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Stochastic Approximation Theory

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November 26, 2015

Plan

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- History and modern formulation of stochastic approximation theory
- In-depth look at stochastic gradient descent (SGD)
- Introduction to key ideas in stochastic approximation theory such as Lyapunov functions, quasimartingales, and also numerical solutions to differential equations.

Bibliography

Stochastic Approximation and Recursive Algorithms and Applications, Kushner & Lin (2003)

Online Learning and Stochastic Approximation, Léon Bottou (1998)

A Stochastic Approximation Algorithm, Robbins & Monro (1951)

Stochastic Estimation of the Maximisation of a Regression Function, Kiefer & Wolfowitz (1952)

Introduction to Stochastic Search and Optimization, Spall (2003)

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Numerical Analysis is a well-established discipline...

c. 1800 - 1600 BC

Babylonians attempted to calculate $\sqrt{2}$, or in modern terms, find the roots of $x^2 - 2 = 0$.

1

[1] http://www.math.ubc.ca/~cass/Euclid/ybc/ybc.html, Yale Babylonian Collection

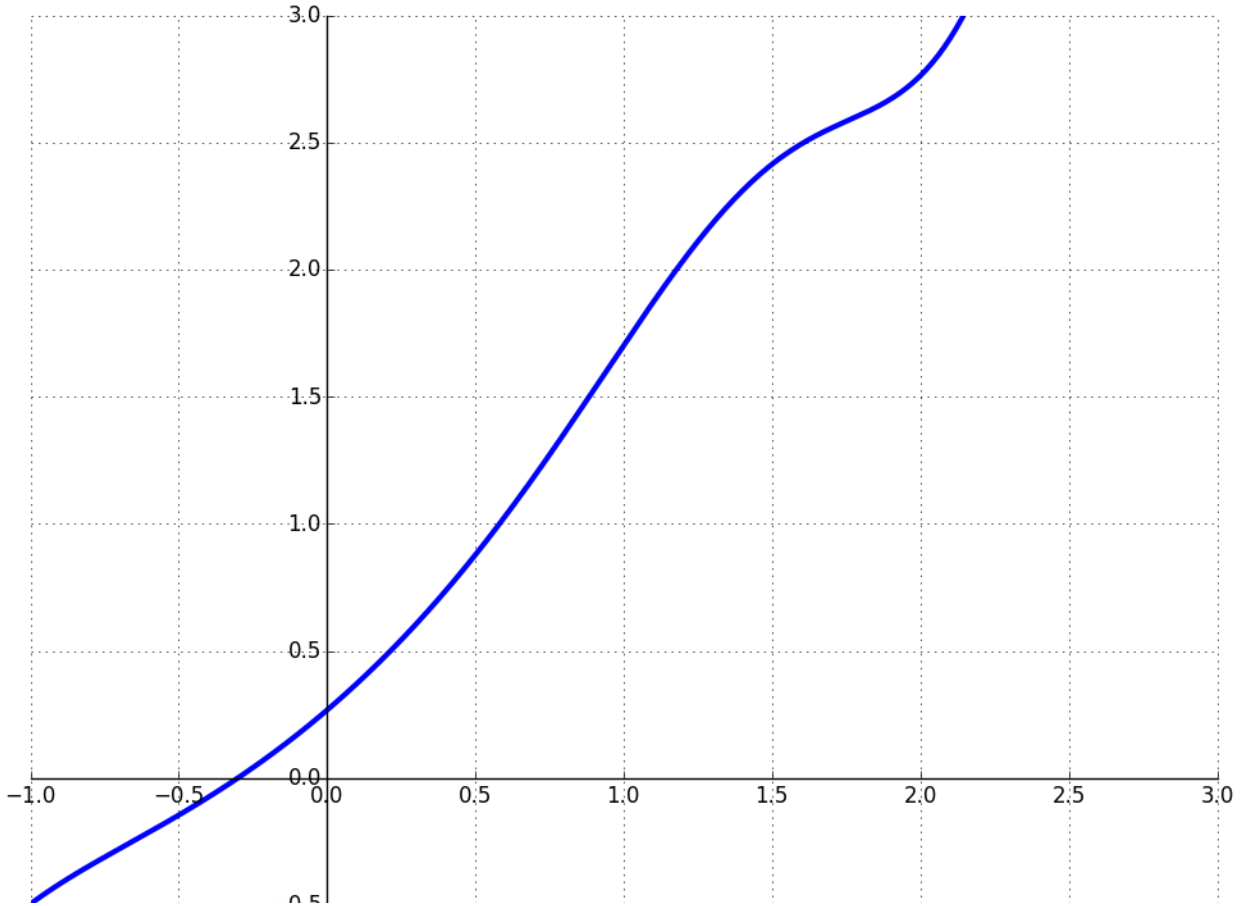
C17-C19

Huge number of numerical techniques developed as tools for the natural sciences:

- Root-finding methods (e.g. Newton-Raphson)
- Numerical integration (e.g. Gaussian Quadrature)
- ODE solution (e.g. Euler method)
- Interpolation (e.g. Lagrange polynomials)

Focus is on situations where function evaluation is deterministic.

1951 Robbins and Monro publish "*A Stochastic Approximation Algorithm*", describing how to find the root of an increasing function $f : \mathbb{R} \to \mathbb{R}$ when only *noisy* estimates of the function's value at a given point are available.



