Outline

- Convex vs Nonconvex Functions
- Coordinate Descent
- Gradient Descent
- Newton’s method
- Stochastic Gradient Descent
Numerical Optimization

- Numerical Optimization:
  \[ \min_X f(X) \]

- Can be applied to computer science, economics, control engineering, operating research, ... 

- **Machine Learning**: find a model that *minimizes* the prediction error.

![Graph showing a function \( f(X) \) with an optimal solution at the bottom of the curve]
Properties of the Function

- Smooth function: a function has continuous derivative.
  
  Example: ridge regression

\[
\arg\min_w \frac{1}{2} \|Xw - y\|^2 + \frac{\lambda}{2} \|w\|^2
\]

- Non-smooth function: Lasso, primal SVM

Lasso: \( \arg\min_w \frac{1}{2} \|Xw - y\|^2 + \lambda \|w\|_1 \)

SVM: \( \arg\min_w \sum_{i=1}^n \max(0, 1 - y_i w^T x_i) + \frac{\lambda}{2} \|w\|^2 \)
Convex Functions

- A function is convex if:
  \[
  \forall x_1, x_2, \forall t \in [0, 1], f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2)
  \]

- No local optimum (why?)

Figure from Wikipedia
Convex Functions

- If \( f(x) \) is twice differentiable, then
  \[ f \text{ is convex if and only if } \nabla^2 f(x) \succeq 0 \]
- Optimal solution may not be unique:
  has a set of optimal solutions \( S \)
- Gradient: capture the first order change of \( f \):
  \[
f(x + \alpha d) = f(x) + \alpha \nabla f(x)^T d + O(\alpha^2)
\]
- If \( f \) is differentiable, we have the following optimality condition:
  \[ x^* \in S \text{ if and only if } \nabla f(x) = 0 \]
Strongly Convex Functions

- \( f \) is strongly convex if there exists a \( m > 0 \) such that
  \[
  f(y) \geq f(x) + \nabla f(x)^T(y - x) + \frac{m}{2} \|y - x\|^2
  \]

- A strongly convex function has a unique global optimum \( x^* \) (why?)

- If \( f \) is twice differentiable, then
  \[
  f \text{ is strongly convex if and only if } \nabla^2 f(x) \succ mI > 0 \text{ for all } x
  \]

- Gradient descent, coordinate descent will converge linearly (will see later)
Nonconvex Functions

- If $f$ is nonconvex, most algorithms can only converge to stationary points.
- $\bar{x}$ is a stationary point if and only if $\nabla f(\bar{x}) = 0$.
- Three types of stationary points:
  1. Global optimum
  2. Local optimum
  3. Saddle point
- Example: matrix completion, neural network, …
- Example: $f(x, y) = \frac{1}{2}(xy - a)^2$
Coordinate Descent
Coordinate Descent

- Update one variable at a time
- Coordinate Descent: repeatedly perform the following loop
  
  Step 1: pick an index $i$
  
  Step 2: compute a step size $\delta^*$ by (approximately) minimizing
  
  $$\arg\min_{\delta} f(x + \delta e_i)$$

  Step 3: $x_i \leftarrow x_i + \delta^*$
Three types of updating order:

- Cyclic: update sequence

\[ X_1, X_2, \ldots, X_n, \quad X_1, X_2, \ldots, X_n, \ldots \]

1st outer iteration \quad 2nd outer iteration

A more general setting: update each variable at least once within every \( T \) steps

Randomly permute the sequence for each outer iteration (faster convergence in practice)
Coordinate Descent (update sequence)

- Three types of updating order:
  - Cyclic: update sequence
    
    $$X_1, X_2, \ldots, X_n, \quad X_1, X_2, \ldots, X_n, \ldots$$
    
    1st outer iteration 2nd outer iteration

- A more general setting: update each variable at least once within every $T$ steps
- Randomly permute the sequence for each outer iteration (faster convergence in practice)

- Random: each time pick a random coordinate to update
  - Typical way: sample from uniform distribution
  - Sample from uniform distribution vs sample from biased distribution

P. Zhao and T. Zhang, Stochastic Optimization with Importance Sampling for Regularized Loss Minimization. In ICML 2015

D. Csiba, Z. Qu and P. Richtarik, Stochastic Dual Coordinate Ascent with Adaptive Probabilities. In ICML 2015
Greedy Coordinate Descent

