Statistical Machine Learning: Dynamical, Stochastic and Economic Perspectives

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Musings on Computation in Statistics

- Two main perspectives: Optimization and Sampling

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- Two main perspectives: Optimization and Sampling
  - underlying mathematical objects: derivatives and integrals
- Are they just incommensurate? Frequentist vs Bayesian?
- Surely not---mature disciplines blend the two
  - cf. vector-field and Lagrangian/Hamiltonian perspectives in mechanics

Musings (Cont)

- In the current era, work on optimization and sampling is quite different
  - the latter focuses on equilibrium states
  - the former focuses on trajectories

Musings (Cont)

- In the current era, work on optimization and sampling is quite different
  - the latter focuses on equilibrium states
  - the former focuses on trajectories
- Glimmers of relationships
  - hybrid Monte Carlo
  - geometric connections (Riemannian and symplectic)
  - analyses of SDEs that include dimension dependence
  - variational inference

Statistics and Computation

- A Grand Challenge of our era: tradeoffs between statistical inference and computation
  - most data analysis problems have a time budget
  - and they're often 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 insights

Statistics and Computation (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

Statistics and Computation (cont)

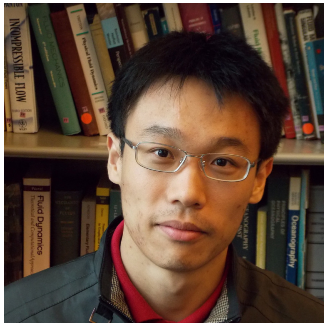
- Modern large-scale statistics has posed new challenges for optimization
  - millions of variables, millions of terms, sampling issues, nonconvexity, need for confidence intervals, parallel—distributed platforms, etc
- Current focus: what can we do with the following ingredients?
  - gradients
  - stochastics
  - acceleration

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

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
- Is it really true?

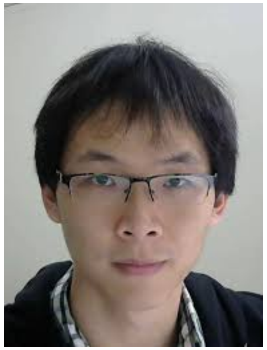


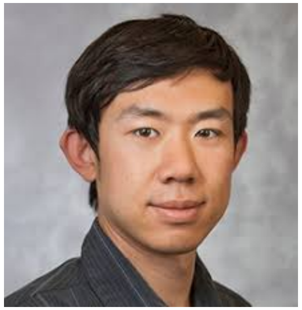
Sampling vs. Optimization: The Tortoise and the Hare

- I'll present a class of problems for which a discretized Langevin diffusion has a polynomial convergence rate in terms of dimension
- Whereas any gradient-based optimization procedure necessarily has an exponential convergence rate

Part I: How to Escape Saddle Points Efficiently

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

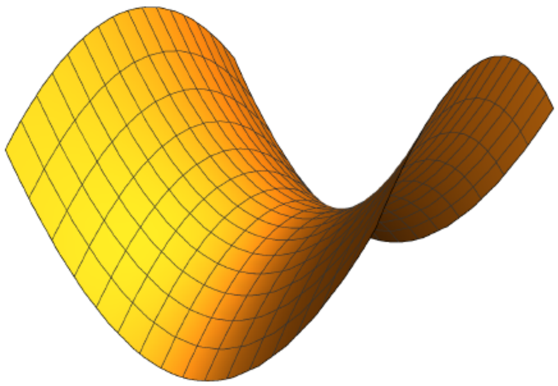


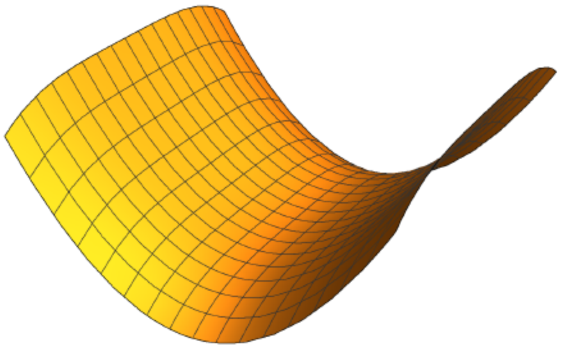



Nonconvex Optimization in Machine Learning

- Bad local minima used to be thought of as the main problem on the optimization side of machine learning
- But many machine learning architectures either have no local minima (see list later), or stochastic gradient seems to have no trouble (eventually) finding global optima
- But saddle points abound in these architectures, and they cause the learning curve to flatten out, perhaps (nearly) indefinitely

The Importance of Saddle Points


Strict saddle point


Non-strict saddle point

- 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?