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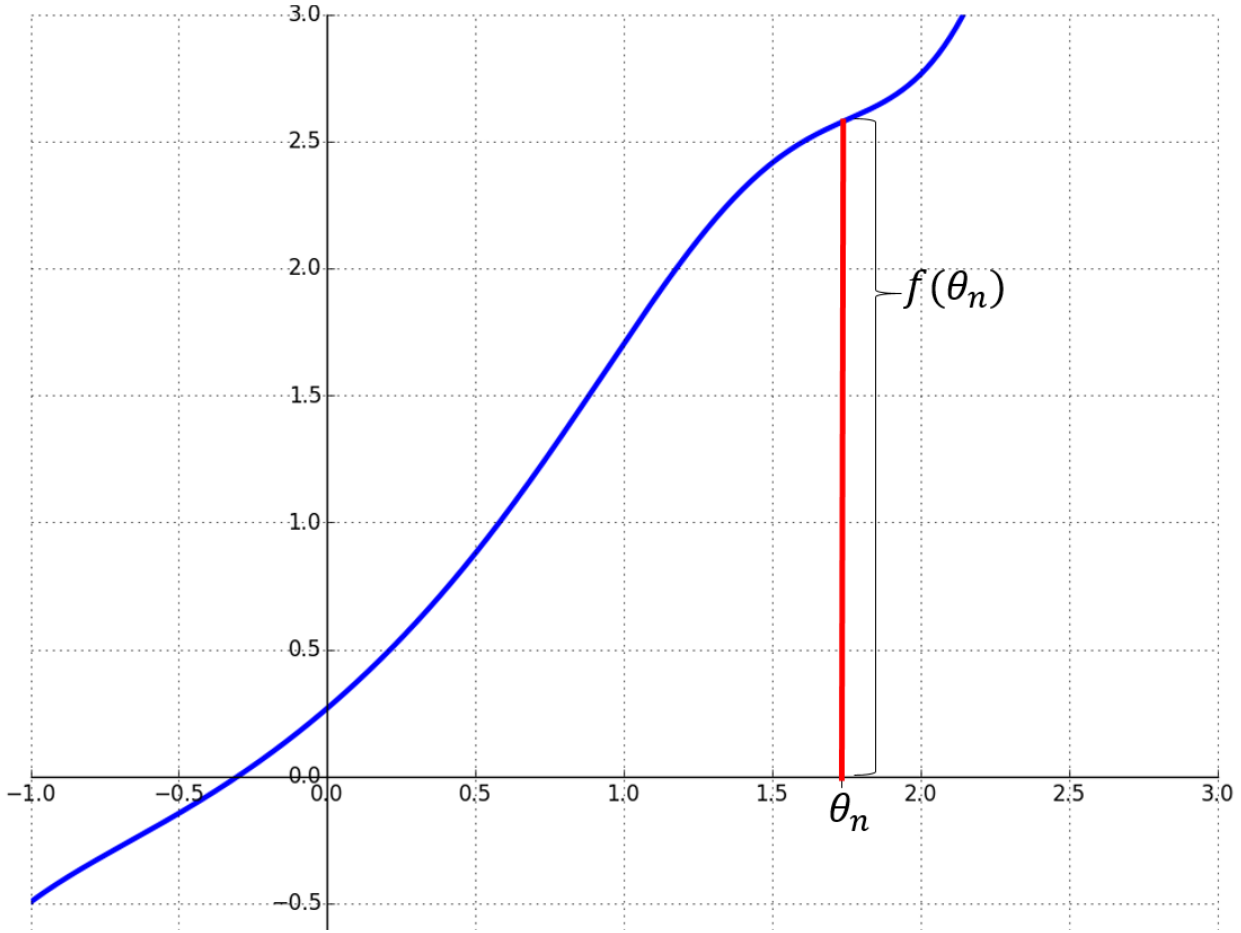

