Machine Learning: Dynamics, Economics and Stochastics

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> > December 16, 2018

What Intelligent Systems Currently Exist?

• Brains and Minds



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Markets







Chapter 1: History and Perspective

Machine Learning (aka, AI) Successes

- First Generation ('90-'00): the backend
 - e.g., fraud detection, search, supply-chain management
- Second Generation ('00-'10): the human side
 e.g., recommendation systems, commerce, social media
- Third Generation ('10-now): pattern recognition
 - e.g., speech recognition, computer vision, translation
- Fourth Generation (emerging): decisions and markets
 - not just one agent making a decision or sequence of decisions
 - rather, a huge interconnected web of data, agents, decisions
 - many new challenges!

Perspectives on Al

- The classical "human-imitative" perspective
 - cf. AI in the movies, interactive home robotics
- The "intelligence augmentation" (IA) perspective
 - cf. search engines, recommendation systems, natural language translation
 - the system need not be intelligent itself, but it reveals patterns that humans can make use of
- The "intelligent infrastructure" (II) perspective
 - cf. transportation, intelligent dwellings, urban planning
 - large-scale, distributed collections of data flows and looselycoupled decisions

M. Jordan (2018), "Artificial Intelligence: The Revolution Hasn't Happened Yet", *Medium.*

Human-Imitative AI Isn't the Right Goal

- Problems studied from the "human-imitative" perspective aren't necessarily the same as those that arise in the IA or II perspectives
 - unfortunately, the "AI solutions" being deployed for the latter are often those developed in service of the former
- "Autonomy" shouldn't be our main goal; rather our goal should be the development of small intelligences that work well with each other and with humans
- To make an overall system behave intelligently, it is neither necessary or sufficient to make each component of the system be intelligent

Near-Term Challenges in II

- Error control for multiple decisions
- Systems that create markets
- Designing systems that can provide meaningful, calibrated notions of their uncertainty
- Achieving real-time performance goals
- Managing cloud-edge interactions
- Designing systems that can find abstractions quickly
- Provenance in systems that learn and predict
- Designing systems that can explain their decisions
- Finding causes and performing causal reasoning
- Systems that pursue long-term goals, and actively collect data in service of those goals
- Achieving fairness and diversity
- Robustness in the face of unexpected situations
- Robustness in the face of adversaries
- Sharing data among individuals and organizations
- Protecting privacy and issues of data ownership

Multiple Decisions: The Load-Balancing Problem

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 - those decisions often interact

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 - those decisions often interact
 - they interact when there is a scarcity of resources
- To manage scarcity of resources in large-scale decision making, "AI" isn't enough; we need concepts from market design

Classical Recommendation Systems

- A record is kept of each customer's purchases
- Customers are "similar" if they buy similar sets of items
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- In existing systems, recommendations are made independently
- That won't work in the real world!

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- Is it OK to recommend the same movie to everyone?

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- Is it OK to recommend the same stock purchase to everyone?
- Such problems are best approached via the creation of markets
 - restaurants bid on customers
 - street segments bid on drivers

The Consequences

- By creating a market based on the data flows, new jobs are created!
- So here's a way that AI can be a job creator, and not (mostly) a job killer
- This can be done in a wide range of other domains, not just music
 - entertainment
 - information services
 - personal services
 - etc

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Chapter 2: In the Engine Room

Algorithmic and Theoretical Progress

- Nonconvex optimization
 - avoidance of saddle points
 - rates that have dimension dependence
 - acceleration, dynamical systems and lower bounds
 - statistical guarantees from optimization guarantees
- Computationally-efficient sampling
 - nonconvex functions
 - nonreversible MCMC
 - links to optimization
- Market design
 - approach to saddle points
 - recommendations and two-way markets

Computation and Statistics

- A Grand Challenge of our era: tradeoffs between statistical inference and computation
 - most data analysis problems have a time budget
 - and often they're embedded in a control problem
- Optimization has provided the computational model for this effort (computer science, not so much)

it's provided the algorithms and the insight

- On the other hand, modern large-scale statistics has posed new challenges for optimization
 - millions of variables, millions of terms, sampling issues, nonconvexity, need for confidence intervals, parallel/distributed platforms, etc

