Tutorial:
Optimization for Machine Learning

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“Instead of trying to produce a programme to simulate the adult mind, why not rather try to produce one which simulates the child's?”

A.M Turing, 1950
ML paradigm

Distribution over \( \{a\} \in \mathbb{R}^n \)

Machine

Chair/car

This tutorial - training the machine
• Efficiency
• generalization

label \( b = f_{\text{parameters}}(a) \)
Agenda

1. Learning as mathematical optimization
   • Empirical Risk Minimization
   • Basics of mathematical optimization
   • Gradient descent + SGD

2. Regularization and Generalization
   • Convex, non-smooth opt.
   • Regret minimization in games, PAC learnability

3. Gradient Descent++
   • Regularization, Adaptive Regularization and AdaGrad
   • Momentum and variance reduction
   • Second order methods
   • Constraints and the Frank-Wolfe algorithm

4. A touch of state-of-the-art

Agenda

NOT touch upon:

- Parallelism/distributed computation (asynchronous optimization, HOGWILD etc.), Bayesian inference in graphical models, Markov Chain Monte Carlo, Partial information and bandit algorithms, optimization for RL (policy and value iteration, policy gradient, ...), Hyperparameter optimization, ...
Mathematical optimization

Input: function $f: K \mapsto R$, for $K \subseteq \mathbb{R}^d$
Output: minimizer $x \in K$, such that $f(x) \leq f(y) \forall y \in K$

Accessing $f$?
- Value oracle (0-order opt.)
- Gradient (1st order opt.), k’th differentials (k’th order...)

Accessing $K$? (separation/membership oracle, explicit constraints)
Generally NP-hard, given full access to function.
NP-hardness of Mathematical optimization

Max Cut over $G=(V,E)$:

$$\max_{x \in [-1,1]^V} \sum_{(i,j) \in E} \frac{1 - x_i x_j}{2}$$
Supervised Learning = optimization over data (a.k.a. Empirical Risk Minimization)

Fitting the parameters of the model ("training") = optimization problem:

\[
\arg \min_{x \in \mathbb{R}^k} \frac{1}{m} \sum_{i=1 \to m} \ell(x, a_i, b_i) + R(x)
\]

\( m = \# \text{ of examples} \quad (a,b) = \text{(features, labels)} \)
\( d = \text{dimension} \)
Example: linear classification

Given a sample $S = \{(a_1, b_1), \ldots, (a_m, b_m)\}$, find hyperplane (through the origin w.l.o.g.) such that:

$$x = \arg\min_{|x| \leq 1} \# \text{ of mistakes} = \arg\min_{|x| \leq 1} \left| \{i \text{ s.t. } \text{sign} \left( x^T a_i \right) \neq b_i \} \right|$$

$$\arg\min_{|x| \leq 1} \frac{1}{m} \sum_i \ell(x, a_i, b_i) \quad \text{for} \quad \ell(x, a_i, b_i) = \begin{cases} 1 &, \quad x^T a \neq b \\ 0 &, \quad x^T a = b \end{cases}$$

NP hard!
Example: deep neural net classification

Given a sample $S = \{(a_1, b_1), \ldots, (a_m, b_m)\}$, find a depth $N$ ResNet such that:

$W = \arg \min_{|W| \leq K} \# \text{ of mistakes} =$

$$\arg \min_{|W| \leq K} |\{i \text{ s.t. } \text{sign}(\text{Net}_W(a_i)) \neq b_i\}|$$

$$\arg \min_{|W| \leq K} \frac{1}{m} \sum_i \ell(W, a_i, b_i) \quad \text{for } \ell(W, a_i, b_i) = \begin{cases} 1 & \text{Net}_W(a) \neq b \\ 0 & \text{Net}_W(a) = b \end{cases}$$
Sum of signs $\rightarrow$ global optimization NP-hard!

Local property that ensures global optimality?
Convexity

A function $f : \mathbb{R}^d \mapsto \mathbb{R}$ is convex if and only if:

$$f \left( \frac{1}{2} x + \frac{1}{2} y \right) \leq \frac{1}{2} f(x) + \frac{1}{2} f(y)$$

- Informally: smiley 😊
- Alternative definition:

$$f(y) \geq f(x) + \nabla f(x)^T (y - x)$$
Convex sets

Set $K$ is convex if and only if:

$x, y \in K \Rightarrow (\frac{1}{2}x + \frac{1}{2}y) \in K$
Loss functions $\ell(x, a_i, b_i) = \ell(x^T a_i \cdot b_i)$
Convex relaxations for linear classification

\[ x = \arg \min_{|x| \leq 1} \left\{ i \mid \text{s.t. } \text{sign} \left( x^T a_i \right) \neq b_i \right\} \]

1. Ridge / linear regression \( \ell(x^T a_i, y_i) = (x^T a_i - b_i)^2 \)
2. SVM \( \ell(x^T a_i, y_i) = \max\{0, 1 - b_i x^T a_i\} \)
3. Logistic regression \( \ell(x^T a_i, y_i) = \log(1 + e^{-b_i x^T a_i}) \)
Non-Convex Optimization

Multiple unsurpassable hurdles.
- Global optimization is NP-hard
- Even deciding whether you are at a local minimum is NP-hard
So what can we hope to do?