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

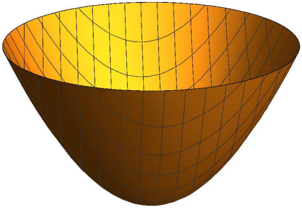
Consider problem:

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

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 $\mathbf{x}$ 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:

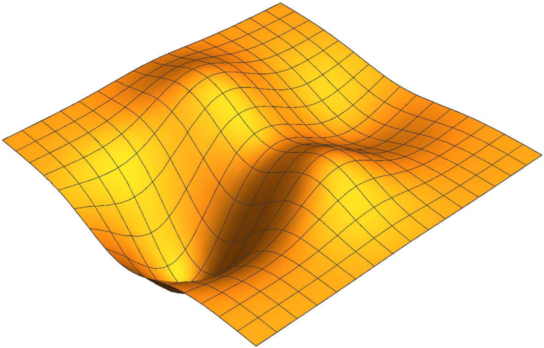
$$\frac{2\ell(f(\mathbf{x}_0) - f^\star)}{\epsilon^2}$$

*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 $\mathbf{x}$ is an ϵ-**second-order stationary point** (ϵ-SOSP) if

$$\|\nabla f(\mathbf{x})\| \le \epsilon, \qquad \text{and} \qquad \lambda_{\min}(\nabla^2 f(\mathbf{x})) \ge -\sqrt{\rho\epsilon}$$

Definitions and Algorithm

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Algorithm Perturbed Gradient Descent (PGD)

1. **for** $t = 0, 1, \ldots$ **do**
2. **if** perturbation condition holds **then**
3. $\mathbf{x}_t \leftarrow \mathbf{x}_t + \xi_t, \qquad \xi_t$ 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:

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

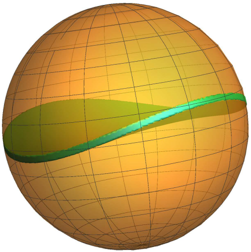
*Dimension dependence in iteration is $\log^4(d)$ (almost dimension free).

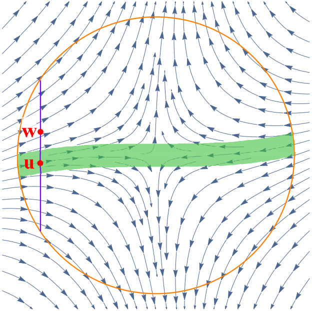
	GD(Nesterov 1998)	**PGD**(This Work)
Assumptions	ℓ-grad-Lip	ℓ-grad-Lip + ρ-Hessian-Lip
Guarantees	ϵ-FOSP	ϵ-SOSP
Iterations	$2\ell(f(\mathbf{x}_0) - f^\star)/\epsilon^2$	$\tilde{O}(\ell(f(\mathbf{x}_0) - f^\star)/\epsilon^2)$

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.





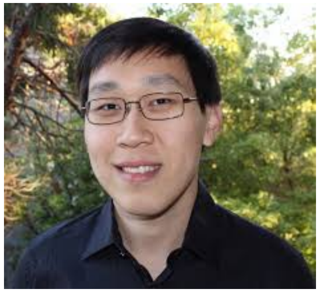
Key Observation: although we don't know its shape, we know it's thin!
(Based on an analysis of two nearly coupled sequences)

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 $O(1/k)$

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- Classical gradient descent:

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

obtains a convergence rate of $O(1/k)$

- Accelerated gradient descent:

$$\begin{aligned} y_{k+1} &= x_k - \beta \nabla f(x_k) \\ x_{k+1} &= (1 - \lambda_k) y_{k+1} + \lambda_k y_k \end{aligned}$$

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

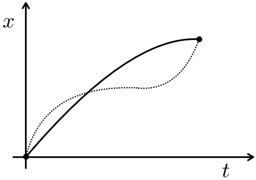
A systematic discretization methodology

Bregman Lagrangian

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

Variational problem over curves:

$$\min_X \int \mathcal{L}(X_t, \dot{X}_t, t)\, dt$$



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:

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

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?

