Stochastic Gradient Descent

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Review: Statistical Learning Theory Framework

Our Setup from Statistical Learning Theory

The Spaces

- $\mathcal{X}$: input space
- $\mathcal{Y}$: outcome space
- $\mathcal{A}$: action space

Prediction Function (or "decision function")

A **prediction function** (or **decision function**) gets input $x \in \mathcal{X}$ and produces an action $a \in \mathcal{A}$:

$$\begin{aligned} f: \quad \mathcal{X} &\to \mathcal{A} \\ x &\mapsto f(x) \end{aligned}$$

Loss Function

A **loss function** evaluates an action in the context of the outcome y.

$$\begin{aligned} \ell: \quad \mathcal{A} \times \mathcal{Y} &\to \mathbf{R} \\ (a,y) &\mapsto \ell(a,y) \end{aligned}$$

Risk and the Bayes Prediction Function

Definition

The **risk** of a prediction function $f : \mathcal{X} \to \mathcal{A}$ is

$$R(f) = \mathbb{E}\ell(f(x), y).$$

In words, it's the **expected loss** of f on a new exampe (x, y) drawn randomly from $P_{\mathcal{X}\times\mathcal{Y}}$.

Definition

A **Bayes prediction function** $f^* : \mathcal{X} \to \mathcal{A}$ is a function that achieves the *minimal risk* among all possible functions:

$$f^* \in \operatorname*{arg\,min}_f R(f),$$

where the minimum is taken over all functions from $\mathcal{X}$ to $\mathcal{A}$.

- The risk of a Bayes prediction function is called the **Bayes risk**.

The Empirical Risk

Let $\mathcal{D}_n = ((x_1, y_1), \ldots, (x_n, y_n))$ be drawn i.i.d. from $\mathcal{P}_{\mathcal{X} \times \mathcal{Y}}$.

Definition

The **empirical risk** of $f : \mathcal{X} \to \mathcal{A}$ with respect to $\mathcal{D}_n$ is

$$\hat{R}_n(f) = \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i).$$

- But we saw that the **unconstrained** empirical risk minimizer overfits.
  - i.e. if we minize $\hat{R}_n(f)$ over **all functions**, we overfit.

Constrained Empirical Risk Minimization

Definition

A **hypothesis space** $\mathcal{F}$ is a set of functions mapping $\mathcal{X} \to \mathcal{A}$.

- It is the collection of prediction functions we are choosing from.

- **Empirical risk minimizer** (ERM) in $\mathcal{F}$ is

$$\hat{f}_n \in \operatorname*{arg\,min}_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i).$$

- From now on "ERM" always means "constrained ERM".
- So we should always specify the hypothesis space when we're doing ERM.

Example: Linear Least Squares Regression

Setup

- Input space $\mathcal{X} = \mathbf{R}^d$
- Output space $\mathcal{Y} = \mathbf{R}$
- Action space $\mathcal{Y} = \mathbf{R}$
- Loss: $\ell(\hat{y}, y) = (y - \hat{y})^2$
- **Hypothesis space:** $\mathcal{F} = \left\{ f : \mathbf{R}^d \to \mathbf{R} \mid f(x) = w^T x,\ w \in \mathbf{R}^d \right\}$

,

- Given data set $\mathcal{D}_n = \{(x_1, y_1), \ldots, (x_n, y_n)\}$,
    - Let's find the ERM $\hat{f} \in \mathcal{F}$.

Example: Linear Least Squares Regression

Objective Function: Empirical Risk

The function we want to minimize is the empirical risk:

$$\hat{R}_n(w) = \frac{1}{n}\sum_{i=1}^{n}\left(w^T x_i - y_i\right)^2,$$

where $w \in \mathbf{R}^d$ parameterizes the hypothesis space $\mathcal{F}$.

- Now let's think more generally...

Gradient Descent for Empirical Risk - Scaling Issues

Gradient Descent for Empirical Risk and Averages

- Suppose we have a hypothesis space of functions $\mathcal{F} = \left\{ f_w : \mathcal{X} \to \mathcal{A} \mid w \in \mathbf{R}^d \right\}$
  - Parameterized by $w \in \mathbf{R}^d$.
- ERM is to find w minimizing

$$\hat{R}_n(w) = \frac{1}{n} \sum_{i=1}^{n} \ell(f_w(x_i), y_i)$$

- Suppose $\ell(f_w(x_i), y_i)$ is differentiable as a function of w.
- Then we can do gradient descent on $\hat{R}_n(w)$...

Gradient Descent: How does it scale with n?

- At every iteration, we compute the gradient at current w:

$$\nabla \hat{R}_n(w) = \frac{1}{n}\sum_{i=1}^{n} \nabla_w \ell(f_w(x_i), y_i)$$

- We have to touch all n training points to take a single step. $[O(n)]$
- Will this scale to “big data”?
- Can we make progress without looking at all the data?

Stochastic Gradient Descent

“Noisy” Gradient Descent

- We know gradient descent works.
- But the gradient may be slow to compute.
- What if we just use an estimate of the gradient?
- Turns out that can work fine.
- **Intuition**:
  - Gradient descent is an interative procedure anyway.
  - At every step, we have a chance to recover from previous missteps.

Minibatch Gradient

- The **full gradient** is

$$\nabla \hat{R}_n(w) = \frac{1}{n}\sum_{i=1}^{n} \nabla_w \ell(f_w(x_i), y_i)$$

- It's an average over the **full batch** of data $\mathcal{D}_n = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.
- Let's take a random subsample of size N (called a **minibatch**):

$$(x_{m_1}, y_{m_1}), \ldots, (x_{m_N}, y_{m_N})$$

- The **minibatch gradient is**

$$\nabla \hat{R}_N(w) = \frac{1}{N}\sum_{i=1}^{N} \nabla_w \ell(f_w(x_{m_i}), y_{m_i})$$

- What can we say about the minibatch gradient? It's random. What's its expectation?