Computation and Statistics (cont)

- Modern large-scale statistics has posed new challenges for optimization
 - millions of variables, millions of terms, sampling issues, nonconvexity, need for confidence intervals, parallel/distributed platforms, etc
- Current algorithmic focus: what can we do with the following ingredients?
 - gradients
 - stochastics
 - acceleration
- Current theoretical focus: placing lower bounds from statistics and optimization in contact with each other

Part I: How to Escape Saddle Points Efficiently

with Chi Jin, Praneeth Netrapalli, Rong Ge, and Sham Kakade









The Importance of Saddle Points



• How to escape?

- need to have a negative eigenvalue that's strictly negative

- How to escape efficiently?
 - in high dimensions how do we find the direction of escape?
 - should we expect exponential complexity in dimension?

Some Well-Behaved Nonconvex Problems

- PCA, CCA, Matrix Factorization
- Orthogonal Tensor Decomposition (Ge, Huang, Jin, Yang, 2015)
- Complete Dictionary Learning (Sun et al, 2015)
- Phase Retrieval (Sun et al, 2015)
- Matrix Sensing (Bhojanapalli et al, 2016; Park et al, 2016)
- Symmetric Matrix Completion (Ge et al, 2016)
- Matrix Sensing/Completion, Robust PCA (Ge, Jin, Zheng, 2017)
- The problems have no spurious local minima and all saddle points are strict

A Few Facts

- Gradient descent will asymptotically avoid saddle points (Lee, Simchowitz, Jordan & Recht, 2017)
- Gradient descent can take exponential time to escape saddle points (Du, Jin, Lee, Jordan, & Singh, 2017)
- Stochastic gradient descent can escape saddle points in polynomial time (Ge, Huang, Jin & Yuan, 2015)
 - but that's still not an explanation for its practical success
- Can we prove a stronger theorem?

Optimization

Consider problem:

$$\min_{\mathbf{x}\in\mathbb{R}^d} f(\mathbf{x})$$

Gradient Descent (GD):

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \eta \nabla f(\mathbf{x}_t).$$

Convex: converges to global minimum; dimension-free iterations.



Convergence to FOSP

Function $f(\cdot)$ is ℓ -smooth (or gradient Lipschitz)

$$\forall \mathbf{x}_1, \mathbf{x}_2, \ \|\nabla f(\mathbf{x}_1) - \nabla f(\mathbf{x}_2)\| \leq \ell \|\mathbf{x}_1 - \mathbf{x}_2\|.$$

Point **x** is an ϵ -first-order stationary point (ϵ -FOSP) if

 $\|\nabla f(\mathbf{x})\| \leq \epsilon$

Theorem [GD Converges to FOSP (Nesterov, 1998)] For ℓ -smooth function, GD with $\eta = 1/\ell$ finds ϵ -FOSP in iterations:

$$\frac{2\ell(f(\mathbf{x}_0) - f^\star)}{\epsilon^2}$$

*Number of iterations is dimension free.

Nonconvex Optimization

Non-convex: converges to Stationary Point (SP) $\nabla f(\mathbf{x}) = 0$.

SP : local min / local max / saddle points



Many applications: no spurious local min (see full list later).

Definitions and Algorithm

Function $f(\cdot)$ is ρ -Hessian Lipschitz if

$$\forall \mathbf{x}_1, \mathbf{x}_2, \ \|\nabla^2 f(\mathbf{x}_1) - \nabla^2 f(\mathbf{x}_2)\| \le \rho \|\mathbf{x}_1 - \mathbf{x}_2\|.$$

Point x is an ϵ -second-order stationary point (ϵ -SOSP) if

$$\|
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 and $\lambda_{\min}(
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Algorithm Perturbed Gradient Descent (PGD)

- **1**. for t = 0, 1, ... do
- 2. if perturbation condition holds then
- 3. $\mathbf{x}_t \leftarrow \mathbf{x}_t + \xi_t$, ξ_t uniformly $\sim \mathbb{B}_0(r)$

4.
$$\mathbf{x}_{t+1} \leftarrow \mathbf{x}_t - \eta \nabla f(\mathbf{x}_t)$$

Adds perturbation when $\|\nabla f(\mathbf{x}_t)\| \leq \epsilon$; no more than once per T steps.

