# Big Data and Open Data Science

Neil D. Lawrence

UCLID Workshop

2nd July 2014

#### data

 data: observations, could be actively or passively acquired (meta-data).

data +

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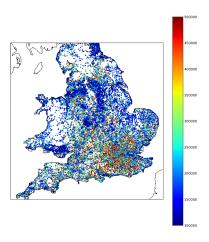
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- model: assumptions, based on previous experience (other data! transfer learning etc), or beliefs about the regularities of the universe. Inductive bias.

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- prediction: an action to be taken or a categorization or a quality score.

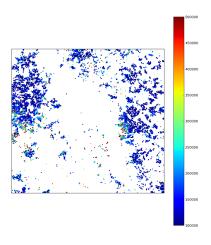
# Nonparametrics for Very Large Data Sets

## Modern data availability



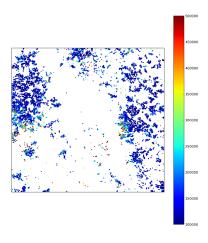
# Nonparametrics for Very Large Data Sets

Proxy for index of deprivation?



# Nonparametrics for Very Large Data Sets

Actually index of deprivation is a proxy for this ...





## Hensman et al. (2013)

#### Gaussian Processes for Big Data

#### James Hensman\*

Dept. Computer Science The University of Sheffield Sheffield, UK

#### Nicolò Fusi\*

Dept. Computer Science The University of Sheffield Sheffield, UK

#### Neil D. Lawrence\*

Dept. Computer Science The University of Sheffield Sheffield, UK

#### Abstract

We introduce stochastic variational inference for Gaussian process models. This enables the application of Gaussian process (GP) models to data sets containing millions of data points. We show how GPs can be varistically decomposed to depend on a set Even to accommodate these data sets, various approximate techniques are required. One approach is to partition the data set into separate groups [e.g. Snelson and Ghahramani, 2007, Urtasun and Darrell, 2008]. An alternative is to build a low rank approximation to the covariance matrix based around 'inducing variables' [see e.g. Csató and Opper, 2002, Seeger et al., 2003. Oniinopero Candela and Rasmussen, 2005. Title



### Hensman et al. (2013)

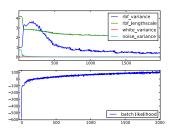


Figure 4: Convergence of the SVIGP algorithm on the two dimensional toy data

land-registry-monthly-price-paid-data/, which covers England and Wales, and filtered for apartments. This resulted in a data set with 75,000 entries,

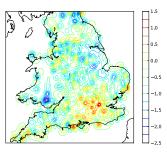


Figure 5: Variability of apartment price (logarithmically!) throughout England and Wales.

ted a CD with the same accordance function as our

# What's Changed (Changing) for Medical Data?

► Try Googling for: "patient data "...



Image from Wikimedia Commons



Image from Wikimedia Commons





# A brief history of Registration

For more information go to: www.direct.gov.uk/motoring

#### A brief history of registration

#### The early days

Prior to the appearance of the first railways in Britain, there was a brief development and interest in steam powered road going vehicles. In 1834, a Mr Hancock started a steam coach called the "Era", carrying up to 14 passengers from Paddington to Regents Park and the City at 6d a head. And in the following year, a Mr Church built an omnibus capable of carrying 40 passengers for

the London and Birmingham Steam Carriage Company.

However, the success of the railway movement drove all such traffic off the roads.

A Parliamentary Commission of Enquiry in 1836 reported "strongly in favour of steam carriages on roads", but subsequent Acts of Parliament tended to have a discouraging and restrictive effect. The Locomotive Act 1861 limited the weight of steam engines to 12 tons and imposed a speed limit of 10 mph.

The Locomotive Act 1865 set a speed limit of 4 mph in the country and 2 mph in towns. The 1865 Act also provided for the famous "man with a red flag". Walking 60 yards ahead

The 1865 Act also provided for the famous "man with a red flag". Walking 60 yards ahead of each vehicle, a man with a red flag or lantern enforced a walking pace, and warned horse riders and horse drawn traffic of the approach of a self propelled machine.

The Locomotive Amendment Act 1878 made the red flag optional under local regulations, and

[Grown Copyright Reserved.]