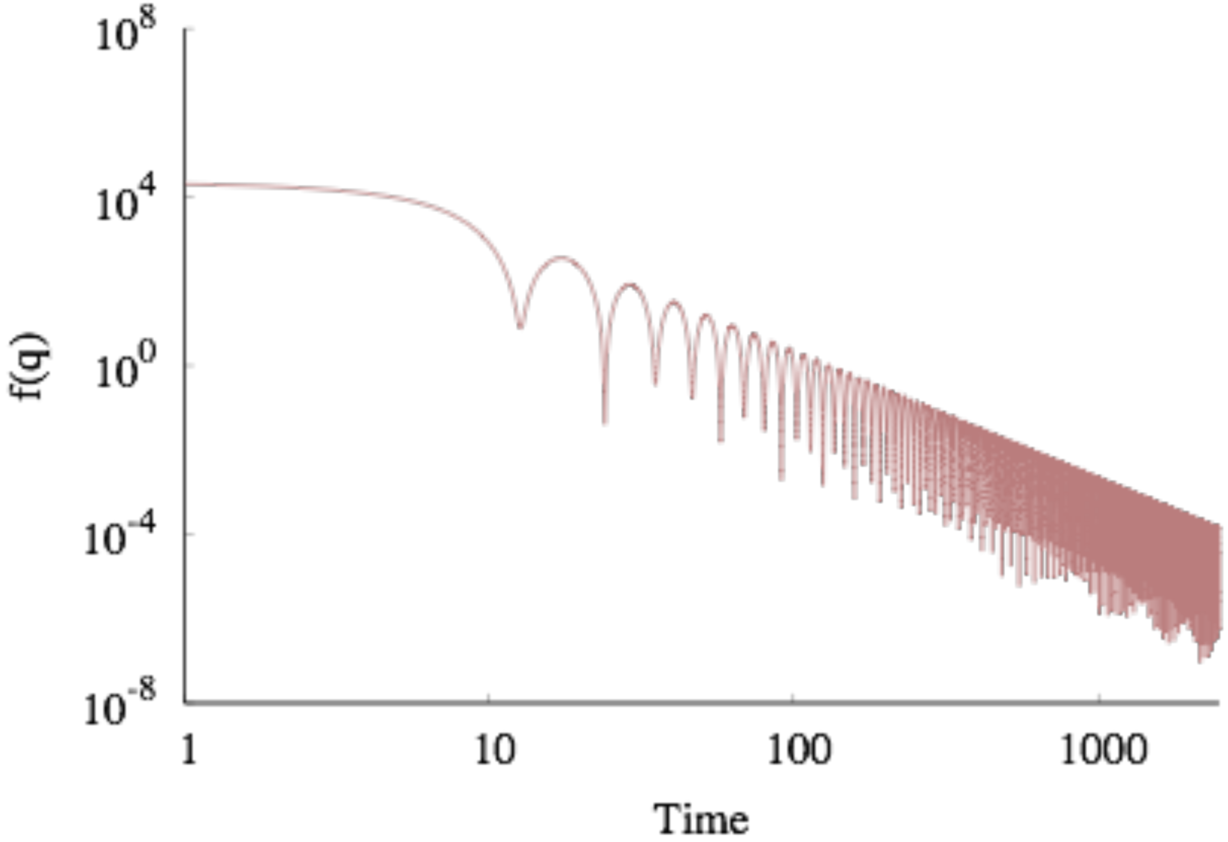
Towards A Symplectic Perspective

- 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:

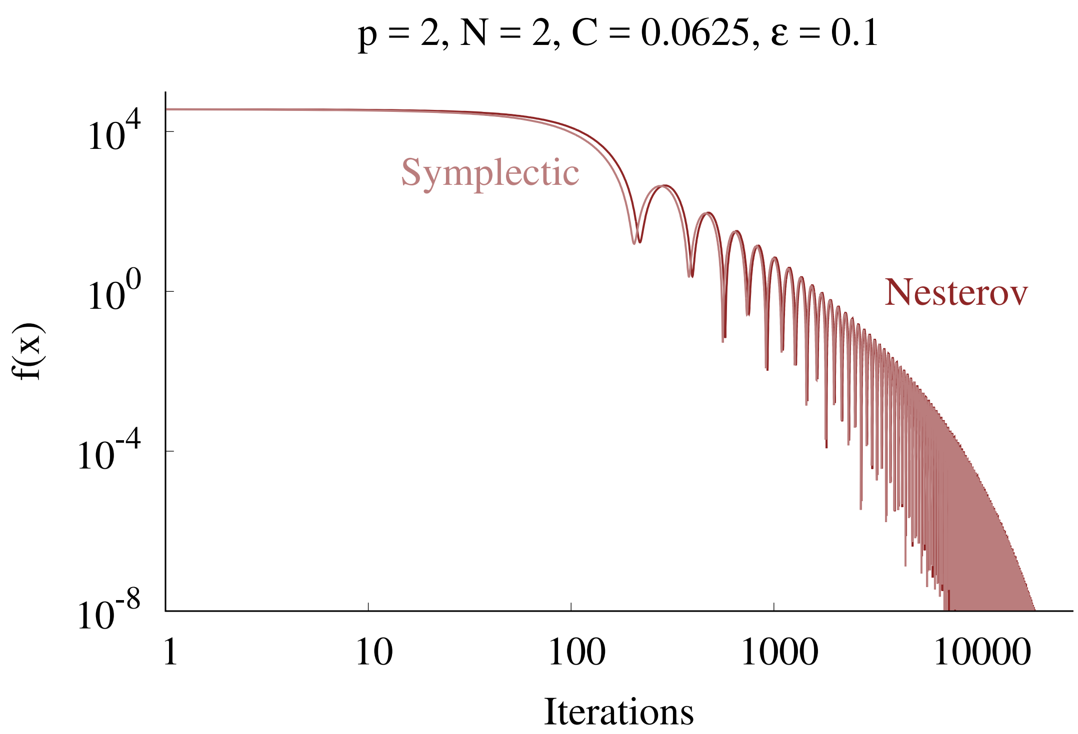
$$L(q, v, t) \to H(q, p, t, \mathcal{E})$$