- First Order Critical Points

\[ \{ h \mid \| \nabla f(h) \| \leq \epsilon \} \]

Good enough

\[ \lambda_{\text{min}}(\nabla^2 f(h)) > 0 \]

or

Less ideal

\[ \lambda_{\text{min}}(\nabla^2 f(h)) < 0 \]

4th order critical points: NP-hard!

\[ f(x) - f(x^*) = O(|x - x^*|^{k+1}) \]
A better baseline

• \( \epsilon \)-approximate local minimum (Nesterov and Polyak)

\[
|| \nabla f(h) || \leq \epsilon \quad \text{and} \quad \nabla^2 f(h) \succeq -\sqrt{\epsilon} I
\]

• Does not guarantee a local minimum even with \( \epsilon = 0 \) (but for some functions)
We have:
1. motivated learning as mathematical optimization
2. convexity $\rightarrow$ locally verify global optimality
3. Non-convex opt $\rightarrow$ $k^{th}$-order local opt.  
   (2$^{nd}$ is reasonable, 4$^{th}$ is NP-hard)

Next $\rightarrow$ algorithms!
Unconstrained Gradient Descent

$$-\left[\nabla f(x)\right]_i = -\frac{\partial}{\partial x_i} f(x)$$

$$x_{t+1} \leftarrow x_t - \eta \nabla f(x_t)$$
Smooth functions

$\beta = \text{smoothness, simplified}:$

$$-\frac{\beta}{2} I \leq \nabla^2 f(x) \leq \frac{\beta}{2} I$$

Why is this important?

For gradients to be meaningful at all...

Remark: any function can be “smoothed” by local integration
Convergence of gradient descent

\[ x_{t+1} \leftarrow x_t - \eta \nabla f(x_t) \]

Theorem: for \( \beta \)-smooth M-bounded functions, step size \( \eta = \frac{1}{\beta} \),

\[ \frac{1}{T} \sum_t |\nabla f(x_t)|^2 \leq \frac{2M\beta}{T} \]

Thus, there exists a time for which:

\[ |\nabla f(x_t)|^2 \leq \frac{2M\beta}{T} \]

convex \( f \) \( \rightarrow \) global convergence:

\[ f(x_t) - f(x^*) \leq |x_t - x^*| |\nabla f(x_t)| = O\left(\frac{D}{\sqrt{T}}\right) \]
Proof:

1. The \textbf{descent lemma}:

\[
\begin{align*}
    f(x_t) - f(x_{t+1}) &\geq -\nabla f(x_t)(x_{t+1} - x_t) - \frac{1}{2} \beta |x_t - x_{t+1}|^2 \\
    &= \eta |\nabla_t|^2 - \frac{1}{2} \beta \eta^2 |\nabla_t|^2 \\
    &= \frac{1}{2\beta} |\nabla_t|^2
\end{align*}
\]

2. Summing over all iterations:

\[
\begin{align*}
    M &\geq f(x_1) - f(x^*) \geq \sum_t f(x_t) - f(x_{t+1}) \geq \frac{1}{2\beta} \sum_t |\nabla_t|^2 \\
    \text{and thus,} \quad \frac{1}{T} \sum_t |\nabla f(x_t)|^2 &\leq \frac{2M \beta}{T}
\end{align*}
\]
For convex functions:

\[ f(x) - f(x^*) \leq \nabla f(x)(x^* - x) \leq D|\nabla f(x)| \]

Thus, in \( T \) iterations, exists an iterate \( t \) for which:

\[ f(x) - f(x^*) \leq \frac{D \sqrt{2M\beta}}{\sqrt{T}} \]
Our objective function:

\[
    f(x) = \arg \min_{x \in \mathbb{R}^d} \frac{1}{m} \sum_{i=1}^{m} \ell_i(x, a_i, b_i) + R(x)
\]

\(m = \# \text{ of examples } (a,b) = (\text{features, labels}). \quad d = \text{dimension}\)

→ Gradients are expensive! (entire data set per iteration)
→ What about non-smooth functions? (non-convex: infeasible)
→ How good is a local minimum in terms of \textbf{generalization}?
→ Can we get faster rates?
Stochastic gradient descent

\[
\arg \min_{x \in \mathbb{R}^d} f(x) = \mathbb{E}_{(a_i, b_i)}[\ell_i(x, a_i, b_i)]
\]

“Random approximation” (Robbins/Monro ’51)

estimate the gradient using a single example: \( f_t(x) = \ell_i(x, a_i, b_i) \)

\[
\hat{\nabla} = \mathbb{E}[\nabla f(x)] = \mathbb{E}_{(a_i, b_i)}[\nabla \ell_i(x, a_i, b_i)]
\]

move in the direction of estimator! \( x_{t+1} \leftarrow x_t - \eta \hat{\nabla}(x_t) \)

Convergence?

Variance of gradient estimator: \( \mathbb{E}[||\nabla||^2] = \sigma^2 \)
Stochastic vs. full gradient descent
Convergence of SGD

\[ x_{t+1} \leftarrow x_t - \eta \nabla f(x_t) \]

Theorem: for \( \beta \)-smooth M-bounded functions, step size

\[ \eta = \sqrt{\frac{M}{T \beta \sigma^2}}, \]

\[
\frac{1}{T} \sum_t \| \nabla f(x_t) \|^2 \leq \sqrt{\frac{M \beta \sigma^2}{T}}
\]
Proof:

1. The **descent lemma**: 

   \[ E[f(x_t) - f(x_{t+1})] \geq E\left[ -\nabla f(x_t)(x_{t+1} - x_t) - \frac{1}{2}\beta|x_t - x_{t+1}|^2 \right] \]

   \[ = E\left[ \nabla_t \cdot \eta \nabla_t - \frac{1}{2}\beta \eta^2 |\nabla_t|^2 \right] = \eta |\nabla_t|^2 - \frac{1}{2}\beta \eta^2 \sigma^2 \]

2. Summing over all iterations:

   \[ M \geq f(x_1) - f(x^*) \geq \sum_t f(x_t) - f(x_{t+1}) \geq \eta \sum_t |\nabla_t|^2 - \frac{1}{2}\beta \eta^2 \sigma^2 T \]

   and thus, \( \frac{1}{T} \sum_t |\nabla f(x_t)|^2 \leq \frac{M}{\eta T} + \eta \beta \sigma^2 \leq \sqrt{\frac{M \beta \sigma^2}{T}} \)
Our objective function:

\[ f(x) = \arg \min_{x \in \mathbb{R}^d} \frac{1}{m} \sum_{i=1}^{m} \ell_i(x, a_i, b_i) + R(x) \]