- Greedy: choose the most “important” coordinate to update
- How to measure the importance?
  - By first derivative: $|\nabla_i f(x)|$
  - By first and second derivative: $|\nabla_i f(x)/\nabla^2_{ii} f(x)|$
  - By maximum reduction of objective function

$$i^* = \arg\max_{i=1,\ldots,n} \left(f(x) - \min_\delta f(x + \delta e_i)\right)$$

- Need to consider the time complexity for variable selection
- Useful for kernel SVM (see lecture 6)
Variables are divided into blocks $\{X_1, \ldots, X_p\}$, where each $X_i$ is a subset of variables and

$$X_1 \cup X_2, \ldots, X_p = \{1, \ldots, n\}, \quad X_i \cap X_j = \emptyset, \quad \forall i, j$$

Each time update a $X_i$ by (approximately) solving the subproblem within the block.

Example: alternating minimization for matrix completion (2 blocks). (See lecture 7)
Coordinate Descent (convergence)

- Converge to an optimum if \( f(\cdot) \) is convex and smooth
- Has a linear convergence rate if \( f(\cdot) \) is strongly convex
- Linear convergence: error \( f(x^t) - f(x^*) \) decays as
  \[
  \beta, \beta^2, \beta^3, \ldots
  \]
  for some \( \beta < 1 \).
- Local linear convergence: an algorithm converges linearly after
  \( \|x - x^*\| \leq K \) for some \( K > 0 \)
Coordinate Descent (nonconvex)

- Block coordinate descent with 2 blocks:
  converges to stationary points
- With $> 2$ blocks:
  converges to stationary points if each subproblem has a unique minimizer.
Coordinate Descent: other names

- Alternating minimization (matrix completion)
- Iterative scaling (for log-linear models)
- Decomposition method (for kernel SVM)
- Gauss Seidel (for linear system when the matrix is positive definite)
- ...
Gradient Descent
Gradient Descent

- Gradient descent algorithm: repeatedly conduct the following update:
  \[ x^{t+1} \leftarrow x^t - \alpha \nabla f(x^t) \]
  where \( \alpha > 0 \) is the step size
- It is a fixed point iteration method:
  \[ x - \alpha \nabla f(x) = x \] if and only if \( x \) is an optimal solution
- Step size too large \( \Rightarrow \) diverge; too small \( \Rightarrow \) slow convergence
Gradient Descent: successive approximation

- At each iteration, form an approximation of $f(\cdot)$:

$$f(x^t + d) \approx \tilde{f}_{x^t}(d) := f(x^t) + \nabla f(x^t)^T d + \frac{1}{2} d^T \left( \frac{1}{\alpha} I \right) d$$

$$= f(x^t) + \nabla f(x^t)^T d + \frac{1}{2\alpha} d^T d$$

- Update solution by $x^{t+1} \leftarrow x^t + \arg\min_d \tilde{f}_{x^t}(d)$

- $d^* = -\alpha \nabla f(x^t)$ is the minimizer of $\arg\min_d \tilde{f}_{x^t}(d)$

- $d^*$ may not decrease the original objective function $f$
Gradient Descent: successive approximation

- However, the function value will decrease if
  
  Condition 1: $\tilde{f}_x(d) \geq f(x + d)$ for all $d$
  
  Condition 2: $\tilde{f}_x(0) = f(x)$

- Why?

  $$f(x^t + d^*) \leq \tilde{f}_{x^t}(d^*)$$
  $$\leq \tilde{f}_{x^t}(0)$$
  $$= f(x^t)$$

Condition 2 is satisfied by construction of $\tilde{f}_{x^t}$

Condition 1 is satisfied if $\frac{1}{\alpha} I \succeq \nabla^2 f(x)$ for all $x$ (why?)
A function has $L$-Lipschitz continuous gradient if

$$\|\nabla f(x) - \nabla f(y)\| \leq L \|x - y\| \quad \forall x, y$$

If $f$ is twice differentiable, this implies

$$\nabla^2 f(x) \leq LI \quad \forall x$$

In this case, Condition 2 is satisfied if $\alpha \leq \frac{1}{L}$

**Theorem:** gradient descent converges if $\alpha \leq \frac{1}{L}$

**Theorem:** gradient descent converges linearly with $\alpha \leq \frac{1}{L}$ if $f$ is strongly convex
Gradient Descent

- In practice, we do not know $L$.
- Step size $\alpha$ too large: the algorithm diverges
- Step size $\alpha$ too small: the algorithm converges very slowly
Gradient Descent: line search