Ministry of Transport.

## THE

## HIGHWAY CODE

Issued by the Minister of Transport with the authority of Parliament in pursuance of Section 45 of the Road Traffic Act, 1930.

#### LONDON:

PRINTED AND FUBLISHED IN VIEW MAJESTYPES STATIONERY OFFICE To be pushed distorth from I.M. Stating Older at the Johnshine address Adderstrained Station I.M. Stating Older at the Johnshine address York S. eet, Manchester; v. St. Andrew's Crescent, Cardiff; 5, Donesult Square West, Belfant; or through any Booksider.

1931.

Price 1d. net.

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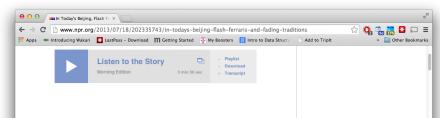
#### Image from Wikimedia Commons

## What are the Issues?

- ▶ Who owns our data?
- ► Is it 'finders keepers'?
- ► Does ownership proliferate?
- What does data protection offer?
- Who has the right to share our data?
- Can we withdraw this right?

# Moral Panics: Perhaps Rightly







road in Beijing, on April 7, 2011.

Before it became China's capital in 1949, Beijing was a fairly provincial little city of 2 million people.



Image from Wikimedia Commons

# What's Changed (Changing) for Medical Data?

- Genotyping.
- ► Epigenotyping.
- ► Transcriptome: detailed characterization of phenotype.
  - Stratification of patients.
- Massive unstructured data sources.

# Open Data

- Automatic data curation: from curated data to curation of publicly available data.
- ► Open Data: http://www.openstreetmap.org/?lat=53. 38086&lon=-1.48545&zoom=17&layers=M.

# Open Data

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# Open Data

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► Social network data, music information (Spotify), exercise.

# UK Government Stipulation on Data Availability



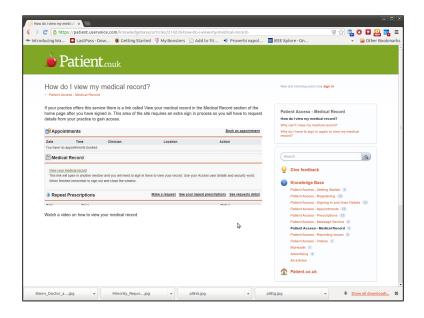
# Patient Online: Roadmap



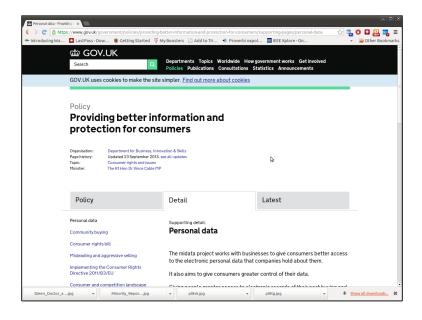
# **PULSE Report**



## **EMIS Patient Access**



## midata project

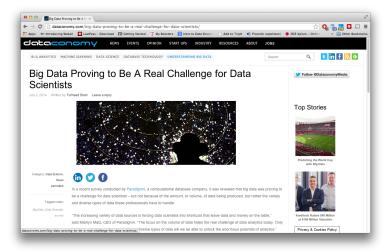


## Outline

Data Heterogenity

Deep Learning

# Not the Scale it's the Diversity



# Massive Missing Data

- ► If missing at random it can be marginalized.
- ► As data sets become very large (39 million in EMIS) data becomes extremely sparse.
- ► Imputation becomes impractical.

# Missing Data

- ► If missing at random it can be marginalized.
- ► As data sets become very large (39 million in EMIS) data becomes extremely sparse.
- ► Imputation becomes impractical.

# **Imputation**

- Expectation Maximization (EM) is gold standard imputation algorithm.
- ► Exact EM optimizes the log likelihood.
- Approximate EM optimizes a lower bound on log likelihood.
  - e.g. variational approximations (VIBES, Infer.net).
- Convergence is guaranteed to a local maxima in log likelihood.