\( m = \# \) of examples \((a,b) = (\text{features, labels})\). \( d = \) dimension

→ Gradients are expensive! (entire data set per iteration)
→ What about non-smooth functions? (non-convex: infeasible)
→ How good is a local minimum in terms of generalization?
→ Can we get faster rates?
Tutorial: PART 2

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4. A touch of state-of-the-art
→ What about non-smooth functions? (non-convex: infeasible)
→ Gradients are expensive! (entire data set per iteration)
→ How good is a local minimum in terms of generalization?
→ Can we get faster rates?

→ convex optimization
Statistical (PAC) learning

Nature: i.i.d from distribution $D$ over $A \times B = \{(a, b)\}$

- learner:
- Hypothesis $h$
- Loss, e.g. $\ell(h, (a, b)) = (h(a) - b)^2$

$$err(h) = \mathbb{E}_{a,b \sim D}[\ell(h, (a, b))]$$

Hypothesis class $H: X \to Y$ is learnable if $\forall \epsilon, \delta > 0$ exists algorithm s.t. after seeing $m$ examples, for $m = poly(\delta, \epsilon, dimension(H))$ finds $h$ s.t. w.p. $1 - \delta$:

$$err(h) \leq \min_{h^* \in \mathcal{H}} err(h^*) + \epsilon$$
More powerful setting: Online Learning in Games

Iteratively, for $t = 1, 2, \ldots, T$

Player: $h_t \in H$

Adversary: $(a_t, b_t) \in A$

Loss $\ell(h_t, (a_t, b_t))$

Goal: minimize (average, expected) regret:

$$\frac{1}{T} \left[ \sum_t \ell(h_t, (a_t, b_t)) - \min_{h^* \in H} \sum_t \ell(h^*, (a_t, b_t)) \right] \xrightarrow{T \to \infty} 0$$

Vanishing regret $\rightarrow$ generalization in PAC setting! (online2batch)

From this point onwards: $f_t(x) = \ell(x, a_t, b_t) = \text{loss for one example}$

Can we minimize regret efficiently?
Online gradient descent

\[ y_{t+1} = x_t - \eta \nabla f_t(x_t) \]

\[ x_{t+1} = \arg \min_{x \in K} \| y_{t+1} - x_t \| \]

Theorem: \( \text{Regret} = \sum_t f_t(x_t) - \sum_t f_t(x^*) = O(\sqrt{T}) \)
Online gradient descent

\[ y_{t+1} \leftarrow x_t - \eta \nabla f_t(x_t) \]
\[ x_{t+1} = \arg\min_{x \in K} |y_{t+1} - x| \]

Theorem: for step size \( \eta = \frac{D}{G \sqrt{T}} \), NO SMOOTHNESS REQUIRED!!

\[
\sum_t f_t(x_t) - \min_{x^*} \sum_t f_t(x^*) \leq DG \sqrt{T}
\]

Where:
- \( G = \) upper bound on norm of gradients
  \[ |\nabla f_t(x_t)| \leq G \]
- \( D = \) diameter of constraint set
  \[ \forall x, y \in K \text{ . } |x - y| \leq D \]
Proof:

1. **Observation 1:**
\[
|x^* - y_{t+1}|^2 = |x^* - x_t|^2 - 2\eta \nabla f_t(x_t)(x_t - x^*) + \eta^2 |\nabla f_t(x_t)|^2
\]

2. **Observation 2:**
\[
|x^* - x_{t+1}|^2 \leq |x^* - y_{t+1}|^2
\]

This is the Pythagorean theorem:
Proof:

1. Observation 1:
   \[ |x^* - y_{t+1}|^2 = |x^* - x_t|^2 - 2\eta \nabla f_t(x_t)(x_t - x^*) + \eta^2 |\nabla f_t(x_t)|^2 \]

2. Observation 2:
   \[ |x^* - x_{t+1}|^2 \leq |x^* - y_{t+1}|^2 \]

Thus:
   \[ |x^* - x_{t+1}|^2 \leq |x^* - x_t|^2 - 2\eta \nabla f_t(x_t)(x_t - x^*) + \eta^2 G^2 \]

And hence:
   \[
   \frac{1}{T} \sum_t [f_t(x_t) - f_t(x^*)] \leq \frac{1}{T} \sum_t \nabla f_t(x_t)(x_t - x^*) \\
   \leq \frac{1}{T} \sum_t \frac{1}{2\eta} \left( |x^* - x_{t+1}|^2 - |x^* - x_t|^2 \right) + \frac{\eta}{2} G^2 \\
   \leq \frac{1}{T \cdot 2\eta} D^2 + \frac{\eta}{2} G^2 \leq \frac{DG}{\sqrt{T}}
   \]

\[ y_{t+1} \leftarrow x_t - \eta \nabla f(x_t) \]

\[ x_{t+1} = \arg \min_{x \in K} |y_{t+1} - x| \]
Lower bound

\[ \text{Regret} = \Omega(\sqrt{T}) \]

- 2 loss functions, \( T \) iterations:
  - \( K = [-1,1] \), \( f_1(x) = x \), \( f_2(x) = -x \)
  - Second expert loss = first \(* -1\)
- Expected loss = 0 (any algorithm)
- Regret = (compared to either -1 or 1)

\[ E[|\#1's - \#(-1)'s|] = \Omega(\sqrt{T}) \]
SGD: non-smooth case

Learning problem \[ \arg \min_{x \in \mathbb{R}^d} F(x) = E_{(a_i, b_i)}[\ell_i(x, a_i, b_i)] \]

random example: \[ f_t(x) = \ell_i(x, a_i, b_i) \]