Main Result

Theorem [PGD Converges to SOSP]

For ℓ -smooth and ρ -Hessian Lipschitz function f, PGD with $\eta = O(1/\ell)$ and proper choice of r, T w.h.p. finds ϵ -SOSP in iterations:

$$\tilde{O}\left(\frac{\ell(f(\mathbf{x}_0)-f^{\star})}{\epsilon^2}\right)$$

*Dimension dependence in iteration is $\log^4(d)$ (almost dimension free).
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	GD(Nesterov 1998)	PGD (This Work)
Assumptions	ℓ-grad-Lip	ℓ -grad-Lip + ρ -Hessian-Lip
Guarantees Iterations	ϵ -FOSP $2\ell(f(\mathbf{x}_0) - f^*)/\epsilon^2$	$ ilde{\epsilon}$ -SUSP $ ilde{O}(\ell(f(\mathbf{x}_0) - f^*)/\epsilon^2)$

Geometry and Dynamics around Saddle Points

Challenge: non-constant Hessian + large step size $\eta = O(1/\ell)$.

Around saddle point, **stuck region** forms a non-flat "pancake" shape.





Key Observation: although we don't know its shape, we know it's thin! (Based on an analysis of two nearly coupled sequences)

How Fast Can We Go?

- Important role of lower bounds (Nemirovski & Yudin)
 - strip away inessential aspects of the problem to reveal fundamentals
- The acceleration phenomenon (Nesterov)
 - achieve the lower bounds
 - second-order dynamics
 - a conceptual mystery
- Our perspective: it's essential to go to continuous time
 - the notion of "acceleration" requires a continuum topology to support it

Part II: Variational, Hamiltonian and Symplectic Perspectives on Acceleration

with Andre Wibisono, Ashia Wilson and Michael Betancourt







Accelerated gradient descent

Setting: Unconstrained convex optimization

 $\min_{x\in\mathbb{R}^d} f(x)$

Classical gradient descent:

$$x_{k+1} = x_k - \beta \nabla f(x_k)$$

obtains a convergence rate of O(1/k)

Accelerated gradient descent

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Accelerated gradient descent:

$$y_{k+1} = x_k - \beta \nabla f(x_k)$$

$$x_{k+1} = (1 - \lambda_k) y_{k+1} + \lambda_k y_k$$

obtains the (optimal) convergence rate of $O(1/k^2)$

Accelerated methods: Continuous time perspective

Gradient descent is discretization of gradient flow

 $\dot{X}_t = -\nabla f(X_t)$

(and mirror descent is discretization of natural gradient flow)

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 Su, Boyd, Candes '14: Continuous time limit of accelerated gradient descent is a second-order ODE

$$\ddot{X}_t + \frac{3}{t}\dot{X}_t + \nabla f(X_t) = 0$$

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These ODEs are obtained by taking continuous time limits. Is there a deeper generative mechanism?

Our work: A general variational approach to acceleration A systematic discretization methodology

Bregman Lagrangian

$$\mathcal{L}(x, \dot{x}, t) = e^{\gamma_t + \alpha_t} \left(D_h(x + e^{-\alpha_t} \dot{x}, x) - e^{\beta_t} f(x) \right)$$



Optimal curve is characterized by Euler-Lagrange equation:

$$\frac{d}{dt}\left\{\frac{\partial \mathcal{L}}{\partial \dot{x}}(X_t, \dot{X}_t, t)\right\} = \frac{\partial \mathcal{L}}{\partial x}(X_t, \dot{X}_t, t)$$

E-L equation for Bregman Lagrangian under ideal scaling:

$$\ddot{X}_t + (e^{\alpha_t} - \dot{\alpha}_t)\dot{X}_t + e^{2\alpha_t + \beta_t} \Big[\nabla^2 h(X_t + e^{-\alpha_t}\dot{X}_t)\Big]^{-1} \nabla f(X_t) = 0$$

Mysteries

- Why can't we discretize the dynamics when we are using exponentially fast clocks?
- What happens when we arrive at a clock speed that we can discretize?
- How do we discretize once it's possible?