# **Expectation Maximization**

Require: An initial guess for missing data

**Require:** An initial guess for missing data repeat

Require: An initial guess for missing data repeat

Update model parameters

(M-step)

Require: An initial guess for missing data repeat

Update model parameters
Update guess of missing data

(M-step) (E-step)

```
Require: An initial guess for missing data
  repeat
     Update model parameters
```

Update guess of missing data

until convergence

(M-step) (E-step)

### Imputation is Impractical

- ► In very sparse data imputation is impractical.
- ► EMIS: 39 million patients, thousands of tests.
- ► For most people, most tests are missing.
- ► M-step becomes confused by poor imputation.

### Direct Marginalization is the Answer

Perhaps we need joint distribution of two test outcomes,

$$p(y_1, y_2)$$

Obtained through marginalizing over all missing data,

$$p(y_1, y_2) = \int p(y_1, y_2, y_3, \dots, y_p) dy_3, \dots dy_p$$

- ▶ Where  $y_3, ..., y_p$  contains:
  - 1. all tests not applied to this patient
  - 2. all tests not yet invented!!

# Magical Marginalization in Gaussians

#### **Multi-variate Gaussians**

- ► Given 10 dimensional multivariate Gaussian,  $\mathbf{y} \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$ .
- ► Generate a single correlated sample  $\mathbf{y} = [y_1, y_2 \dots y_{10}].$
- ▶ How do we find the marginal distribution of  $y_1, y_2$ ?

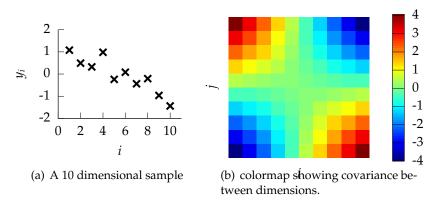


Figure : A sample from a 10 dimensional correlated Gaussian distribution.

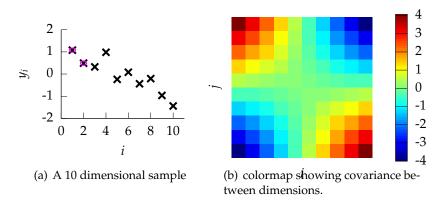


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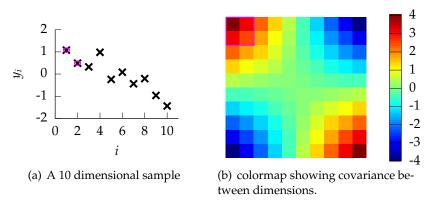


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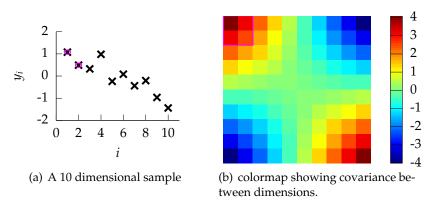


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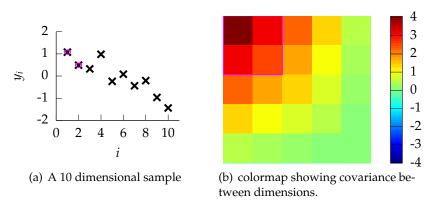


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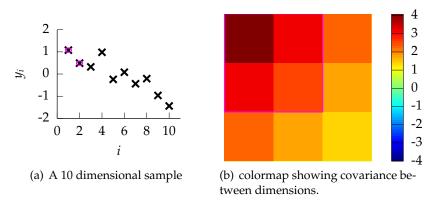


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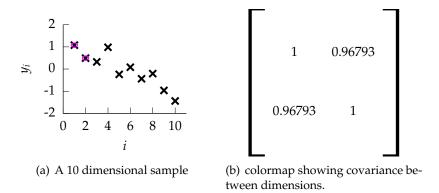


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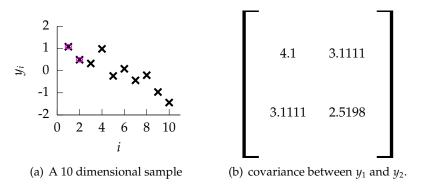


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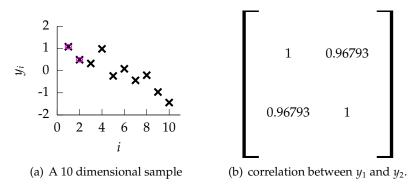


Figure : A sample from a 10 dimensional correlated Gaussian distribution.