1. We have proved: (for any sequence of \( \nabla_t \))

\[
\frac{1}{T} \sum_t \nabla_t^T x_t \leq \min_{x^* \in \mathbb{R}^d} \frac{1}{T} \sum_t \nabla_t^T x^* + \frac{D_G}{\sqrt{T}}
\]

2. Taking (conditional) expectation:

\[
E \left[ F \left( \frac{1}{T} \sum_t x_t \right) - \min_{x^* \in \mathbb{R}^d} F(x^*) \right] \leq E \left( \frac{1}{T} \sum_t \nabla_t^T (x_t - x^*) \right) \leq \frac{D_G}{\sqrt{T}}
\]

One example per step, same convergence as GD, & gives direct generalization!
(formally needs martingales)

\[ O \left( \frac{d}{\epsilon^2} \right) \text{ vs. } O \left( \frac{md}{\epsilon^2} \right) \text{ total running time for } \epsilon \text{ generalization error.} \]
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4. A touch of state of the art
Regularization & Gradient Descent++
Why “regularize”?

- Statistical learning theory / Occam’s razor:
  # of examples needed to learn hypothesis class ~ it’s “dimension”
  - VC dimension
  - Fat-shattering dimension
  - Rademacher width
  - Margin/norm of linear/kernel classifier

- PAC theory: Regularization  \(<->\) reduce complexity
- Regret minimization: Regularization  \(<->\) stability
Condition number of convex functions

defined as $\gamma = \frac{\beta}{\alpha}$, where (simplified)

$$0 < \frac{\alpha}{2} I \leq \nabla^2 f(x) \leq \frac{\beta}{2} I$$

$\alpha = \text{strong convexity}, \beta = \text{smoothness}$

Non-convex smooth functions: (simplified)

$$-\frac{\beta}{2} I \leq \nabla^2 f(x) \leq \frac{\beta}{2} I$$

Why do we care?

well-conditioned functions exhibit much faster optimization!

Important for regularization
Minimize regret: best-in-hindsight

\[
\text{Regret} = \sum_{t} f_t(x_t) - \min_{x^* \in K} \sum_{t} f_t(x^*)
\]

• Most natural:

\[
x_t = \arg \min_{x \in K} \sum_{i=1}^{t-1} f_i(x)
\]

• Provably works [Kalai-Vempala’05]:

\[
x_t' = \arg \min_{x \in K} \sum_{i=1}^{t} f_i(x) = x_{t+1}
\]

• So if \( x_t \approx x_{t+1} \), we get a regret bound
• But instability \(|x_t - x_{t+1}|\) can be large!
Fixing FTL: Follow-The-Regularized-Leader (FTRL)

- Linearize: replace $f_t$ by a linear function, $\nabla f_t(x_t)^T x$
- Add regularization:

$$x_t = \arg\min_{x \in K} \sum_{i=1 \ldots t-1} \nabla_t^T x + \frac{1}{\eta} R(x)$$

- $R(x)$ is a strongly convex function, ensures stability:

$$\nabla_t^T (x_t - x_{t+1}) = O(\eta)$$
FTRL vs. gradient descent

• \( R(x) = \frac{1}{2} \| x \|^2 \)

\[
x_t = \arg \min_{x \in K} \sum_{i=1}^{t-1} \nabla f_i(x_i)^\top x + \frac{1}{\eta} R(x)
\]

\[
= \Pi_K \left( -\eta \sum_{i=1}^{t-1} \nabla f_i(x_i) \right)
\]

• *Essentially* OGD: starting with \( y_1 = 0 \), for \( t = 1, 2, \ldots \)

\[
x_t = \Pi_K(y_t)
\]

\[
y_{t+1} = y_t - \eta \nabla f_t(x_t)
\]
FTRL vs. Multiplicative Weights

- Experts setting: $K = \Delta_n$ distributions over experts
- $f_t(x) = c_t^T x$, where $c_t$ is the vector of losses
- $R(x) = \sum_i x_i \log x_i$: negative entropy

$$x_t = \arg \min_{x \in K} \sum_{i=1}^{t-1} \nabla f_i(x_i)^\top x + \frac{1}{\eta} R(x)$$

$$= \exp \left( -\eta \sum_{i=1}^{t-1} c_i \right) / Z_t$$

- Gives the Multiplicative Weights method!

**Entrywise exponential**

**Normalization constant**
FTRL $\Leftrightarrow$ Online Mirror Descent

$$x_t = \arg\min_{x \in K} \sum_{i=1}^{t-1} \nabla f_i(x_i) \top x + \frac{1}{\eta} R(x)$$

**Bregman Projection:**

$$\Pi^K_R(y) = \arg\min_{x \in K} B_R(x \| y)$$

$$B_R(x \| y) := R(x) - R(y) - \nabla R(y) \top (x - y)$$

$$x_t = \Pi^K_R(y_t)$$

$$y_{t+1} = (\nabla R)^{-1}(\nabla R(y_t) - \eta \nabla f_t(x_t))$$
GD++

#1: Adaptive Regularization
Adaptive Regularization: AdaGrad

- Consider generalized linear model, prediction is function of $a^T x$
  \[ \nabla f_t(x) = \ell(a_t, b_t, x)a_t \]

- OGD update: $x_{t+1} = x_t - \eta \nabla_t = x_t - \eta \ell(a_t, b_t, x)a_t$

- features treated equally in updating parameter vector

- In typical text classification tasks, feature vectors $a_t$ are very sparse, Slow learning!

