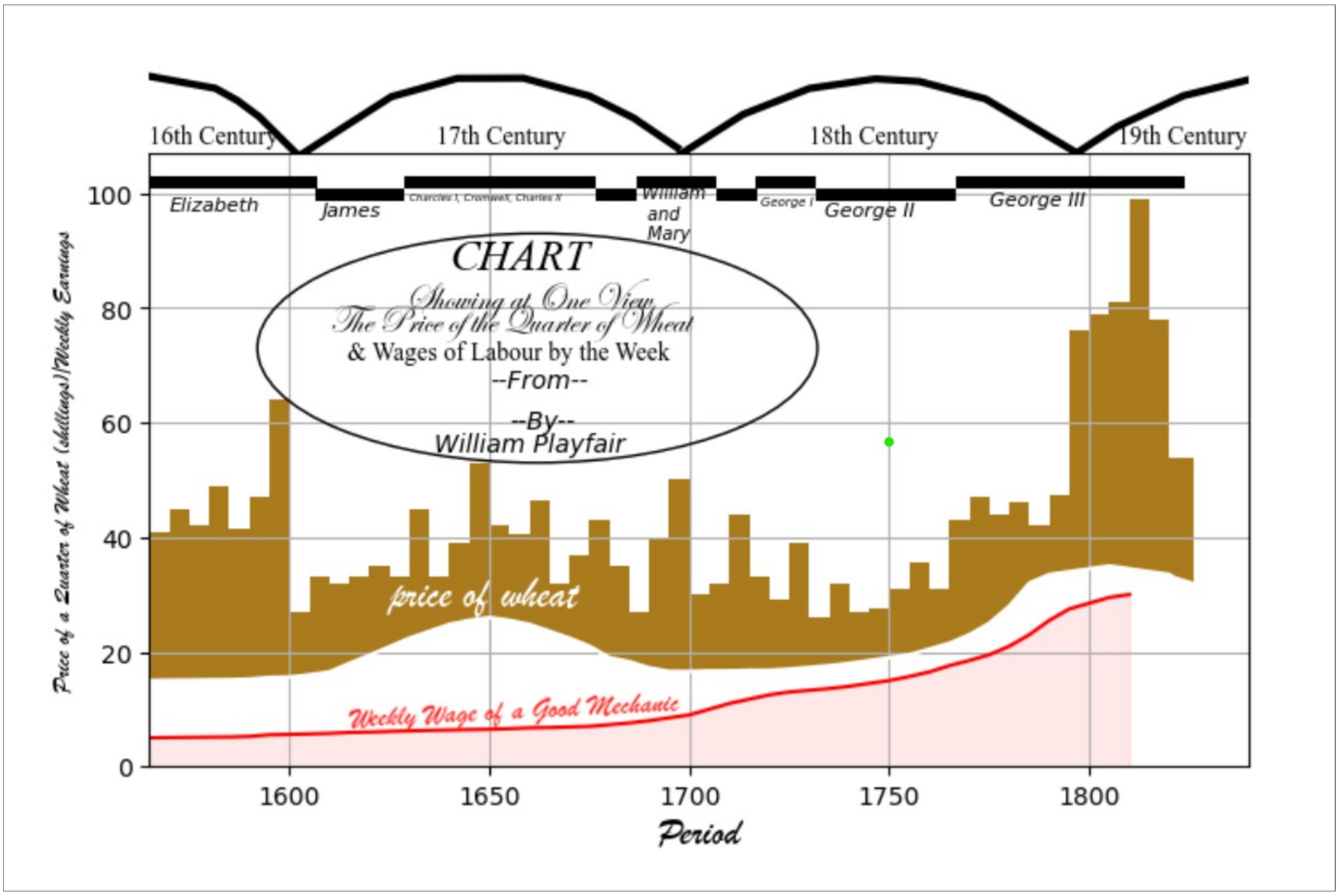
Lecture 12: Manifolds, Dimensionality Reduction

Historical Timeseries: Ryan McNeil



Historical Timeseries: Paul Ayamah



Historical Timeseries: Neh Majmudar

Historical Timeseries: Sean Sudol

Historical Timeseries: Giacomo Radaelli

Historical Timeseries: Joshua Rollins

Historical Timeseries: Jordan Matuszewski

Historical Timeseries: Garima Goyal

Manifold Learning

1. set with notion of nearness
2. a set of subsets whose union is the entire thing
3. indistinguishable with the tools of topology

Manifolds

Formal Definition

A topological space[1] is a manifold if it can be equipped with an **atlas**: a cover[2] where each element of the cover is homeomorphic[3] to (an open subset of) $\mathbb{R}^n$.

Intuitive Description

A shape is a manifold if it has the same dimension everywhere and neither self-intersections, nor boundaries, nor other kinds of pathological behavior.

Manifolds are a particular way of defining what it means for a shape to be nice in a theoretical sense

The Manifold Hypothesis

Geometric/Topological machine learning and data science operate under the **manifold hypothesis**: an assumption that data typically lies on (or near) a relatively low-dimensional manifold embedded in a higher-dimensional ambient space.

Example: Linear Regression assumes data lies near a hyperplane.

If we can shift from **ambient dimension** to **intrinsic dimension** it may be a lot easier to work with the data.

For visualization purposes, it would be best to get down to the range of 2-5 actually relevant dimensions, to limit the number of visual channels we need to use.

Dimensionality Reduction

Dealing with high-dimensional data

A selection of Dimensionality Reduction methods

PCA - Principal Component Analysis
: Use **eigenvectors of the sample covariance matrix** of the data to find a linear change of basis that **concentrates variability** into a few basis vectors.

MDS - Multi-Dimensional Scaling
: Use optimization of a **stress value** (sum-of-squares of differences between distances before projecting and distances after projecting) to find a map as close to **isometric** as possible.

Random Projection
: Create a random projection matrix by generating a set of orthonormal random vectors and multiply data matrix with the projection matrix.

: **Johnson-Lindenstrauss Lemma:** If your target dimension is $d > 8\log(N)/\epsilon^2$, then there is some map f whose squared norm distortion is no more than ϵ.

Time to read

Divide into three groups.
Each group picks one (a different one) of:

- Isomap: Tenenbaum, de Silva, Langford, A global geometric framework for nonlinear dimensionality reduction, Science 290 (2000) pp 2319-2323. **http://doi.org/10.1126/science.290.5500.2319**
- t-SNE: van der Maaten, Hinton, Visualizing data using t-SNE, JMLR, 9 (2008) pp 2579-2605 **http://jmlr.org/papers/volume9/vandermaaten08a/vandermaaten08a.pdf**
- UMAP: McInnes, Healy, Melville, Uniform manifold approximation and projection for dimension reduction, arXiv:1802.03426 **https://arxiv.org/pdf/1802.03426.pdf**

1. Everyone reads their article alone.
2. Discuss within your article group. Make sure everyone in your group understand the method and what distinguishes it.
3. Divide into groups of 3 (one from each group) and explain your paper to the other 2.

Dimensionality Reduction in Action

From a database (collected by van Hateren) of naturally occurring images, draw 3x3 pixel patches at random.
Most such pixel patches will be almost constant - discard those.
D Mumford et al. used PCA to identify a **primary circle** of high density in this data.
Turns out to trace linear gradients in different orientations.
G Carlsson et al. used Topological Data Analysis to study the high-density structure more carefully. They identify a high-density **Klein bottle** in the data, with a direct correspondence to quadratic gradients (ridges and valleys) in different orientations.

Homework

Read **https://handsondataviz.org/how-to-lie-with-charts.html**