### Avoid Imputation: Marginalize Directly



- ► Our approach: Avoid Imputation, Marginalize Directly.
- Explored in context of Collaborative Filtering.
- Similar challenges:
  - many users (patients),
  - many items (tests),
  - sparse data
- ► Implicitly marginalizes over all future tests too.

Work with Raquel Urtasun (Lawrence and Urtasun, 2009) and recent submission with Nicoló Fusi.

### Methods that Interrelate Covariates

- Need Class of models that interrelates data.
- Common assumption: high dimensional data lies on low dimensional manifold.
- Want to retain the marginalization property of Gaussians but deal with non-Gaussian data!

### Linear Dimensionality Reduction

#### Linear Latent Variable Model

- ► Represent data, **Y**, with a lower dimensional set of latent variables **X**.
- ► Assume a linear relationship of the form

$$\mathbf{y}_{i,:} = \mathbf{W}\mathbf{x}_{i,:} + \boldsymbol{\epsilon}_{i,:},$$

where

$$\epsilon_{i,:} \sim \mathcal{N}\left(\mathbf{0}, \sigma^2 \mathbf{I}\right).$$

#### Linear Latent Variable Model II

Probabilistic PCA Max. Likelihood Soln (Tipping and Bishop, 1999)



$$p(\mathbf{Y}|\mathbf{W}) = \prod_{i=1}^{n} \mathcal{N}(\mathbf{y}_{i,:}|\mathbf{0}, \mathbf{W}\mathbf{W}^{\top} + \sigma^{2}\mathbf{I})$$

### Linear Latent Variable Model II

Probabilistic PCA Max. Likelihood Soln (Tipping and Bishop, 1999)

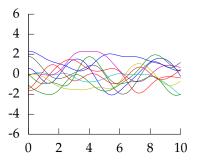
$$p(\mathbf{Y}|\mathbf{W}) = \prod_{i=1}^{n} \mathcal{N}(\mathbf{y}_{i,:}|\mathbf{0},\mathbf{C}), \quad \mathbf{C} = \mathbf{W}\mathbf{W}^{\top} + \sigma^{2}\mathbf{I}$$

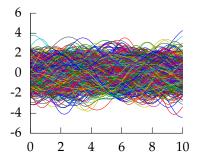
$$\log p(\mathbf{Y}|\mathbf{W}) = -\frac{n}{2}\log|\mathbf{C}| - \frac{1}{2}\operatorname{tr}\left(\mathbf{C}^{-1}\mathbf{Y}^{\mathsf{T}}\mathbf{Y}\right) + \operatorname{const.}$$

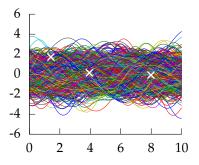
If  $\mathbf{U}_q$  are first q principal eigenvectors of  $n^{-1}\mathbf{Y}^{\top}\mathbf{Y}$  and the corresponding eigenvalues are  $\mathbf{\Lambda}_q$ ,

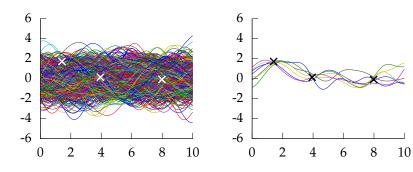
$$\mathbf{W} = \mathbf{U}_q \mathbf{L} \mathbf{R}^{\mathsf{T}}, \quad \mathbf{L} = \left(\mathbf{\Lambda}_q - \sigma^2 \mathbf{I}\right)^{\frac{1}{2}}$$

where **R** is an arbitrary rotation matrix.









## Dealing with Non Gaussian Data

- Marginalization property of Gaussians very attractive.
- ► How to incorporate non-Gaussian data?
  - Data which isn't missing at random.
  - Binary data.
  - Ordinal categorical data.
  - ▶ Poisson counts.
  - Outliers.