- Adaptive regularization: per-feature learning rates
Optimal regularization

• The general RFTL form

\[ x_t = \arg \min_{x \in K} \sum_{i=1 \ldots t-1} f_i(x) + \frac{1}{\eta} R(x) \]

• Which regularizer to pick?
• AdaGrad: treat this as a learning problem!
  Family of regularizations:

\[ R(x) = |x|^2_A \quad s.t. \quad A \succeq 0 , \text{Trace}(A) = d \]

• Objective in matrix world: best regret in hindsight!
AdaGrad

• Set $x_1 \in K$ arbitrarily

• For $t = 1, 2, \ldots$,

  1. use $x_t$ obtain $f_t$, and gradient $g_t = \nabla f(x_t)$
  2. compute $x_{t+1}$ as follows:

\[
G_t = \sum_{i=1}^{t} g_i g_i^\top
\]

\[
x_{t+1} = x_t - \eta G_t^{-1/2} g_t \text{ or diagonal version } x_{t+1} = x_t - \eta \text{ diag}(G_t)^{-1/2} g_t
\]

\[
y_{t+1} = \arg \min_{x \in K} (y_{t+1} - x)^\top G_t (y_{t+1} - x)
\]
Intuition: Adaptive Preconditioning

- Per-coordinate scaling matrix $D_t = \left[ \sum_{s=1}^{t} \text{diag}(g_s[i])^2 \right]^{-1/2}$
- Adaptive methods learn $D$ which makes the loss surface more isotropic

$f(x) \mapsto f(Dx)$
The ratio of adaptivity

- Theorem 1: (informal) AdaGrad has regret within factor at most $O(d)$ from the best regularization in hindsight from the family
  
  $R(x) = |x|^2_A \quad s.t. \quad A \succeq 0, \text{Trace}(A) = d$

- Define ratio of adaptivity

  $\mu := \frac{\sum_{t=1}^T \langle g_t, x_t - x^* \rangle}{\|x_1 - x^*\| \sqrt{\sum_{t=1}^T \|g_t\|^2}} = \frac{\text{AdaGrad regret}}{\text{worst-case OGD regret}}$

- Theorem 2: $\mu = O \left( \sum_i \sqrt{\sum_t \nabla^2_{t,i}} \right) \in \left[ \frac{1}{\sqrt{d}}, \sqrt{d} \right]$

- Infrequently occurring, or small-scale, features have small influence on regret (and therefore, convergence to optimal parameter)
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Accelerating gradient descent?

1. Adaptive regularization (AdaGrad) works for non-smooth & non-convex

2. Variance reduction uses special ERM structure very effective for smooth & convex

3. Acceleration/momentum smooth convex only, general purpose optimization since 80’s
GD++

#2: Variance Reduction
Recall: smooth gradient descent

The descent lemma, \( \beta \)-smooth functions: (algorithm: \( x_{t+1} = x_t - \eta \nabla_t \))

\[
f(x_{t+1}) - f(x_t) \leq \nabla_t (x_{t+1} - x_t) + \beta |x_t - x_{t+1}|^2
\]

\[
= -(\eta + \beta \eta^2) |\nabla_t|^2 = -\frac{1}{4\beta} |\nabla_t|^2
\]

Thus, for \( M \)-bounded functions: (\(|f(x_t)| \leq M\))

\[
-2M \leq f(x_T) - f(x_1) = \sum_t [f(x_{t+1}) - f(x_t)] \leq -\frac{1}{4\beta} \sum_t |\nabla_t|^2
\]

Thus, exists a \( t \) for which,

\[
|\nabla_t|^2 \leq \frac{8M\beta}{T}
\]
Smooth gradient descent

Conclusions: for $x_{t+1} = x_t - \eta \nabla_t$ and $T = \Omega \left( \frac{1}{\epsilon} \right)$, finds

$$\left| \nabla_t \right|^2 \leq \epsilon$$

Holds even for non-convex functions
Non-convex stochastic gradient descent

The descent lemma, $\beta$-smooth functions: (algorithm: $x_{t+1} = x_t - \eta \nabla_t$)

$$E[f(x_{t+1}) - f(x_t)] \leq E[\nabla_t(x_{t+1} - x_t) + \beta |x_t - x_{t+1}|^2]$$

$$= E\left[-\nabla_t \cdot \eta \nabla_t + \beta |\nabla_t|^2\right] = -\eta \nabla_t^2 + \eta^2 \beta E|\nabla_t|^2$$

$$= -\eta \nabla_t^2 + \eta^2 \beta (\nabla_t^2 + \text{var}(\nabla_t))$$

Thus, for $M$-bounded functions: ($|f(x_t)| \leq M$)

$$T = O\left(\frac{M\beta}{\epsilon^2}\right) \quad \Rightarrow \quad \exists t \leq T . \ |\nabla_t|^2 \leq \epsilon$$
Controlling the variance: Interpolating GD and SGD

Model: both full and stochastic gradients. Estimator combines both into lower variance RV:

\[ x_{t+1} = x_t - \eta [\tilde{V} f(x_t) - \tilde{V} f(x_0) + \nabla f(x_0)] \]

Every so often, compute full gradient and restart at new \( x_0 \).