- \( \mathbf{d}^* \) is a “descent direction” if and only if \( (\mathbf{d}^*)^T \nabla f(\mathbf{x}) < 0 \)
- Armijo rule backtracking line search:
  - Try \( \alpha = 1, \frac{1}{2}, \frac{1}{4}, \ldots \) until it satisfies

\[
    f(\mathbf{x} + \alpha \mathbf{d}^*) \leq f(\mathbf{x}) + \gamma \alpha (\mathbf{d}^*)^T \nabla f(\mathbf{x})
\]

where \( 0 < \gamma < 1 \)

Figure from http://ool.sourceforge.net/ool-ref.html
Gradient Descent: line search

- Gradient descent with line search:
  - Converges to optimal solutions if $f$ is smooth
  - Converges linearly if $f$ is strongly convex
- However, each iteration requires evaluating $f$ several times
- Several other step-size selection approaches
  (an ongoing research topic, especially for stochastic gradient descent)
Gradient Descent: applying to ridge regression

Input: $X \in \mathbb{R}^{N \times d}$, $y \in \mathbb{R}^N$, initial $w^{(0)}$

Output: Solution $w^* := \arg\min_w \frac{1}{2} \|Xw - y\|^2 + \frac{\lambda}{2} \|w\|^2$

1: $t = 0$
2: while not converged do
3: Compute the gradient
   
   $g = X^T(Xw - y) + \lambda w$
4: Choose step size $\alpha^t$
5: Update $w \leftarrow w - \alpha^t g$
6: $t \leftarrow t + 1$
7: end while

Time complexity: $O(\text{nnz}(X))$ per iteration
Proximal Gradient Descent

- How can we apply gradient descent to solve the Lasso problem?

\[ \arg\min_w \frac{1}{2} \|Xw - y\|^2 + \lambda \|w\|_1 \]

general composite function minimization:

\[ \arg\min_x f(x) := \{g(x) + h(x)\} \]

where \(g\) is smooth and convex, \(h\) is convex but may be non-differentiable

- Usually assume \(h\) is simple (for computational efficiency)
Proximal Gradient Descent: successive approximation

At each iteration, form an approximation of $f(\cdot)$:

$$f(x^t + d) \approx \tilde{f}_{x^t}(d) := g(x^t) + \nabla g(x^t)^T d + \frac{1}{2} d^T \left( \frac{1}{\alpha} I \right) d + h(x^t + d)$$

$$= g(x^t) + \nabla g(x^t)^T d + \frac{1}{2\alpha} d^T d + h(x^t + d)$$

Update solution by $x^{t+1} \leftarrow x^t + \text{argmin}_d \tilde{f}_{x^t}(d)$

This is called “proximal” gradient descent

Sometimes $d^* = \text{argmin}_d \tilde{f}_{x^t}(d)$ has a closed form solution
Proximal Gradient Descent: $\ell_1$-regularization (*)

The subproblem:

$$x^{t+1} = x^t + \arg\min_d \nabla g(x^t)^T d + \frac{1}{2\alpha} d^T d + \lambda \|x^t + d\|_1$$

$$= \arg\min_u \frac{1}{2} \|u - (x^t - \alpha \nabla g(x^t))\|^2 + \lambda \alpha \|u\|_1$$

$$= S(x^t - \alpha \nabla g(x^t), \alpha \lambda),$$

where $S$ is the soft-thresholding operator defined by

$$S(a, z) = \begin{cases} 
    a - z & \text{if } a > z \\
    a + z & \text{if } a < -z \\
    0 & \text{if } a \in [-z, z]
\end{cases}$$
Proximal Gradient: soft-thresholding

Figure from http://jocelynchi.com/soft-thresholding-operator-and-the-lasso-solution/
Proximal Gradient Descent for Lasso

**Input:** \( X \in \mathbb{R}^{N \times d}, \ y \in \mathbb{R}^N, \) initial \( w^{(0)} \)

**Output:** Solution \( w^* := \arg\min_w \frac{1}{2} \|Xw - y\|^2 + \lambda \|w\|_1 \)

1. \( t = 0 \)
2. **while** not converged **do**
3. Compute the gradient

\[
g = X^T(Xw - y)
\]

4. Choose step size \( \alpha^t \)
5. Update \( w \leftarrow S(w - \alpha^t g, \alpha^t \lambda) \)
6. \( t \leftarrow t + 1 \)
7. **end while**