Towards A Symplectic Perspective

- We've discussed discretization of Lagrangian-based dynamics
- Discretization of Lagrangian dynamics is often fragile and requires small step sizes
- We can build more robust solutions by taking a Legendre transform and considering a *Hamiltonian* formalism:

$$\begin{split} L(q,v,t) &\to H(q,p,t,\mathcal{E}) \\ \left(\frac{\mathrm{d}q}{\mathrm{d}t},\frac{\mathrm{d}v}{\mathrm{d}t}\right) &\to \left(\frac{\mathrm{d}q}{\mathrm{d}\tau},\frac{\mathrm{d}p}{\mathrm{d}\tau},\frac{\mathrm{d}t}{\mathrm{d}\tau},\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}\tau}\right) \end{split}$$

Symplectic Integration of Bregman Hamiltonian



Symplectic vs Nesterov



Symplectic vs Nesterov



Part III: Acceleration and Saddle Points

with Chi Jin and Praneeth Netrapalli



PAGD Converges to SOSP Faster (Jin et al. 2017)

For ℓ -gradient Lipschitz and ρ -Hessian Lipschitz function f, PAGD with proper choice of η , θ , r, T, γ , s w.h.p. finds ϵ -SOSP in iterations:

$$ilde{O}\left(rac{\ell^{1/2}
ho^{1/4}(f(\mathbf{x}_0)-f^{\star})}{\epsilon^{7/4}}
ight)$$

	Strongly Convex	Nonconvex (SOSP)
Assumptions	$\ell ext{-grad-Lip}$ & $lpha ext{-str-convex}$	$\ell ext{-grad-Lip}$ & $ ho ext{-Hessian-Lip}$
(Perturbed) GD	$\tilde{O}(\ell/\alpha)$	$\tilde{O}(\Delta_f \cdot \ell/\epsilon^2)$
(Perturbed) AGD	$ ilde{O}(\sqrt{\ell/lpha})$	$ ilde{O}(\Delta_f\cdot\ell^{rac{1}{2}} ho^{rac{1}{4}}/\epsilon^{rac{7}{4}})$
Condition κ	$\ell/lpha$	$\ell/\sqrt{ ho\epsilon}$
Improvement	$\sqrt{\kappa}$	$\sqrt{\kappa}$

Part IV: Acceleration and Stochastics

with Xiang Cheng, Niladri Chatterji and Peter Bartlett

Acceleration and Stochastics

- Can we accelerate diffusions?
- There have been negative results...
- ...but they've focused on classical overdamped diffusions

Acceleration and Stochastics

- Can we accelerate diffusions?
- There have been negative results...
- ...but they've focused on classical overdamped diffusions
- Inspired by our work on acceleration, can we accelerate underdamped diffusions?

Overdamped Langevin MCMC

Described by the Stochastic Differential Equation (SDE): $dx_t = -\nabla U(x_t)dt + \sqrt{2}dB_t$

where $U(x): \mathbb{R}^d \to \mathbb{R}$ and B_t is standard Brownian motion. The stationary distribution is $p^*(x) \propto \exp(U(x))$

Corresponding Markov Chain Monte Carlo Algorithm (MCMC):

$$\tilde{x}_{(k+1)\delta} = \tilde{x}_{k\delta} - \nabla U(\tilde{x}_{k\delta}) + \sqrt{2\delta}\xi_k$$

where δ is the *step-size* and $\xi_k \sim N(0, I_{d \times d})$

Guarantees under Convexity

Assuming U(x) is *L*-smooth and *m*-strongly convex:

Dalalyan'14: Guarantees in Total Variation If $n \ge O\left(\frac{d}{\epsilon^2}\right)$ then, $TV(p^{(n)}, p^*) \le \epsilon$