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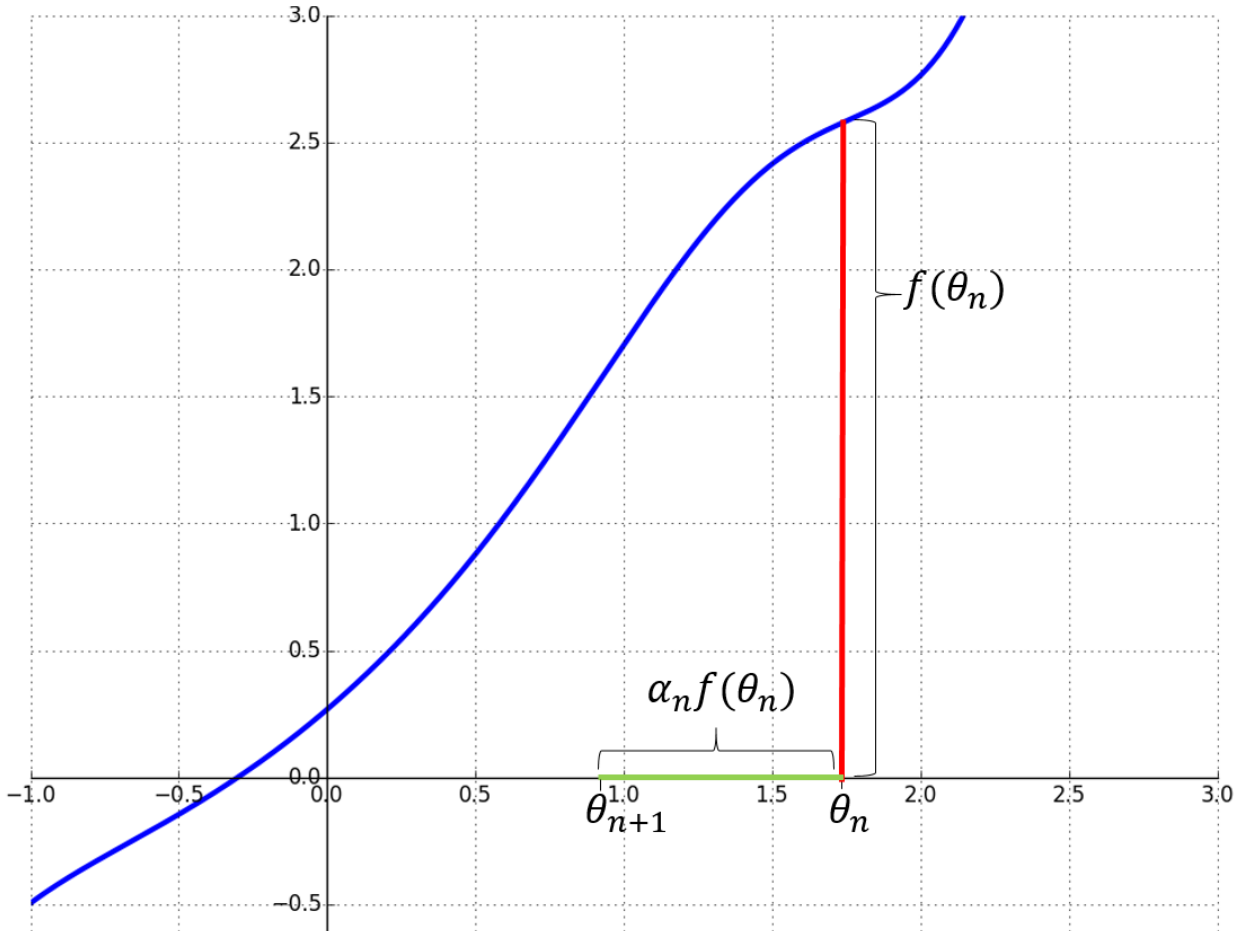

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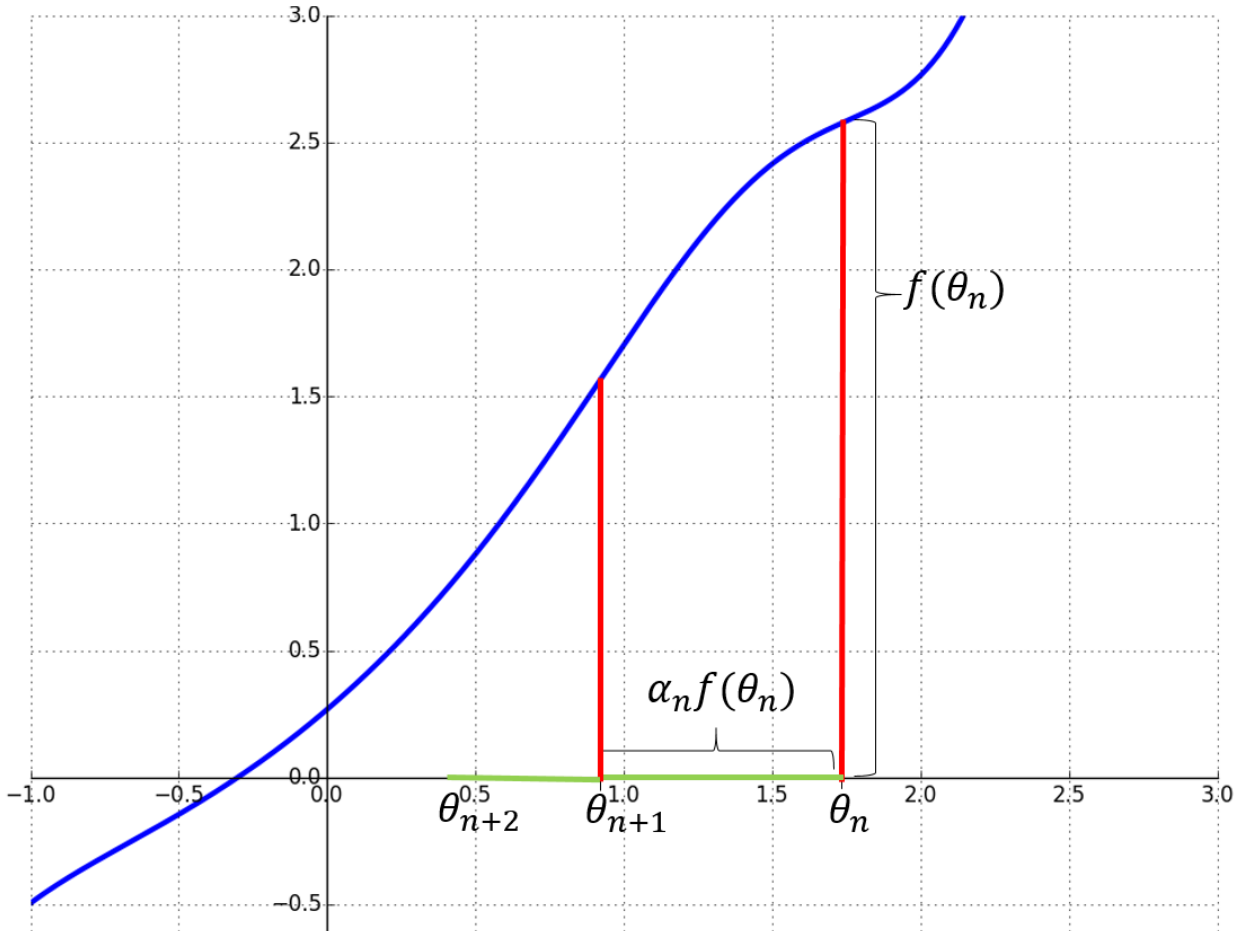

They provide an iterative scheme for root estimation in this context and prove convergence of the resulting estimate in L^2 and in probability.