### Project Back into Gaussian

- Combine non-Gaussian likelihood with Gaussian prior.
- ► Either:
  - Project back to Gaussian posterior that is nearest in KL sense.
  - Expectation propagation.
- Or:
  - Fit a locally valid Gaussian approximation.
  - Laplace Approximation.





Ongoing work with Ricardo Andrade Pacheco (EP) and Alan Saul (Laplace) also James Hensman.

#### Gaussian Noise

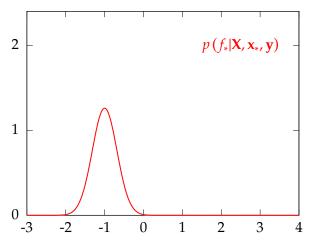


Figure: Inclusion of a data point with Gaussian noise.

#### Gaussian Noise

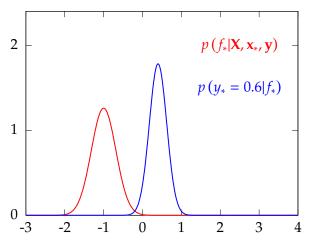


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#### Gaussian Noise

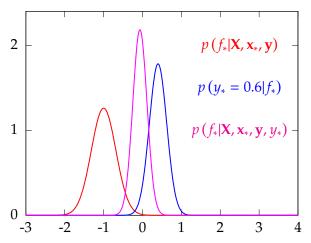


Figure: Inclusion of a data point with Gaussian noise.

### Classification Noise Model

Probit Noise Model

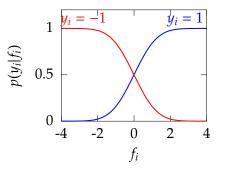


Figure : The probit model (classification). The plot shows  $p(y_i|f_i)$  for different values of  $y_i$ . For  $y_i = 1$  we have  $p(y_i|f_i) = \phi(f_i) = \int_{-\infty}^{f_i} \mathcal{N}(z|0,1) \, \mathrm{d}z$ .

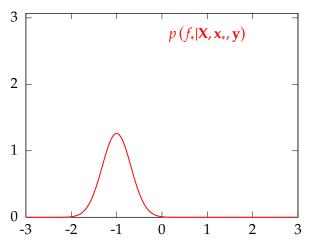


Figure : An EP style update with a classification noise model.

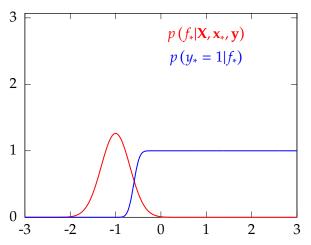


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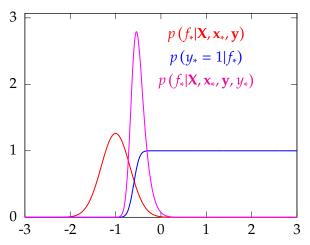


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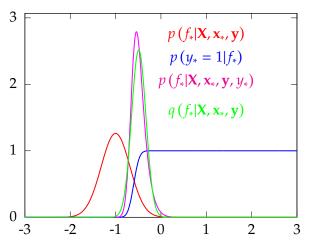


Figure : An EP style update with a classification noise model.

#### Ordinal Noise Model

#### **Ordered Categories**

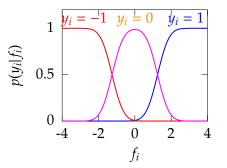


Figure : The ordered categorical noise model (ordinal regression). The plot shows  $p(y_i|f_i)$  for different values of  $y_i$ . Here we have assumed three categories.

## Other Challenges



 Spatial Data (workshops in November 2013 and January 2014with Peter Diggle, work with Ricardo Andrade Pacheco and John Quinn's group).

#### Survival Data



Survival Data (work with Alan Saul and Aki Vehtari's group and HeRC).

#### Other Data

- Image Data (work with Teo de Campos, Fariba Yousefi, Zhenwen Dai, GaussianFace)
- Text Data (long time planned collaboration with Trevor Cohn)

## Example: Prediction of Malaria Incidence in Uganda

- Work with John Quinn and Martin Mubaganzi (Makerere University, Uganda)
- ► See http://cit.mak.ac.ug/cs/aigroup/.