Durmus & Moulines'16: Guarantees in 2-Wasserstein If $n \ge O\left(\frac{d}{\epsilon^2}\right)$ then, $W_2(p^{(n)}, p^*) \le \epsilon$

Cheng and Bartlett'17: Guarantees in KL divergence

If
$$n \ge O\left(\frac{d}{\epsilon^2}\right)$$
 then, $\mathsf{KL}(p^{(n)}, p^*) \le \epsilon$

Underdamped Langevin Diffusion

Described by the *second-order* equation:

$$dx_t = v_t dt$$

$$dv_t = -\gamma v_t dt + \lambda \nabla U(x_t) dt + \sqrt{2\gamma\lambda} dB_t$$

The stationary distribution is $p^*(x, v) \propto \exp\left(-U(x) - \frac{|v|_2^2}{2\lambda}\right)$

Intuitively, x_t is the position and v_t is the velocity

 $\nabla U(x_t)$ is the force and γ is the drag coefficient

Quadratic Improvement

Let $p^{(n)}$ denote the distribution of $(\tilde{x}_{n\delta}, \tilde{v}_{n\delta})$. Assume U(x) is strongly convex

Cheng, Chatterji, Bartlett, Jordan '17: If $n \ge O\left(\frac{\sqrt{d}}{\epsilon}\right)$ then $W_2(p^{(n)}, p^*) \le \epsilon$

Compare with Durmus & Moulines '16 (Overdamped) If $n \ge 0$ $\left(\frac{d}{\epsilon^2}\right)$ then $W_2(p^{(n)}, p^*) \le \epsilon$

Proof Idea: Reflection Coupling

Tricky to prove continuous-time process contracts. Consider two processes,

$$dx_t = -\nabla U(x_t)dt + \sqrt{2} \, dB_t^x$$
$$dy_t = -\nabla U(y_t)dt + \sqrt{2} \, dB_t^y$$

where $x_0 \sim p_0$ and $y_0 \sim p^*$. Couple these through Brownian motion

$$dB_{t}^{\mathcal{Y}} = \left[I_{d \times d} - \frac{2 \cdot (x_{t} - y_{t})(x_{t} - y_{t})^{\mathsf{T}}}{|x_{t} - y_{t}|_{2}^{2}} \right] dB_{t}^{\mathcal{X}}$$

"reflection along line separating the two processes"

Reduction to One Dimension

By Itô's Lemma we can monitor the evolution of the separation distance

$$d|x_t - y_t|_2 = -\left\langle \frac{x_t - y_t}{|x_t - y_t|_2}, \nabla U(x_t) - \nabla U(y_t) \right\rangle dt + 2\sqrt{2}dB_t^1$$

'Drift' '1-d random walk'

Two cases are possible

1. If $|x_t - y_t|_2 \le R$ then we have strong convexity; the drift helps. 2. If $|x_t - y_t|_2 \ge R$ then the drift hurts us, but Brownian motion helps stick

Rates not exponential in d as we have a 1-d random walk

*Under a clever choice of Lyapunov function.

Part V: Optimization vs. Sampling

With Yi-An Ma, Yuansi Chen, Chi Jin and Nicolas Flammarion

Sampling vs. Optimization: The Tortoise and the Hare

- Folk knowledge: Sampling is slow, while optimization is fast
 - but sampling provides inferences, while optimization only provides point estimates
- But there hasn't been a clear theoretical analysis that establishes this folk knowledge as true

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- Folk knowledge: Sampling is slow, while optimization is fast
 - but sampling provides inferences, while optimization only provides point estimates
- But there hasn't been a clear theoretical analysis that establishes this folk knowledge as true
- Is it really true?
- Define the *mixing time*:

$$\tau(\epsilon, p^0) = \min\{k \mid \|p^k - p^*\|_{\mathrm{TV}} \le \epsilon\}$$

 We'll study the Unadjusted Langevin Algorithm (ULA) and the Metropolis-Adjusted Langevin Algorithm (MALA)