Note also that if we treat f as the gradient of some function F, the Robbins-Monro algorithm can be viewed a minimisation procedure.

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1952

Motivated by the Robbins-Monro paper the year before, Kiefer and Wolfowitz publish "*Stochastic Estimation of the Maximisation of a Regression Function*".

Their algorithm is phrased as a maximisation procedure, in contrast to the Robbins-Monro paper, and uses central-difference approximations of the gradient to update the optimum estimator.

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Present day

Stochastic approximation widely researched and used in practice:

- Original applications in root-finding and optimisation, often in the guise of stochastic gradient descent:
  - Neural networks
  - K-Means
  - ...
- Related ideas are used in :
  - Stochastic variational inference (Hoffman et al. (2013))
  - Psuedo-marginal Metropolis-Hastings (Beaumont (2003), Andrieu & Roberts (2009))
  - Stochastic Gradient Langevin Dynamics (Welling & Teh (2011))

Textbooks:

Stochastic Approximation and Recursive Algorithms and Applications, Kushner & Yin (2003)

Introduction to Stochastic Search and Optimization, Spall (2003)

Modern-day formulation

Stochastic approximation is now a mature area of numerical analysis, and the general problem it seeks to solve has the following form:

$$\text{Minimise } f(w) = \mathbb{E}\left[F(w, \xi)\right]$$

(over w in some domain W, and some random variable ξ).

This is an immensely flexible framework:

- $F(w, \xi) = f(w) + \xi$ models experimental/measurement error.
- $F(x, \xi) = (w^\top \phi(\xi_X) - \xi_Y)^2$ corresponds to (least squares) linear regression
- If $f(w) = \frac{1}{N}\sum_{i=1}^{N} g(w, x_i)$ and $F(w, \xi) = \frac{1}{Ks}\sum_{x \in \xi} g(w, x)$, with ξ a randomly-selected subset (of size K) of large data set corresponds to "stochastic" machine learning algorithms.

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Stochastic gradient descent

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We'll focus on proof techniques for stochastic gradient descent (SGD).

We'll derive conditions for SGD to convergence almost surely. We broadly follow the structure of Léon Bottou's paper[2].

Plan:

- Continuous gradient descent
- Discrete gradient descent
- Stochastic gradient descent

[2] *Online Learning and Stochastic Approximations* - Léon Bottou (1998)

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Continuous Gradient Descent

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Let $C : \mathbb{R}^k \longrightarrow \mathbb{R}$ be differentiable. How do solutions $s : \mathbb{R} \to \mathbb{R}^k$ to the following ODE behave?

$$\frac{d}{dt}s(t) = -\nabla C(s(t))$$

Example: $C(\mathbf{x}) = 5(x_1 + x_2)^2 + (x_1 - x_2)^2$

We can analytically solve the gradient descent equation for this example:

$$\nabla C(\mathbf{x}) = (12x_1 + 8x_2, 8x_1 + 12x_2)$$

So $(s_1', s_2') = (12s_1 + 8s_2, 8s_1 + 12s_2)$, and solving with $(s_1(0), s_2(0)) = (1.5, 0.5)$ gives

$$\begin{pmatrix} s_1(t) \\ s_2(t) \end{pmatrix} = \begin{pmatrix} e^{-20t} + 1.5e^{-4t} \\ e^{-20t} - 0.5e^{-4t} \end{pmatrix}$$

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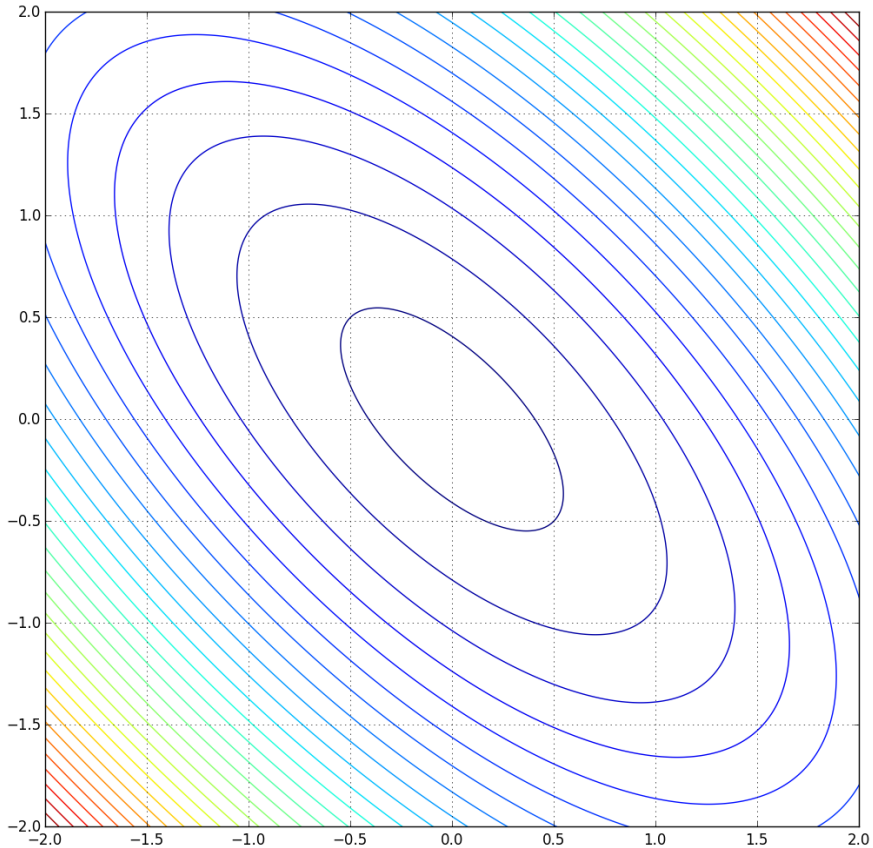