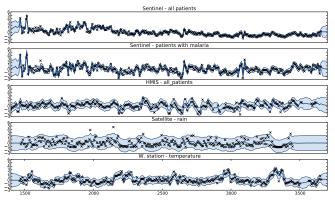
# Malaria Prediction in Uganda



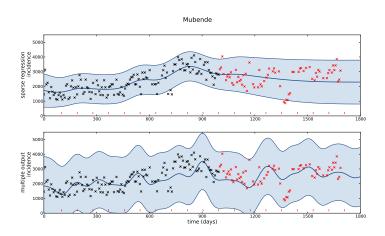


#### Malaria Prediction in Uganda





## Malaria Prediction in Uganda



# Visit to Uganda



#### Outline

Data Heterogenity

Deep Learning

direction for further research.

#### 11.1. HAVE WE THROWN THE BABY OUT WITH THE BATH WATER?

According to the hype of 1987, neural networks were meant to be intelligent models which discovered features and patterns in data. Gaussian processes in contrast are simply smoothing devices. How can Gaussian processes possibly replace neural networks? What is going on?

I think what the work of Williams and Rasmussen (1996) shows is that many real-world data modelling problems are perfectly well solved by sensible smoothing methods. The most interesting problems, the task of feature discovery for example, are not ones which Gaussian processes will solve. But maybe multilayer perceptrons can't solve them either. On the other hand, it may be that the limit of an infinite number of hidden units, to which Gaussian processes correspond, was a bad limit to take; maybe we should backtrack, or modify the prior on neural network parameters, so as to create new models more interesting than Gaussian processes. Evidence that this infinite limit has lost something compared with finite neural networks comes from the observation that in a finite neural network with more than one output, there are non-trivial correlations between the outputs (since they share inputs from common hidden units); but in the limit of an infinite number of hidden units, these correlations vanish. Radford Neal has suggested the use of non-Gaussian priors in networks with multiple hidden layers. Or perhaps a completely fresh start is needed, approaching the problem of machine learning from a paradigm different from the supervised feedforward mapping.

#### Structure of Priors

MacKay: NIPS Tutorial 1997 "Have we thrown out the baby with the bathwater?" (Published as MacKay, 1998) Also noted by (Wilson et al., 2012)







CI SHARE # 90 fr.

Mar 14, 2013 • 8:23 am | == (10) by Barry Schwartz [3] [5] | Filed Under Google Search Engine

page about it:

If I had to place one search priority above all else, I'd say right now. Google's most ambitious project is the

knowledge graph. Yea, they are pushing Google+ big time, but the knowledge graph is a level above all of that technically. Of course, Google has an outstanding team working on this project lead by one of the smartest people I've

ever met Amit Singhal. To take the knowledge graph to the next level, Google has hired/acquired Geoffrey Hinton and his team at DNNresearch. Geoffrey posted a note on his Google-



Last summer. I spent several months working with Google's Knowledge team in Mountain View, working with Jeff Dean and an incredible group of scientists and engineers who have a real shot at making spectacular progress in machine learning. Together with two of my recent graduate students, Ilya Sutskever and Alex Krizhevsky (who won the 2012 ImageNet competition). I am betting on Google's team to be the epicenter of future breakthroughs. That means we'll soon be joining Google to work with some of the smartest engineering minds to tackle some of the biggest challenges in computer science. I'll remain part-time at the University of Toronto, where I still have a lot of excellent graduate students, but at Google I will get to see what we can do with very large-scale computation.

I know we just scratched the surface of the knowledge graph and I am excited to see where it takes us in the future.

I am just glad I don't have to figure out how to get us there. I get to just sit and enjoy the ride.