Sampling

Theorem. For $p^* \propto e^{-U}$, we assume that U is m-strongly convex outside of a region of radius R and L-smooth. Let $\kappa = L/m$ denote the condition number of U. Let $p^0 = \mathcal{N}(0, \frac{1}{L}I)$ and let $\epsilon \in (0, 1)$. Then ULA satisfies

$$\tau_{ULA}(\epsilon, p^0) \le \mathcal{O}\left(e^{32LR^2}\kappa^2 \frac{d}{\epsilon^2}\ln\left(\frac{d}{\epsilon^2}\right)\right).$$

For MALA,

$$\tau_{MALA}(\epsilon, p^0) \le \mathcal{O}\left(e^{16LR^2}\kappa^{1.5}\left(d\ln\kappa + \ln\left(\frac{1}{\epsilon}\right)\right)^{3/2}d^{1/2}\right)$$

Optimization

Theorem. For any radius R > 0, Lipschitz and strong convexity constants $L \ge 2m > 0$, probability 0 , there exists an objective function <math>U(x) where $x \in \mathbb{R}^d$ and U is L-Lipschitz smooth and m-strongly convex for $||x||_2 > 2R$, such that for any optimization algorithm that inputs $\{U(x), \nabla U(x), \ldots, \nabla^n U(x)\}$, for some n, at least

$$K \ge \mathcal{O}\left(p \cdot (LR^2/\epsilon)^{d/2}\right)$$

steps are required for $\epsilon \leq \mathcal{O}(LR^2)$ so that $P(|U(x_K) - U(x^*)| < \epsilon) \geq p$.

Part VI: Acceleration and Sampling

With Yi-An Ma, Niladri Chatterji, and Xiang Cheng

Acceleration of SDEs

• The underdamped Langevin stochastic differential equation is Nesterov acceleration on the manifold of probability distributions, with respect to the KL divergence (Ma, et al., to appear)

Part VII: Market Design Meets Gradient-Based Learning

with Lydia Liu, Horia Mania and Eric Mazumdar






Two Examples of Current Projects

- How to find saddle points in high dimensions?
 - not just any saddle points; we want to find the Nash equilibria (and only the Nash equilibria)
- Competitive bandits and two-way markets
 - how to find the "best action" when supervised training data is not available, when other agents are also searching for best actions, and when there is conflict (e.g., scarcity)





Chapter 3: Concluding Remarks

Machine Learning (aka, AI)

- First Generation ('90-'00): the backend
 - e.g., fraud detection, search, supply-chain management
- Second Generation ('00-'10): the human side
 e.g., recommendation systems, commerce, social media
- Third Generation ('10-now): pattern recognition
 e.g., speech recognition, computer vision, translation
- Fourth Generation (emerging): decisions and markets
 - not just one agent making a decision or sequence of decisions
 - but a huge interconnected web of data, agents, decisions
 - many new challenges!
- What do these developments have to do with "intelligence"?

AI = Data + Algorithms + Markets

- Computers are currently gathering huge amounts of data, for and about humans, to be fed into learning algorithms
 - often the goal is to learn to imitate humans
 - a related goal is to provide personalized services to humans
 - but there's a lot of guessing going on about what people want
- Services are best provided in the context of a market; market design can eliminate much of the guesswork
 - when data flows in a market, the underlying system can learn from that data, so that the market provides better services
 - fairness arises not from providing the same service to everyone, but by allowing individual utilities to be expressed
- Learning algorithms provide the glue between data and the market

Consequences for IT Business Models

- Many modern IT companies collect data as part of providing a service on a platform
 - often the value provided by these services is limited
 - so the monetization comes from advertising
 - i.e., many companies are in fact creating markets based on data and learning algorithms, but these markets only link the IT company and the advertisers
- Humans are treated as a product, not as a player in a market
 - the results (ads) are not based on the utility (happiness) of the providers of the data, and does not pay them for their data
- This is broken---humans should be able to participate fully in a market in which their data are being used
 - they should not be treated as mere product or mere observers

Executive Summary

- ML (AI) has come of age
- But it is far from being a solid engineering discipline that can yield robust, scalable solutions to modern dataanalytic problems
- There are many hard problems involving uncertainty, inference, decision-making, robustness and scale that are far from being solved

not to mention economic, social and legal issues