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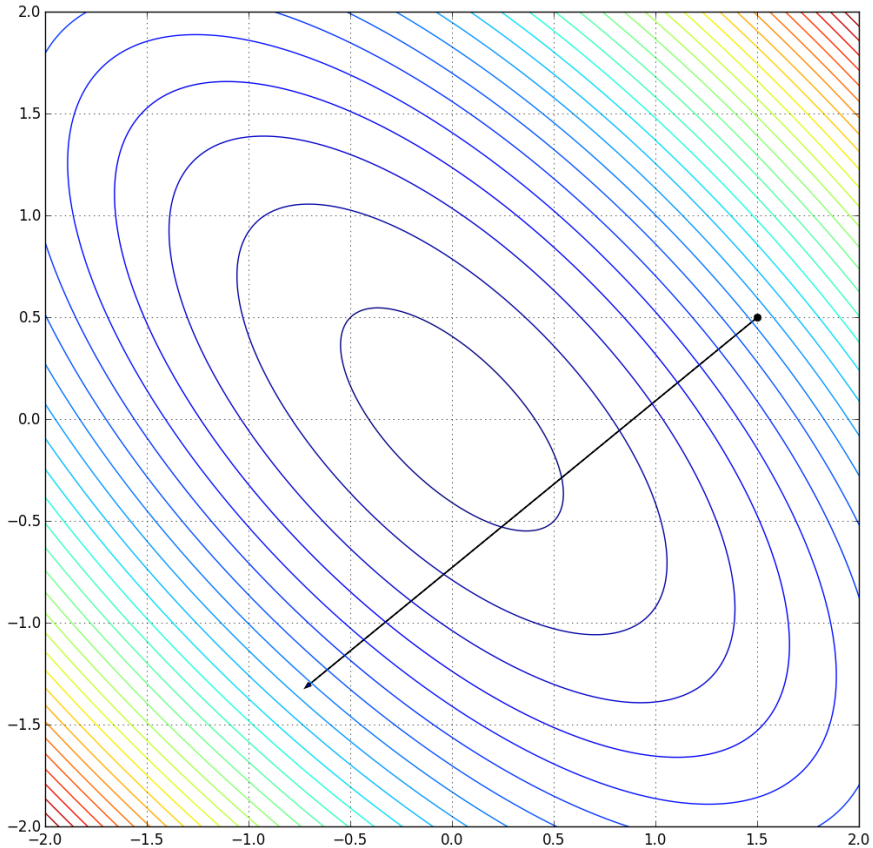

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Exact solution of gradient descent ODE

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We'll start with some simplifying assumptions:

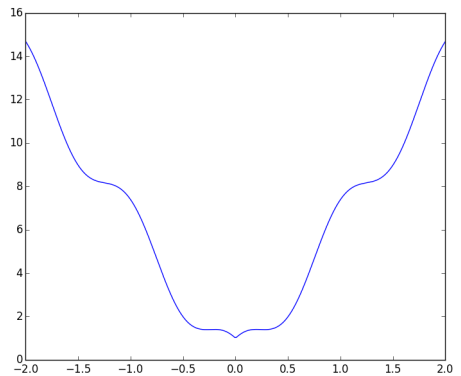
1. C has a unique minimiser $x^\star$
2. $\forall \epsilon > 0, \inf_{\|x-x^\star\|_2^2 > \epsilon} \langle x - x^\star, \nabla C(x) \rangle > 0$

(The second condition is weaker than convexity)

Proposition If $s : [0, \infty) \to X$ satisfies the differential equation

$$\frac{ds(t)}{dt} = -\nabla C(s(t))$$

then $s(t) \to x^\star$ as $t \to \infty$.