Theorem: [Schmidt, LeRoux, Bach ‘12]

Variance reduction for well-conditioned functions

\[ 0 < \alpha I \lesssim \nabla^2 f(x) \lesssim \beta I, \quad \gamma = \frac{\beta}{\alpha} \]

Produces an \( \epsilon \) approximate solution in time

\[ O \left( (m + \gamma) d \log \frac{1}{\epsilon} \right) \]

\( \gamma \) should be interpreted as \( \frac{1}{\epsilon} \)
Variance Reduction: analysis

For smooth functions (non-stochastic):

\[
\frac{1}{\beta} |\nabla_t|^2 \leq h_t = f(x_t) - f(x^*)
\]

Variance-reduced estimator advantage:

\[
|\tilde{\nabla}_t|^2 = |\tilde{\nabla} f(x_t) - \tilde{\nabla} f(x_0) + \nabla f(x_0)|^2 \leq \\
\leq 2|\tilde{\nabla} f(x_t) - \tilde{\nabla} f(x_0)|^2 + 2|\nabla f(x_0)|^2
\]

Since \((a + b)^2 \leq 2a^2 + 2b^2\)

\[
\leq 2G^2 |x_t - x_0|^2 + 2\beta h_t
\]

G-smoothness for \(\tilde{\nabla} f\), smoothness

\[
\leq 2 \frac{G^2}{\alpha} h_t + 2\beta h_t \quad \text{by strong convexity}
\]

\[
= O(\beta h_T)
\]
Variance Reduction: analysis

Regret minimization for strongly convex functions:

\[ h^{k+1} = \frac{1}{T} \sum_t h_t \leq \frac{1}{\alpha T} \sum_t |\tilde{v}_t|^2 \leq \frac{\beta \log T}{\alpha T} h^k \]

Thus, after \( O\left(\gamma = \frac{\beta}{\alpha}\right) \) iterations, we have that the average distance \( \frac{1}{2} \) of what it (on average) was:

\[ E[h^{k+1}] \leq \frac{1}{2} E[h^k] \]

Thus \( O\left(\log \frac{1}{\epsilon}\right) \) epochs. Each epoch: one full gradient, \( T \) stochastic gradients. Total running time:

\[ O\left((m + \gamma)d \log \frac{1}{\epsilon}\right) \]
GD++

#3: Momentum and Nesterov acceleration
Acceleration/momentum [Nesterov ‘83]

• Optimal gradient complexity (smooth, convex)

• modest practical improvements, non-convex “momentum” methods.

• With variance reduction, fastest possible running time of first-order methods:
  \[ O \left( (m + \sqrt{ym}) d \log \frac{1}{\epsilon} \right) \]

[Woodworth, Srebro ’15] – tight lower bound w. gradient oracle
Experiments w. convex losses

Improve upon GradientDescent++?
Next few slides:

Move from first order (GD++) to second order
Higher Order Optimization

- Gradient Descent – Direction of Steepest Descent
- Second Order Methods – Use Local Curvature
Newton’s method (+ Trust region)

\[ x_{t+1} = x_t - \eta \left[ \nabla^2 f(x) \right]^{-1} \nabla f(x) \]

For non-convex function: can move to $\infty$
Solution: solve a quadratic approximation in a local area (trust region)
Newton’s method (+ Trust region)

\[ x_{t+1} = x_t - \eta \left[ \nabla^2 f(x) \right]^{-1} \nabla f(x) \]

\( d^3 \) time per iteration!
Infeasible for ML!!

Till recently...
Speed up the Newton direction computation??

• Spielman-Teng ‘04: diagonally dominant systems of equations in linear time!
  • 2015 Godel prize
  • Used by Daitch-Speilman for faster flow algorithms

• Erdogu-Montanari ‘15: low rank approximation & inversion by Sherman-Morisson
  • Allow stochastic information
  • Still prohibitive: rank * d^2
Stochastic Newton?

\[ x_{t+1} = x_t - \eta \left[ \nabla^2 f(x) \right]^{-1} \nabla f(x) \]

- ERM, rank-1 loss: \( \arg \min_x E_{\{i \sim m\}}[\ell(x^T a_i, b_i) + \frac{1}{2} |x|^2] \)

- unbiased estimator of the Hessian:
  \[ \tilde{\nabla}^2 = a_i a_i^T \cdot \ell'(x^T a_i, b_i) + I \quad i \sim U[1, ..., m] \]

- clearly \( E[\tilde{\nabla}^2] = \nabla^2 f \), but \( E[\tilde{\nabla}^{2^{-1}}] \neq \nabla^2 f^{-1} \)
Circumvent Hessian creation and inversion!

• 3 steps:
  • (1) represent Hessian inverse as infinite series
    \[ \nabla^{-2} = \sum_{i=0}^{\infty} (I - \nabla^2)^i 
    \]
  • (2) sample from the infinite series (Hessian-gradient product), ONCE
    \[ \nabla^2 f^{-1} \nabla f = \sum_i (I - \nabla^2 f)^i \nabla f = E_{i \sim N} (I - \nabla^2 f)^i \nabla f \cdot \frac{1}{\Pr[i]} \]
  • (3) estimate Hessian-power by sampling i.i.d. data examples
    \[ = E_{i \sim N, k \sim [i]} \left[ \prod_{k=1}^{i} (I - \nabla^2 f_k) \nabla f \cdot \frac{1}{\Pr[i]} \right] \]
Linear-time Second-order Stochastic Algorithm (LiSSA)

- Use the estimator $\hat{\nabla}^{-2}f$ defined previously
- Compute a full (large batch) gradient $\nabla f$
- Move in the direction $\hat{\nabla}^{-2}f \nabla f$
- Theoretical running time to produce an $\epsilon$ approximate solution for $\gamma$ well-conditioned functions (convex): [Agarwal, Bullins, Hazan ‘15]

$$0 \left( dm \log \frac{1}{\epsilon} + \sqrt{\gamma d} d \log \frac{1}{\epsilon} \right)$$

1. Faster than first-order methods!
2. Indications this is tight [Arjevani, Shamir ‘16]
What about constraints??

Next few slides – projection free (Frank-Wolfe) methods
### Recommendation systems

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*rating of user $i$ for movie $j$*
**Recommendation systems**

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Recommendation systems

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*get new data*
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Assume low rank of “true matrix”, convex relaxation: bounded trace norm
Bounded trace norm matrices

- Trace norm of a matrix = sum of singular values
- $K = \{ X \mid X \text{ is a matrix with trace norm at most } D \}$