$$\left(\frac{\mathrm{d}q}{\mathrm{d}t}, \frac{\mathrm{d}v}{\mathrm{d}t} \right) \to \left(\frac{\mathrm{d}q}{\mathrm{d}\tau}, \frac{\mathrm{d}p}{\mathrm{d}\tau}, \frac{\mathrm{d}t}{\mathrm{d}\tau}, \frac{\mathrm{d}\mathcal{E}}{\mathrm{d}\tau} \right)$$

Symplectic Integration of Bregman Hamiltonian



Symplectic vs Nesterov



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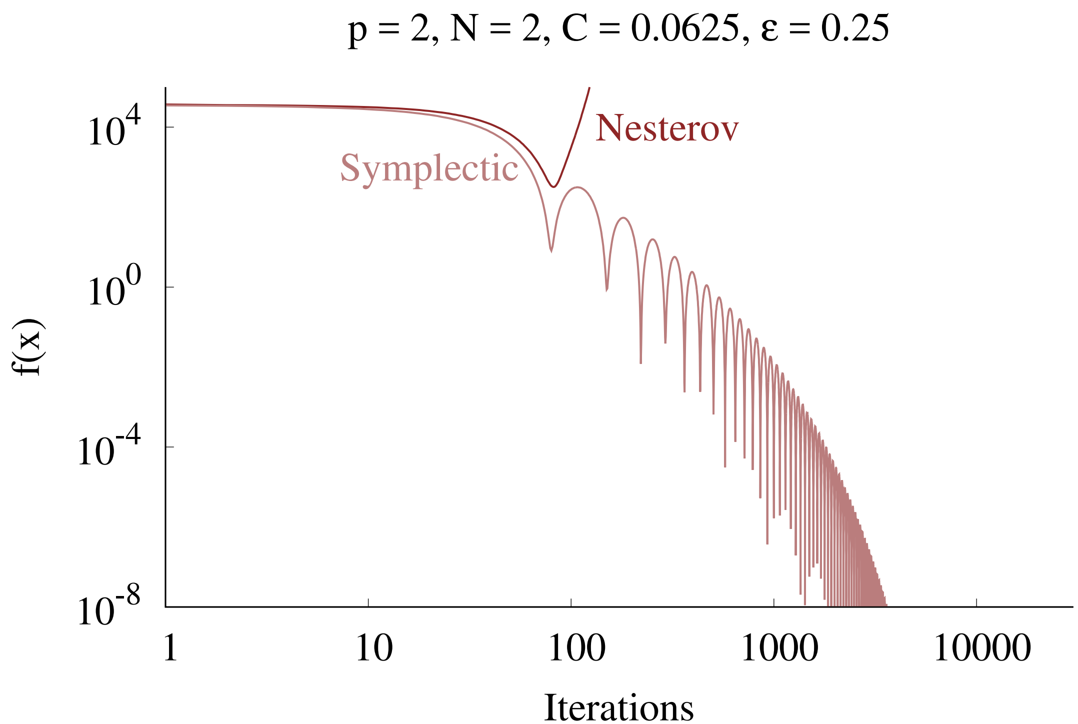
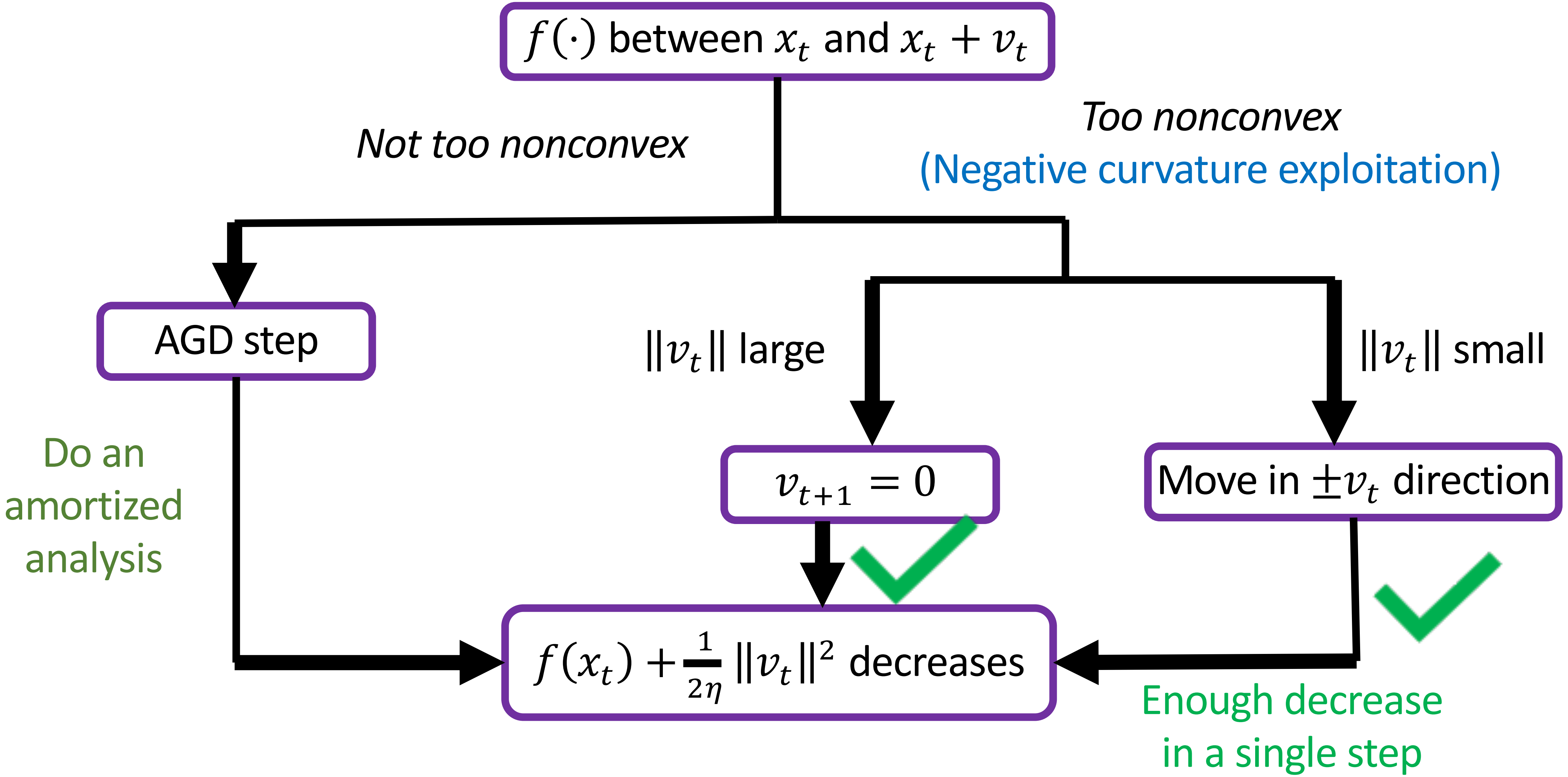