Example of non-convex function satisfying these conditions

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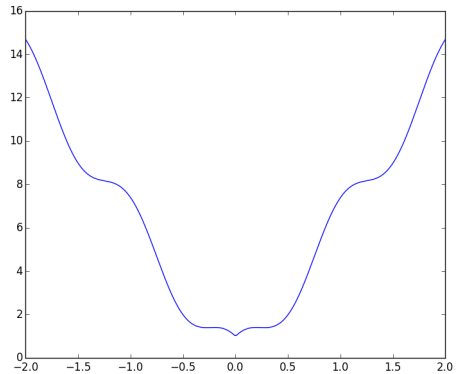

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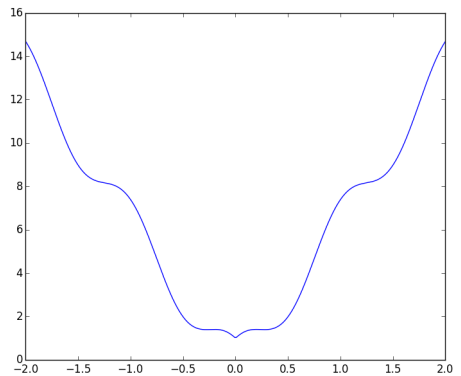

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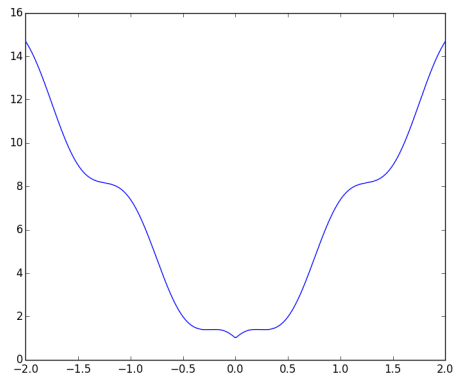

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Continuous Gradient Descent

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1. Define Lyapunov function $h(t) = \|s(t) - x^\star\|_2^2$
2. $h(t)$ is a decreasing function
3. $h(t)$ converges to a limit, and $h'(t)$ converges to 0
4. The limit of $h(t)$ must be 0
5. $s(t) \to x^\star$

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$h(t)$ is a decreasing function

$$\begin{aligned}
\frac{d}{dt}h(t) &= \frac{d}{dt}\|s(t) - x^\star\|_2^2 \\
&= \frac{d}{dt}\langle s(t) - x^\star, s(t) - x^\star\rangle \\
&= 2\left\langle \frac{ds(t)}{dt}, s(t) - x^\star \right\rangle \\
&= -\langle s(t) - x^\star, \nabla C(s(t))\rangle \leq 0
\end{aligned}$$

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The limit of $h(t)$ must be 0

If not, there is some $K > 0$ such that $h(t) > K$ for all t. By assumption,

$$\inf_{x:h(x)>K} \langle x - x^\star, \nabla C(x) \rangle > 0$$

which means that $\inf_t h'(t) < 0$, contradicting the convergence of $h'(t)$ to 0.

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So gradient descent finds the global minimum for functions in the class stated in the theorem.

Solving general ODEs analytically is extremely difficult at best, and usually impossible.

To implement this strategy algorithmically to solve a minimisation problem, we'll need a method of solving the ODE numerically.

There is no one best way to do this!!

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Discrete Gradient Descent

An intuitive, straightforward discretisation of

$$\frac{d}{dt}s(t) = -\nabla C(s(t))$$

is

$$\frac{s_{n+1} - s_n}{\epsilon_n} = -\nabla C(s_n) \qquad (ForwardEuler)$$

Although it is easy and quick to implement, it has theoretical (A-)instability issues.

An alternative method which is (A-)stable is the implicit Euler method:

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So why settle for explicit discretisation? Implicit requires solution of non-linear system at each step, and practically explicit discretisation works.

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Also have multistep methods, e.g.:

$$s_{n+2} = s_{n+1} + \epsilon_{n+2}\left(\frac{3}{2}\nabla C(s_{n+1}) - \frac{1}{2}\nabla C(s_n)\right)$$

This is the 2nd-order Adams-Bashforth method.

Similar (in)stability properties to forward Euler, but discretisation error of a smaller order of magnitude at each step ($\mathcal{O}(\epsilon^3)$ compared with $\mathcal{O}(\epsilon^2)$)

Examples of discretisation with $\epsilon = 0.1$

Examples of discretisation with $\epsilon = 0.07$

Examples of discretisation with $\epsilon = 0.01$

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Proposition If $s_{n+1} = s_n - \epsilon_n \nabla C(s_n)$ and C satisfies

1. C has a unique minimiser $x^\star$
2. $\forall \epsilon > 0, \quad \inf_{\|x - x^\star\|_2^2 > \epsilon} \langle x - x^\star, \nabla C(x) \rangle > 0$
3. $\|\nabla C(x)\|_2^2 \leq A + B\|x - x^\star\|_2^2$ for some $A, B \geq 0$

then subject to $\sum_n \epsilon_n = \infty$ and $\sum_n \epsilon_n^2 < \infty$ we have $s_n \to x^\star$

Proof structure The proof is largely the same as for the continuous case, but the extra conditions in the statement deal with the errors introduced by discretisation.

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2. Consider the positive variations $h_n^+ = \max(0, h_{n+1} - h_n)$
3. Show that $\sum_{n=1}^{\infty} h_n^+ < \infty$
4. Show that this implies that h_n converges
5. Show that h_n must converge to 0
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Because of the error that the discretisation introduced, h_n is not guaranteed to be decreasing - have to adjust proof.

Idea: h_n may fluctuate, but if we can show that the cumulative 'up' movements aren't too big, we can still prove convergence of h_n.