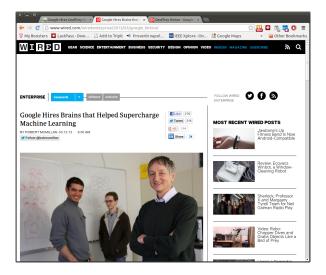
#### ROUNDTABLE SPONSORS

#### BROWSE BY-

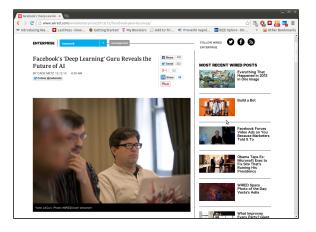
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- > Discover by Author
- > Scan Most Recent > See Comments
- > View Tag Cloud

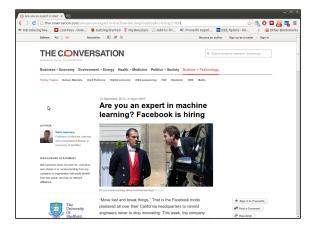
#### SEM FORUM THREADS

WebmasterWorld Forums









## Challenges for Companies

- ► Trying to dominate the modern interconnected data market (e.g. Amazon, Google, Facebook) buying up talent and competitors.
- or trying to exploit current 'data silos' (e.g. Tescos clubcard, Experian) — monetising our data today (limited shelf life?)
- or trying to understand their own systems (the internal google search)
- ▶ or new companies with new ideas that will generate data.

## Challenges for Companies

- ► How do they break the natural data monopoly?
- ► How do they access the necessary expertise?

## Challenges in Science

#### Data sharing is more widely accepted but:

- Most analysis is simple statistical tests or explorative modelling with PCA or clustering.
- ► Few scientists understand these methodologies, apply them as black box.
- ► There is an understanding gap between the data & scientist and the data scientist.

## Challenges in Health

- ► Ensure the privacy of patients is respected.
- ► Leverage the wide range of data available for wider societal benefit.

## International Development

- Exploit new telecommunications infrastructure to develop a leap-frog developed countries.
- Needs mechanisms for data sharing that retain the individual's control.
- Widespread education of *local* talent in code and model development.

#### Common Strands

- Improving access to data whilst balancing against individual's right to privacy against societal needs to advance.
- Advancing methodologies: development of methodologies needed to characterize large interconnected complex data sets.
- Analysis empowerment: giving scientists, clinicians, students, commercial and academic partners ability to analyze their own data with latest methodologies.

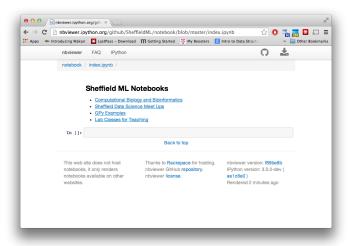
## Open Data Science: A Magic Bullet?

- Make new methodologies available as widely and rapidly as possible with as few conditions on their use as possible.
- Educate commercial, scientific and medical partners in use of these methodologies.
- Act to achieve a balance between data sharing for societal benefit and right of an individual to own their own data.

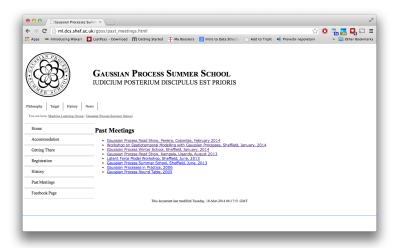
## **Achieving This**

- ▶ Use BSD-like licenses on software.
- ► Educate our partners (summer schools, courses etc).
- ► Act to achieve a balance between data sharing for societal benefit and rights of the individual.

#### Make Analysis Available

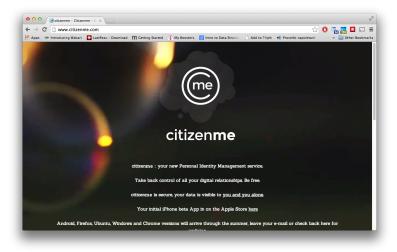


## Educating

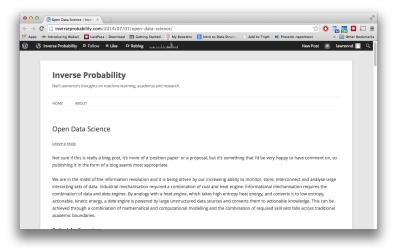


But we need to do much more! (Dan Cornford's User Groups)

## Digital Identity and Data Ownership



#### **Blog Post**



#### Summary

- ► The Challenges of Modern Big Data are Radically Different
- statistics + computer science = data science
- Need to change the way in which we do science.
- Major methodological difficulties, computational difficulties and accessibility difficulties.
- Open Data Science provides and Answer.

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