Part III: Acceleration and Saddle Points

with Chi Jin and Praneeth Netrapalli

Hamiltonian Analysis



Convergence Result

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

For ℓ-gradient Lipschitz and ρ-Hessian Lipschitz function f, PAGD with proper choice of $\eta, \theta, r, T, \gamma, s$ w.h.p. finds ϵ-SOSP in iterations:

$$\tilde{O}\left(\frac{\ell^{1/2}\rho^{1/4}(f(\mathbf{x}_0) - f^\star)}{\epsilon^{7/4}}\right)$$

	Strongly Convex	**Nonconvex (SOSP)**
Assumptions	ℓ-grad-Lip & α-str-convex	ℓ-grad-Lip & ρ-Hessian-Lip
(Perturbed) GD	$\tilde{O}(\ell/\alpha)$	$\tilde{O}(\Delta_f \cdot \ell/\epsilon^2)$
(Perturbed) AGD	$\tilde{O}(\sqrt{\ell/\alpha})$	$\tilde{O}(\Delta_f \cdot \ell^{\frac{1}{2}}\rho^{\frac{1}{4}}/\epsilon^{\frac{7}{4}})$
Condition κ	ℓ/α	$\ell/\sqrt{\rho\epsilon}$
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 $U(x): R^d \to R$ and B_t is standard Brownian motion.