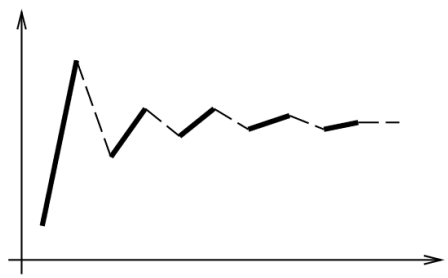

Illustration credit: *Online learning and stochastic approximation*, Léon Bottou (1998)

1. Define Lyapunov sequence $h_n = \|s_n - x^\star\|_2^2$
2. Consider the positive variations $h_n^+ = \max(0, h_{n+1} - h_n)$
3. Show that $\sum_{n=1}^{\infty} h_n^+ < \infty$
4. Show that this implies that h_n converges
5. Show that h_n must converge to 0
6. $s_n \to x^\star$

Consider the positive variations $h_n^+ = \max(0, h_{n+1} - h_n)$

With some algebra, note that

$$\begin{aligned} h_{n+1} - h_n &= \langle s_{n+1} - x^\star, s_{n+1} - x^\star \rangle - \langle s_n - x^\star, s_n - x^\star \rangle \\ &= \langle s_{n+1}, s_{n+1} \rangle - \langle s_n, s_n \rangle - 2 \langle s_{n+1} - s_n, x^\star \rangle \\ &= \langle s_n - \epsilon_n \nabla C(s_n), s_n - \epsilon_n \nabla C(s_n) \rangle - \langle s_n, s_n \rangle + 2\epsilon_n \langle \nabla C(s_n), x^\star \rangle \\ &= -2\epsilon_n \langle s_n - x^\star, \nabla C(s_n) \rangle + \epsilon_n^2 \|\nabla C(s_n)\|_2^2 \end{aligned}$$

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Show that $\sum_{n=1}^{\infty} h_n^+ < \infty$

Assuming $\|\nabla C(x)\|_2^2 \leq A + B\|x - x^\star\|_2^2$, we get

$$\begin{aligned} h_{n+1} - h_n &\leq -2\epsilon_n \langle s_n - x^\star, \nabla C(s_n)\rangle + \epsilon_n^2(A + Bh_n) \\ \implies h_{n+1} - (1 + \epsilon_n^2 B)h_n &\leq -2\epsilon_n \langle s_n - x^\star, \nabla C(s_n)\rangle + \epsilon_n^2 A \\ &\leq \epsilon_n^2 A \end{aligned}$$

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Assuming $\|\nabla C(x)\|_2^2 \leq A + B\|x - x^\star\|_2^2$, we get

$$h_{n+1} - (1 - \epsilon_n^2 B) h_n \leq \epsilon_n^2 A$$

Writing $\mu_n = \prod_{i=1}^{n} \frac{1}{1+\epsilon_i^2 B}$, and $h'_n = \mu_n h_n$, we get

$$h'_{n+1} - h'_n \leq \epsilon_n^2 \mu_n A$$

Assuming $\sum_{n=1}^{\infty} \epsilon_n^2 < \infty$, μ_n converges away from 0, so RHS is summable.

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Show that this implies that h_n converges

If $\sum_{n=1}^{\infty} \max(0, h_{n+1} - h_n) < \infty$, then $\sum_{n=1}^{\infty} \min(0, h_{n+1} - h_n) < \infty$ (why?)

But $h_{n+1} = h_0 + \sum_{k=1}^{n} (\max(0, h_{k+1} - h_k) + \min(0, h_{k+1} - h_k))$

So $(h_n)_{n=1}^{\infty}$ converges.

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Show that h_n must converge to 0 Assume h_n converges to some positive number. Previously, we had

$$h_{n+1} - h_n = -2\epsilon_n \langle s_n - x^\star, \nabla C(s_n)\rangle + \epsilon_n^2 \|\nabla C(s_n)\|_2^2$$

This is summable, and if we assume further that $\sum_{n=1}^{\infty} \epsilon_n = \infty$, then we get

$$\langle s_n - x^\star, \nabla C(s_n)\rangle \to 0$$

contradicting h_n converging away from 0.

Discrete Gradient Descent

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Stochastic Gradient Descent

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We're now ready to introduce the stochastic approximation of the gradient into our algorithm.

If C is a cost function averaged across a data set, often have true gradient of the form

$$\nabla C(x) = \frac{1}{N} \sum_{n=1}^{N} f_n(x)$$

and an approximation is formed by subsampling:

$$\widehat{\nabla C}(x) = \frac{1}{K} \sum_{k \in I_K} f_k(x) \qquad (I_k \sim \mathit{Unif}(\text{subsets of size K}))$$

We'll treat the more general case where the gradient estimates $\widehat{\nabla C}(x)$ are unbiased and independent.

The introduced randomness means that the Lyapunov sequence in our proof will now be a stochastic process, and we'll need some additional machinery to deal with it.

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Let $(X_n)_{n\geq 0}$ be a stochastic process.