Time complexity: \( O(\text{nnz}(X)) \) per iteration
Newton’s Method
Newton’s Method

- Iteratively conduct the following updates:

\[ x \leftarrow x - \alpha \nabla^2 f(x)^{-1} \nabla f(x) \]

where \( \alpha \) is the step size

- If \( \alpha = 1 \): converges quadratically when \( x^t \) is close enough to \( x^* \):

\[ \|x^{t+1} - x^*\| \leq K \|x^t - x^*\|^2 \]

for some constant \( K \). This means the error \( f(x^t) - f(x^*) \) decays quadratically:

\[ \beta, \beta^2, \beta^4, \beta^8, \beta^{16}, \ldots \]

- Only need few iterations to converge in this “quadratic convergence region”
Newton’s Method

However, Newton’s update rule is more expensive than gradient descent/coordinate descent.
Newton’s Method

- Need to compute $\nabla^2 f(x)^{-1} \nabla f(x)$
- Closed form solution: $O(d^3)$ for solving a $d$ dimensional linear system
- Usually solved by another iterative solver:
  - gradient descent
  - coordinate descent
  - conjugate gradient method
  ...
- Useful for the cases where the quadratic subproblem can be solved more efficiently than the original problem
- Examples: primal L2-SVM/logistic regression, $\ell_1$-regularized logistic regression, ...
Newton’s Method(*)

- At each iteration, form an approximation of $f(\cdot)$:
  
  $$f(x^t + d) \approx \tilde{f}_{x^t}(d) := f(x^t) + \nabla f(x^t)^T d + \frac{1}{2\alpha} d^T \nabla^2 f(x) d$$

- Update solution by $x^{t+1} \leftarrow x^t + \text{argmin}_d \tilde{f}_{x^t}(d)$

- When $x$ is far away from $x^*$, needs line search to guarantee convergence

- Assume $L I \succeq \nabla^2 f(x) \succeq m I$ for all $x$, then $\alpha \leq \frac{m}{L}$ guarantee the objective function value decreases because

  $$\frac{L}{m} \nabla^2 f(x) \succeq \nabla^2 f(y) \quad \forall x, y$$

- In practice, we often just use line search.
Proximal Newton (*)

- What if \( f(x) = g(x) + h(x) \) and \( h(x) \) is non-smooth (\( h(x) = \|x\|_1 \))?
- At each iteration, form an approximation of \( f(\cdot) \):

\[
f(x^t + d) \approx \tilde{f}_{x^t}(d) := g(x^t) + \nabla g(x^t)^T d + \frac{\alpha}{2} d^T \nabla^2 g(x) d + h(x + d)
\]

- Update solution by \( x^{t+1} \leftarrow x^t + \text{argmin}_d \tilde{f}_{x^t}(d) \)
- Need another iterative solver for solving the subproblem
Stochastic Gradient
**Stochastic Gradient: Motivation**

- Widely used for machine learning problems (with large number of samples)
- Given training samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$, we usually want to solve the following empirical risk minimization (ERM) problem:
  \[
  \arg\min_{\mathbf{w}} \sum_{i=1}^{n} \ell_i(\mathbf{x}_i),
  \]
  where each $\ell_i(\cdot)$ is the loss function
- Minimize the summation of individual loss on each sample
**Stochastic Gradient**

- Assume the objective function can be written as
  \[ f(x) = \frac{1}{n} \sum_{i=1}^{n} f_i(x) \]

- Stochastic gradient method:
  Iterative conducts the following updates
  1. Choose an index \( i \) (uniform) randomly
  2. \( x^{t+1} \leftarrow x^t - \eta^t \nabla f_i(x^t) \)

- \( \eta^t > 0 \) is the step size
Stochastic Gradient

- Assume the objective function can be written as
  \[ f(x) = \frac{1}{n} \sum_{i=1}^{n} f_i(x) \]

- Stochastic gradient method:
  Iterative conducts the following updates
  1. Choose an index \( i \) (uniform) randomly
  2. \( x^{t+1} \leftarrow x^t - \eta^t \nabla f_i(x^t) \)

- \( \eta^t > 0 \) is the step size
- Why does SG work?

  \[ E_i[\nabla f_i(x)] = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(x) = \nabla f(x) \]
Assume the objective function can be written as:

\[ f(x) = \frac{1}{n} \sum_{i=1}^{n} f_i(x) \]

Stochastic gradient method:

Iterative conducts the following updates:

1. Choose an index \( i \) (uniform) randomly
2. \( x^{t+1} \leftarrow x^t - \eta^t \nabla f_i(x^t) \)

\( \eta^t > 0 \) is the step size

Why does SG work?

\[ E_i[\nabla f_i(x)] = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(x) = \nabla f(x) \]

Is it a fixed point method? No if \( \eta > 0 \) because \( x^* - \eta \nabla_i f(x^*) \neq x^* \)

Is it a descent method? No, because \( f(x^{t+1}) \neq f(x^t) \)
Stochastic Gradient

- Step size $\eta$ has to decay to 0
  (e.g., $\eta^t = Ct^{-a}$ for some constant $a, C$)
- Many variants proposed recently (SVRG, SAGA, \ldots)
- Widely used in online setting
Objective function:

\[ \arg\min_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|^2 \]

How to write as \( \arg\min_w \frac{1}{n} \sum_{i=1}^{n} f_i(w) \)?

How to decompose into \( n \) components?
Objective function:

$$\arg\min_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|^2$$

How to write as $\arg\min_w \frac{1}{n} \sum_{i=1}^{n} f_i(w)$?

First approach: $f_i(w) = (w^T x_i - y_i)^2 + \lambda \|w\|^2$

Update rule:

$$w^{t+1} \leftarrow w^t - 2\eta^t (w^T x_i - y_i)x_i - 2\eta^t \lambda w$$

$$= (1 - 2\eta^t \lambda)w - 2\eta^t (w^T x_i - y_i)x_i$$
Objective function:

$$\arg\min_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|^2$$

How to write as $\arg\min_w \frac{1}{n} \sum_{i=1}^{n} f_i(w)$?

First approach: $f_i(w) = (w^T x_i - y_i)^2 + \lambda \|w\|^2$

Update rule:

$$w^{t+1} \leftarrow w^t - 2\eta^t (w^T x_i - y_i)x_i - 2\eta^t \lambda w$$

$$= (1 - 2\eta^t \lambda)w - 2\eta^t (w^T x_i - y_i)x_i$$

Need $O(d)$ complexity per iteration even if data is sparse
Stochastic Gradient: applying to ridge regression

- Objective function:

\[
\text{argmin}_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|^2
\]

- How to write as \( \text{argmin}_w \frac{1}{n} \sum_{i=1}^{n} f_i(w) \)?
- First approach: \( f_i(w) = (w^T x_i - y_i)^2 + \lambda \|w\|^2 \)
- Update rule:

\[
\begin{align*}
    w^{t+1} &\leftarrow w^t - 2\eta^t (w^T x_i - y_i)x_i - 2\eta^t \lambda w \\
    &= (1 - 2\eta^t \lambda) w - 2\eta^t (w^T x_i - y_i)x_i
\end{align*}
\]

- Need \( O(d) \) complexity per iteration even if data is sparse
- Solution: store \( w = sv \) where \( s \) is a scalar
Objective function:

\[
\text{arg}\min_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|^2
\]

Second approach:

- define \( \Omega_i = \{j \mid X_{ij} \neq 0\} \) for \( i = 1, \ldots, n \)
- define \( n_j = |\{i \mid X_{ij} \neq 0\}| \) for \( j = 1, \ldots, d \)
- define \( f_i(w) = (w^T x_i - y_i)^2 + \sum_{j \in \Omega_i} \frac{\lambda n}{n_j} w_j^2 \)
Stochastic Gradient: applying to ridge regression

**Objective function:**

\[
\arg\min_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|^2
\]

**Second approach:**

define \(\Omega_i = \{j \mid X_{ij} \neq 0\}\) for \(i = 1, \ldots, n\)

define \(n_j = |\{i \mid X_{ij} \neq 0\}|\) for \(j = 1, \ldots, d\)

define \(f_i(w) = (w^T x_i - y_i)^2 + \sum_{j \in \Omega_i} \frac{\lambda n}{n_j} w_j^2\)

**Update rule when selecting index \(i\):**

\[
w_j^{t+1} \leftarrow w_j^t - 2\eta^t (x_i^T w^t - y_i)X_{ij} - \frac{2\eta^t \lambda n}{n_j} w_j^t, \quad \forall j \in \Omega_i
\]

**Solution:** update can be done in \(O(|\Omega_i|)\) operations
Coming up

- Next class: Parallel Optimization Methods

Questions?