The stationary distribution is $p^*(x) \propto \exp\big(U(x)\big)$

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 $n \geq O\left(\frac{d}{\epsilon^2}\right)$ then, $TV(p^{(n)}, p^*) \leq \epsilon$

Durmus & Moulines'16: Guarantees in 2-Wasserstein

If $n \geq O\left(\frac{d}{\epsilon^2}\right)$ then, $W_2(p^{(n)}, p^*) \leq \epsilon$

Cheng and Bartlett'17: Guarantees in KL divergence

If $n \geq O\left(\frac{d}{\epsilon^2}\right)$ then, $\mathrm{KL}(p^{(n)}, p^*) \leq \epsilon$

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 $n \geq O\left(\frac{\sqrt{d}}{\epsilon}\right)$ then $W_2\left(p^{(n)}, p^*\right) \leq \epsilon$

Compare with Durmus & Moulines ’16 (Overdamped)

If $n \geq O\left(\frac{d}{\epsilon^2}\right)$ then $W_2\left(p^{(n)}, p^*\right) \leq \epsilon$

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

$$dB_t^y = \left[I_{d\times d} - \frac{2 \cdot (x_t - y_t)(x_t - y_t)^\top}{|x_t - y_t|_2^2} \right] dB_t^x$$

"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 $|x_t - y_t|_2 \leq R$ then we have strong convexity; the drift helps.
2. If $|x_t - y_t|_2 \geq R$ 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 VI: Acceleration and Sampling

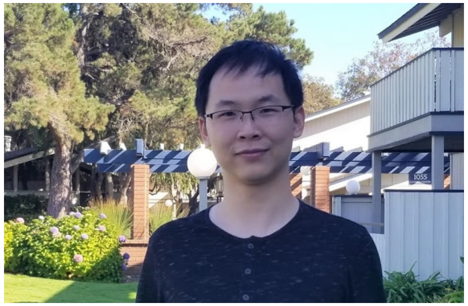
With Yi-An Ma, Niladri Chatterji, and Xiang Cheng

Acceleration of SDEs

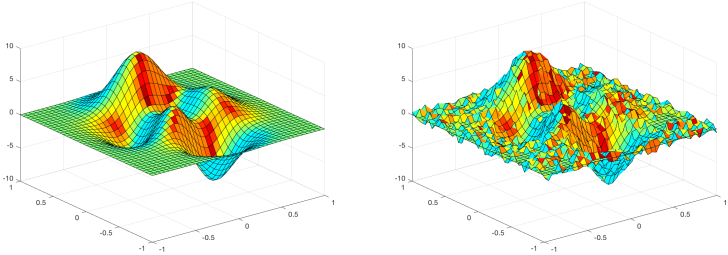
- *The underdamped Langevin stochastic differential equation is Nesterov acceleration on the manifold of probability distributions, with respect to the KL divergence* (Ma, et al., to appear)

Part V: Population Risk and Empirical Risk

with Chi Jin and Lydia Liu



Population Risk vs Empirical Risk



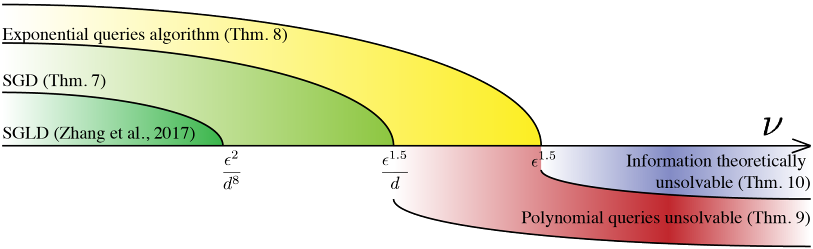
Well-behaved population risk $\Rightarrow$ rough empirical risk

- Even when R is smooth, $\hat{R}_n$ can be **non-smooth** and may even have many **additional local minima** (ReLU deep networks).
- Typically $\|R - \hat{R}_n\|_\infty \leq O(1/\sqrt{n})$ by empirical process results.

Can we finds local min of R given only access to the function value $\hat{R}_n$?

Our Contribution

Our answer: **Yes!** Our SGD approach finds $\epsilon-$SOSP of F if $\nu \leq \epsilon^{1.5}/d$, which is **optimal among all polynomial queries algorithms**.



Complete characterization of error ν vs accuracy ϵ and dimension d.