$\mathcal{F}_n$ denotes "the information describing the stochastic process up to time n" denoted mathematically by $\mathcal{F}_n = \sigma(X_m | m \leq n)$

Definition A stochastic process $(X_n)_{n=0}^{\infty}$ is a martingale[3] if

- $\mathbb{E}[|X_n|] < \infty$ for all n
- $\mathbb{E}[X_n | \mathcal{F}_m] = X_m$ for $n \geq m$

Martingale convergence theorem (Doob, 1953) If $(X_n)_{n=1}^{\infty}$ is a martingale, and $\sup \mathbb{E}[|X_n|] < \infty$, then $X_n \to X_\infty$ almost surely.
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$$\sum_{n=1}^{\infty} \mathbb{E}\left[\left(\mathbb{E}[X_{n+1}|\mathcal{F}_n] - X_n\right) \mathbb{1}_{\{\mathbb{E}[X_{n+1}|\mathcal{F}_n] - X_n > 0\}}\right] < \infty$$

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Proposition If $s_{n+1} = s_n - \epsilon_n H_n(s_n)$, with $H_n(s_n)$ an unbiased estimator for $\nabla C(s_n)$, and C satisfies

1. C has a unique minimiser $x^\star$
2. $\forall \epsilon > 0, \inf_{\|x-x^\star\|_2^2 > \epsilon} \langle x - x^\star, \nabla C(x) \rangle > 0$
3. $\mathbb{E}\left[\|H_n(x)\|_2^2\right] \leq A + B\|x - x^\star\|_2^2$ for some $A, B \geq 0$ independent of n

then subject to $\sum_n \epsilon_n = \infty$ and $\sum_n \epsilon_n^2 < \infty$ we have $s_n \to x^\star$

Proof structure The proof is largely the same as for the deterministic discrete case, but the extra conditions in the statement deal with the control we need over the unbiased gradient estimators.

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1. Define Lyapunov process $h_n = \|s_n - x^\star\|_2^2$
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Consider the positive variations $h_n^+ = \max(0, h_{n+1} - h_n)$
By exactly the same calculation as in the deterministic discrete case:

$$h_{n+1} - h_n = -2\epsilon_n \langle s_n - x^\star, H_n(s_n)\rangle + \epsilon_n^2 \|H_n(s_n)\|_2^2$$

So

$$\mathbb{E}\left[h_{n+1} - h_n | \mathcal{F}_n\right] = -2\epsilon_n \langle s_n - x^\star, \nabla C(s_n)\rangle + \epsilon_n^2 \mathbb{E}\left[\|H_n(s_n)\|_2^2 \middle| \mathcal{F}_n\right]$$

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Show that h_n converges almost surely

Exactly the same as for discrete gradient descent:

- Assume $\mathbb{E}\left[\|H_n(x)\|_2^2\right] \leq A + B\|x - x^\star\|_2^2$
- Introduce $\mu_n = \prod_{i=1}^n \frac{1}{1+\epsilon_i^2 B}$ and $h'_n = \mu_n h_n$

Get:

$$\mathbb{E}\left[h'_{n+1} - h'_n \middle| \mathcal{F}_n\right] \leq \epsilon_n^2 \mu_n A$$

$$\implies \mathbb{E}\left[(h'_{n+1} - h'_n)\mathbb{1}_{\mathbb{E}\left[h'_{n+1} - h'_n \middle| \mathcal{F}_n\right] > 0} \middle| \mathcal{F}_n\right] \leq \epsilon_n^2 \mu_n A$$

$\sum_{n=1}^\infty \epsilon_n^2 < \infty \implies$ Quasimartingale convergence $\implies (h'_n)_{n=1}^\infty$ converges a.s. $\implies (h_n)_{n=1}^\infty$ converges a.s.

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Show that h_n must converge to 0 almost surely

From previous calculations:

$$\mathbb{E}\left[h_{n+1} - (1 - \epsilon_n^2 B)h_n \middle| \mathcal{F}_n\right] = -2\epsilon_n \langle s_n - x^\star, \nabla C(s_n)\rangle + \epsilon_n^2 A$$

$(h_n)_{n=1}^\infty$ converges, so sequence is summable a.s. . Assume $\sum_{n=1}^\infty \epsilon_n^2 < \infty$, so right term is summable a.s., so left term side is also summable a.s. :

$$\sum_{n=1}^{\infty} \epsilon_n \langle s_n - x^\star, \nabla C(s_n)\rangle < \infty \text{almost surely}$$

If we assume in addition that $\sum_{n=1}^\infty \epsilon_n = \infty$, this forces

$$\langle s_n - x^\star, \nabla C(s_n)\rangle \to 0 \text{almost surely}$$

And by our initial assumptions about C, $(h_n)_{n=1}^\infty$ must converge to 0 almost

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Relaxing the pseudo-convexity conditions

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Often the conditions on C in the preceding theorems are not satisfied in practice. One possible way of extending ideas above: Assume:

- C is a non-negative, three-times differentiable function.
- Robbins-Monro learning rate conditions hold: $\sum_{n=1}^{\infty} \epsilon_n = \infty$, $\sum_{n=1}^{\infty} \epsilon_n^2 < \infty$
- Gradient estimate H satisfies: $\mathbb{E}\left[\|H_n(x)\|^k\right] \leq A_k + B_k\|x\|^k$ for $k = 2, 3, 4$.
- There exists $D > 0$ such that $\inf_{\|x\|^2 > D} \langle x, \nabla C(x) \rangle > 0$

Idea for proof is then:

1. For a given start position, the sequence $(s_n)_{n=1}^{\infty}$ is confined to a bounded neighbourhood of 0 almost surely.
2. Introduce the Lyapunov function $h_n = C(s_n)$, and prove its almost-sure convergence.
3. Prove that $\nabla C(s_n)$ necessarily converges almost surely.

Note that this guarantees we settle at some critical point for the function (which may be a maximum, minimum, or saddle), rather than reaching the global optimum.

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