- Computational bottleneck: projections on $K$ require eigendecomposition: $O(n^3)$ operations

- But: linear optimization over $K$ is easier computing top eigenvector; $O(\text{sparsity})$ time
Projections $\rightarrow$ linear optimization

1. Matrix completion ($K =$ bounded trace norm matrices) 
   eigen decomposition

2. Online routing ($K =$ flow polytope) 
   conic optimization over flow polytope

3. Rotations ($K =$ rotation matrices) 
   conic optimization over rotations set

4. Matroids ($K =$ matroid polytope) 
   convex opt. via ellipsoid method
Conditional Gradient algorithm [Frank, Wolfe ’56]

Convex opt problem:
\[
\min_{x \in K} f(x)
\]

- \( f \) is smooth, convex
- linear opt over \( K \) is easy

\[
v_t = \arg \min_{x \in K} \nabla f(x_t)^\top x
\]

\[
x_{t+1} = x_t + \eta_t (v_t - x_t)
\]

1. At iteration \( t \): convex comb. of at most \( t \) vertices (sparsity)
2. No learning rate. \( \eta_t \approx \frac{1}{t} \) (independent of diameter, gradients etc.)
FW theorem

\[ x_{t+1} = x_t + \eta_t (v_t - x_t) , \quad v_t = \arg \min_{x \in K} \nabla_t^T x \]

Theorem: \[ f(x_t) - f(x^*) = O\left(\frac{1}{t}\right) \]

Proof, main observation:

\[
\begin{align*}
&f(x_{t+1}) - f(x^*) = f(x_t + \eta_t (v_t - x_t)) - f(x^*) \\
&\leq f(x_t) - f(x^*) + \eta_t (v_t - x_t)^\top \nabla_t + \frac{\eta_t^2 \beta}{2} \|v_t - x_t\|^2 \\
&\leq f(x_t) - f(x^*) + \eta_t (x^* - x_t)^\top \nabla_t + \frac{\eta_t^2 \beta}{2} \|v_t - x_t\|^2 \\
&\leq f(x_t) - f(x^*) + \eta_t (f(x^*) - f(x_t)) + \frac{\eta_t^2 \beta}{2} \|v_t - x_t\|^2 \\
&\leq (1 - \eta_t)(f(x_t) - f(x^*)) + \frac{\eta_t^2 \beta}{2} D^2.
\end{align*}
\]

Thus: \[ h_t = f(x_t) - f(x^*) \]

\[ h_{t+1} \leq (1 - \eta_t) h_t + O(\eta_t^2) \]

\[ \eta_t, h_t = O\left(\frac{1}{t}\right) \]
Online Conditional Gradient

- Set $x_1 \in K$ arbitrarily
- For $t = 1, 2, \ldots,$
  1. Use $x_t$, obtain $f_t$
  2. Compute $x_{t+1}$ as follows

$$v_t = \arg \min_{x \in K} \left( \sum_{i=1}^{t} \nabla f_i(x_i) + \beta_t x_t \right)^T x$$

$$x_{t+1} \leftarrow (1 - t^{-\alpha}) x_t + t^{-\alpha} v_t$$

Theorem: [Hazan, Kale ’12] \hspace{1cm} \textbf{Regret} = O(T^{3/4})

Theorem: [Garber, Hazan ‘13] For polytopes, strongly-convex and smooth losses,

1. Offline: convergence after $t$ steps: $e^{-\Omega(t)}$
2. Online: $\textbf{Regret} = O(\sqrt{T})$
Agenda

1. Learning as mathematical optimization
   - Empirical Risk Minimization
   - Basics of mathematical optimization
   - Gradient descent + SGD

2. Regularization and Generalization
   - Convex, non-smooth opt.
   - Regret minimization in games, PAC learnability

3. Gradient Descent++
   - Regularization, Adaptive Regularization and AdaGrad
   - Momentum and variance reduction
   - Second order methods
   - Constraints and the Frank-Wolfe algorithm

4. A touch of state of the art
   * Some slides by Cyril Zhang
Non-convex optimization in ML

\[
\arg \min_{x \in \mathbb{R}^d} \frac{1}{m} \sum_{i=1 \text{ to } m} \ell_i(x, a_i, b_i) + R(x)
\]
Stochastic Optimization in ML

- **Problem**: find \( \arg\min_{x \in \mathbb{R}^d} f(x) \)

- **Stochastic first-order oracle**: \( \mathbb{E}[\nabla f(x)] = \nabla f(x), \quad \mathbb{E} \left[ \|\nabla f(x)\|^2 \right] \leq \sigma^2 \)

- **SGD** [Robbins & Monro ‘51]:

\[
f(x) = x^T A x + b^T x
\]
“Modern ML is SGD++”

**Variance Reduction**
[Le Roux et al. ‘12]
[Shalev-Shwartz & Zhang ‘12]
[Johnson & Zhang ‘13]

**Momentum**
[Polyak ‘64]
[Nemirovskii & Yudin ‘77]
[Nesterov ‘83]

**Adaptive Regularization**
[Duchi, Hazan, Singer ‘10]
[Kingma & Ba ‘14]
Adaptive Optimizers: The Usual Recipe

- Each coordinate $x[i]$ gets a learning rate $D_t[i]$
- $D_t[i]$ chosen “adaptively” using $\overline{\overline{f}}(x_{1:t})[i]$ ($g_{1:t}[i]$ for short)

- **AdaGrad**: $D_t[i] := \frac{1}{\sqrt{\sum_{s=1}^{t} (g_s[i])^2}}$

- **RMSprop**: $D_t[i] := \frac{1}{\sqrt{\sum_{s=1}^{t} 0.99^{t-s} (g_s[i])^2}}$

- **Adam**: $D_t[i] := \frac{1}{(1-0.99^t)\sqrt{\sum_{s=1}^{t} 0.99^{t-s} (g_s[i])^2}}$
Intuition: Adaptive Preconditioning

- Per-coordinate scaling matrix $D_t = [\sum_{s=1}^{t} \text{diag}(g_s[i])^2]^{-1/2}$
- Adaptive methods learn $D$ which makes the loss surface more isotropic
What about the other AdaGrad?