Part VII: Market Design Meets Gradient-Based Learning

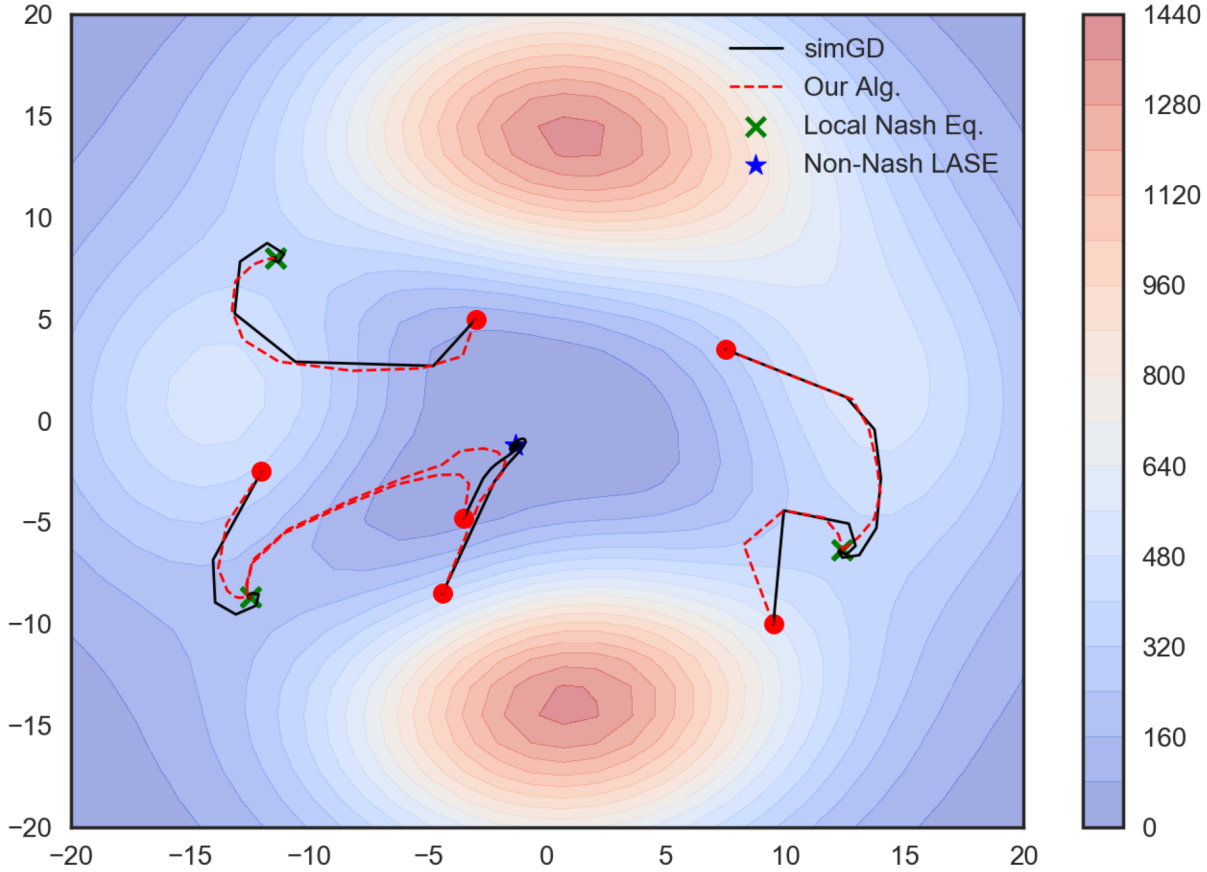
with Lydia Liu, Horia Mania and Eric Mazumdar

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)



simGD
Our Alg.
Local Nash Eq.
Non-Nash LASE
20
15
10
5
0
−5
−10
−15
−20
−20
−15
−10
−5
0
5
10
15
20
1440
1280
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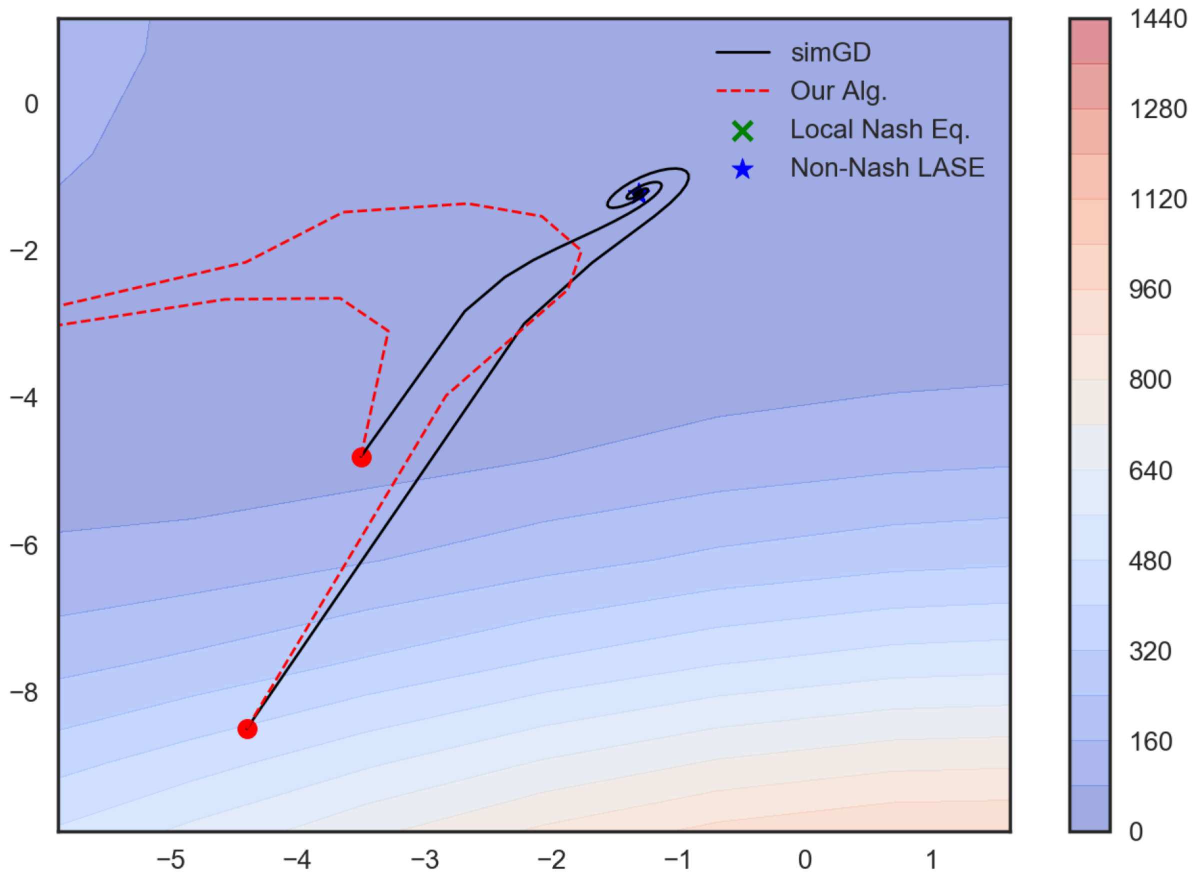
800
640
480
320
160
0