Minibatch Gradient

- What's the expected value of the **minibatch gradient**?

$$\begin{aligned}
\mathbb{E}\left[\nabla \hat{R}_N(w)\right] &= \frac{1}{N}\sum_{i=1}^{N}\mathbb{E}\left[\nabla_w \ell(f_w(x_{m_i}), y_{m_i})\right] \\
&= \mathbb{E}\left[\nabla_w \ell(f_w(x_{m_1}), y_{m_1})\right] \\
&= \sum_{i=1}^{n}\mathbb{P}(m_1 = i)\,\nabla_w \ell(f_w(x_i), y_i) \\
&= \frac{1}{n}\sum_{i=1}^{n}\nabla_w \ell(f_w(x_{m_i}), y_{m_i}) \\
&= \nabla \hat{R}_n(w)
\end{aligned}$$

- *Technical note:* We only assumed that each point in the minibatch is equally likely to be any of the n points in the batch – no independence needed. So still true if we're sampling without replacement. Still true if we sample one point randomly and reuse it N times.

Minibatch Gradient Properties

- Minibatch gradient is an **unbiased estimator** for the [full] batch gradient:

$$\mathbb{E}\left[\nabla \hat{R}_N(w)\right] = \nabla \hat{R}_n(w)$$

- The bigger the minibatch, the better the estimate.

Minibatch Gradient – In Practice

- Tradeoffs of minibatch size:
  - Bigger $N \implies$ Better estimate of gradient, but slower (more data to touch)
  - Smaller $N \implies$ Worse estimate of gradient, but can be quite fast
- Even $N = 1$ works, it's traditionally called **stochastic gradient descent** (SGD).
- These days, people use SGD to refer to minibatch SGD as well.
- If someone says "SGD", you ask – "What's your [mini]batch size?", to avoid ambiguity.

Terminology Review (Rough)

- **Gradient descent** or **"full-batch" gradient descent**
    - Use full data set of size n to determine step direction
- **Minibatch gradient descent**
    - Use a random subset of size N to determine step direction
    - Yoshua Bengio says[1]:
        - N is typically between 1 and few hundred
        - $N = 32$ is a good default value
        - With $N \geqslant 10$ we get computational speedup (per datum touched)
- **Stochastic gradient descent**
    - Minibatch with $m = 1$.
    - Use a single randomly chosen point to determine step direction.

But these days terminology isn't used so consistently, so always clarify the [mini]batch size.

[1] See Yoshua Bengio's "Practical recommendations for gradient-based training of deep architectures" http://arxiv.org/abs/1206.5533.

Minibatch Gradient Descent

Minibatch Gradient Descent (minibatch size N)

- initialize $w = 0$
- repeat
  - randomly choose N points $\{(x_i, y_i)\}_{i=1}^{N} \subset \mathcal{D}_n$
  - $w \leftarrow w - \eta \left[\frac{1}{N}\sum_{i=1}^{N} \nabla_w \ell(f_w(x_i), y_i)\right]$

Stochastic Gradient Descent (SGD)

Stochastic Gradient Descent

- initialize $w = 0$
- repeat
  - randomly choose training point $(x_i, y_i) \in \mathcal{D}_n$
  - $w \leftarrow w - \eta \underbrace{\nabla_w \ell(f_w(x_i), y_i)}_{\text{Grad(Loss on i'th example)}}$

Step Size: In practice

- For SGD, fixed step size can work well in practice.
- *Typical approach:* Fixed step size reduced by constant factor whenever validation performance stops improving.
- But no theorem for this giving performance guarantees (to my knowledge).

Robbins-Monro conditions

- For convergence guarantee, use decreasing step sizes (dampens noise in step direction).
- Let η_t be the step size at the t'th step.

Robbins-Monro Conditions

Many classical convergence results depend on the following two conditions:

$$\sum_{t=1}^{\infty} \eta_t^2 < \infty \qquad \sum_{t=1}^{\infty} \eta_t = \infty$$

- As fast as $\eta_t = O\left(\frac{1}{t}\right)$ would satisfy this... but should be faster than $O\left(\frac{1}{\sqrt{t}}\right)$.
- A useful reference for practical techniques: Leon Bottou's "Tricks": http://research.microsoft.com/pubs/192769/tricks-2012.pdf

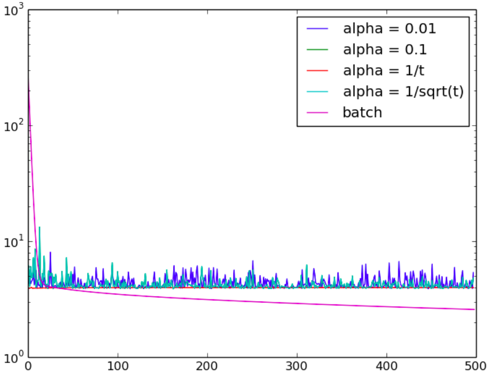
Practical Comparison of GD vs SGD

Practical Comparison of GD vs SGD

- For huge data, GD isn't practical.
- In a theoretical sense, GD is much faster than SGD... (i.e. better convergence rates)
  - but most of that benefit happens once you're already pretty close to the solution
  - much faster to add an extra decimal place of accuracy on the minimum

Does SGD Catch Up to GD?

- Ridge regression objective function value for GD and SGD with various stepsizes



- Why doesn't SGD catch up to batch GD? It does, just takes a **very** long time.
- Is it worth the wait? As we discuss in next module, probably not...