**diagonal** preconditioning

$O(d)$ time per iteration

**full-matrix** preconditioning

$> O(d^2)$ time per iteration
What does adaptive regularization even do?! 

**Theorem 5** Let the sequence $\{x_t\}$ be defined by Algorithm 1. For $x_t$ generated using the primal-dual subgradient update (3) with $\delta \geq \max_t \|g_t\|_\infty$, for any $x^* \in X$,

$$R_q(T) \leq \frac{\delta}{\eta} \|x^*\|_2^2 + \frac{1}{\eta} \|x^*\|_\infty^2 \sum_{i=1}^{d} \|g_{1:T,i}\|_2 + \eta \sum_{i=1}^{d} \|g_{1:T,i}\|_2.$$ 

Main theorem, AdaGrad

- No analysis for *non-convex* optimization
The Case for Full-Matrix Adaptive Regularization

- **GGT**, a new adaptive optimizer
- Efficient full-matrix (low-rank) AdaGrad

- **Theory**: “Adaptive” convergence rate on convex & non-convex $f$

- **Experiments**: viable in the deep learning era
  - GPU-friendly; not much slower than SGD on deep models
  - Accelerates training in deep learning benchmarks
  - Empirical insights on anisotropic loss surfaces, real and synthetic
The GGT Algorithm

- **SGD**: \( x_{t+1} \leftarrow x_t - \eta_t \cdot g_t \)
- **AdaGrad**: \( x_{t+1} \leftarrow x_t - \left[ \text{diag} \left( \sum_{s=1}^{t} g_s^2 \right) \right]^{-1/2} \cdot g_t \)
- **Full-Matrix AdaGrad**: \( x_{t+1} \leftarrow x_t - \left[ \sum_{s=1}^{t} g_s g_s^T \right]^{-1/2} \cdot g_t \)
- **GGT**: \( x_{t+1} \leftarrow x_t - \left[ G_t G_t^T \right]^{-1/2} \cdot g_t \)

\[
\begin{align*}
G_t & \approx 200 \\
d & \approx 10^7 \\
\begin{bmatrix}
G_t \\
g_t & \beta g_{t-1} & \beta^2 g_{t-2} & \cdots & \beta^{r-1} g_{t-r+1}
\end{bmatrix}
\end{align*}
\]
Why a low-rank preconditioner?

- **Answer 1**: want to forget stale gradients (like Adam)
- **Synthetic experiments**: logistic regression, polytope analytic center
Why a low-rank preconditioner?

Matrix ops: $O(rd^2)$
Huge SVD: $O(d^3)$

Matrix ops: $O(r^2d)$
Tiny SVD: $O(r^3)$
Large-Scale Experiments (CIFAR-10, PTB)
Visualizing Gradient Spectra

\[ \text{eigs}(\mathbf{G}_t^T \mathbf{G}_t) \]

\[ @ t = 150 \]

26-layer ResNet
CIFAR-10

3-layer LSTM
Penn Treebank
(char-level)
Theory: Convergence of Non-Convex SGD

- **Convex:** \( f(x_T) \leq \arg\min_x f(x) + \varepsilon \) in \( O\left(\frac{\sigma^2}{\varepsilon^2}\right) \) steps
- **Non-convex:** \( \exists t: \|\nabla f(x_t)\| \leq \varepsilon \) within \( O\left(\frac{\sigma^2}{\varepsilon^4}\right) \) steps
- Reduction via **modified descent lemma:**

\[
\begin{align*}
\frac{1}{\varepsilon^2} \times: \\ f(x_t) + \langle \nabla f(x), x - x_t \rangle + L\|x - x_t\|^2 &\geq f(x) \\
\end{align*}
\]

\[
\begin{align*}
\frac{1}{\varepsilon^2} \times: \\ f(x) + 2L\|x - x_t\|^2 &\geq f(x) \\
\end{align*}
\]
Theory: Adaptive Convergence Rate of GGT

- Define the *adaptivity ratio* $\mu$:

$$\mu := \frac{\sum_{t=1}^{T} g_t^\top (x_t - x^*)}{\|x_1 - x^*\| \sqrt{\sum_{t=1}^{T} \|g_t\|^2}} = \frac{\text{AdaGrad regret}}{\text{worst-case OGD regret}}$$

- [DHS10]: $\mu \leq \left[\frac{1}{\sqrt{d}}, \sqrt{d}\right]$ for diag-AdaGrad, sometimes smaller for full AdaGrad

- **Strongly convex losses**: GGT* converges in $\tilde{O}\left(\frac{\mu^2 \sigma^2}{\varepsilon}\right)$ steps

- **Non-convex reduction**: GGT* converges in $\tilde{O}\left(\frac{\mu^2 \sigma^2}{\varepsilon^4}\right)$ steps

- First step towards analyzing adaptive methods in non-convex optimization
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4. A touch of state of the art
   * Some slides by Cyril Zhang
Recap

1. Basic non-convex optimization
   - GD and SGD
2. Online learning and stochastic optimization
   - Online gradient descent, non-smooth optimization
3. Regularization and generalization
   - Multiplicative update, mirrored-descent
4. Advanced optimization
   - Adaptive Regularization, Acceleration, variance reduction, second order methods, Frank-Wolfe
5. New algorithms: GGT
collaborators: & Google Princeton-Brain

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Bibliography & more information, see:


Thank you!