simGD
Our Alg.
Local Nash Eq.
Non-Nash LASE
0
−2
−4
−6
−8
−5
−4
−3
−2
−1
0
1
1440
1280
1120
960
800
640
480
320
160
0

Perspectives on AI

- 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 loosely-coupled decisions

M. Jordan (2018), “Artificial Intelligence: The Revolution Hasn’t Happened Yet”, *Medium.*

What Intelligent Systems Currently Exist?

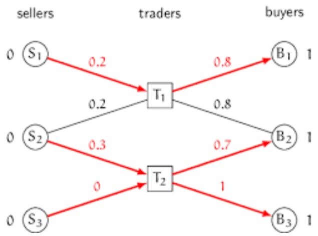
What Intelligent Systems Currently Exist?

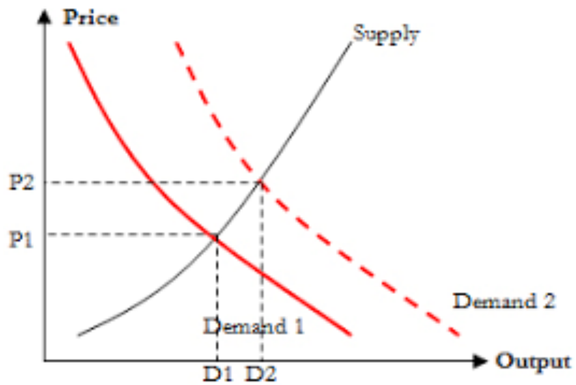
- Brains and Minds

What Intelligent Systems Currently Exist?

- Brains and Minds

- Markets





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

Consider 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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- Recommendations are made on the basis of these similarities
- These systems have become a commodity

Multiple Decisions with Competition

- Suppose that recommending a certain movie is a good business decision (e.g., because it’s very popular)
- Is it OK to recommend the same movie to everyone?
- Is it OK to recommend the same book to everyone?
- Is it OK to recommend the same restaurant to everyone?
- Is it OK to recommend the same street to every driver?
- Is it OK to recommend the same stock purchase to everyone?

The Alternative: Create a Market

- A two-way market between consumers and producers
  - based on recommendation systems on both sides
- E.g., diners are one side of the market, and restaurants on the other side
- E.g., drivers are one side of the market, and street segments on the other side

- This isn't just classical microeconomics; the use of recommendation systems is key

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Social 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

- The markets-meets-learning approach deals with other problems that a pure learning approach does not
  - e.g., recommendations when there is scarcity

Example: Music in the Data Age

- More people are making music than ever before, placing it on sites such as SoundCloud
- More people are listening to music than ever before
- But there is no economic value being exchanged between producers and consumers
- And, not surprisingly, most people who make music cannot do it as their full-time job
  - i.e., human happiness is being left on the table

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- There do exist companies who make money off of this; they stream data from SoundCloud to listeners, and they make their money … from advertising! ☹

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- Use data to provide a dashboard to musicians, letting them learn where their audience is
- The musician can give shows where they have an audience
- And they can make offers to their fans
- I.e., consumers and producers become linked, and value flows: a market is created
  - the company that creates this market profits simply by taking a cut from the transactions

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 data-analytic 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