COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Andrew McGregor
Lecture 22
Last Class: Fast computation of the SVD/eigendecomposition.

• Power method for computing the top singular vector of a matrix.
• Power method is a simple iterative algorithm for solving the *non-convex* optimization problem \( \max_{\vec{v} : \|\vec{v}\|^2 = 1} |\vec{v}^T A \vec{v}| \)

Final Two Weeks of Class:

• More general iterative algorithms for optimization, specifically gradient descent and its variants.
• What are these methods, when are they applied, and how do you analyze their performance?
• Small taste of what you can find in COMPSCI 590OP or 690OP.
Discrete (Combinatorial) Optimization: (traditional CS algorithms)

- Graph Problems: min-cut, max-cut, max flow, shortest path, matchings, maximum independent set, traveling salesman problem
- Problems with discrete constraints or outputs: bin-packing, scheduling, sequence alignment, submodular maximization
- Generally searching over a finite but exponentially large set of possible solutions. Many of these problems are NP-Hard.

Continuous Optimization: (maybe seen in ML/advanced algorithms)

- Unconstrained convex and non-convex optimization.
- Linear programming, quadratic programming, semidefinite programming
CONTINUOUS OPTIMIZATION EXAMPLES

\[ f(\theta) \]
\[ \theta \in \mathbb{R} \]

\[ f(\theta) \]
\[ \theta \in \mathbb{R} \]
MATHEMATICAL SETUP

Given some function $f : \mathbb{R}^d \rightarrow \mathbb{R}$, find $\vec{\theta}^\ast$ with:

$$f(\vec{\theta}^\ast) = \min_{\vec{\theta} \in \mathbb{R}^d} f(\vec{\theta})$$

Typically up to some small additive approximation term $\epsilon$.

Often under some constraints:

- $\|\vec{\theta}\|_2 \leq 1$, $\|\vec{\theta}\|_1 \leq 1$.
- $\vec{\theta} \leq \vec{b}$, $\vec{\theta}^T \vec{A} \geq 0$.
- $\sum_{d_i=1} \vec{\theta}(i) \leq c$. 

Given some function $f : \mathbb{R}^d \to \mathbb{R}$, find $\vec{\theta}_\star$ with:

$$f(\vec{\theta}_\star) = \min_{\vec{\theta} \in \mathbb{R}^d} f(\vec{\theta}) + \epsilon$$

Typically up to some small additive approximation term $\epsilon$. 
Given some function $f : \mathbb{R}^d \rightarrow \mathbb{R}$, find $\vec{\theta}_\star$ with:

$$f(\vec{\theta}_\star) = \min_{\vec{\theta} \in \mathbb{R}^d} f(\vec{\theta}) + \epsilon$$

Typically up to some small additive approximation term $\epsilon$.

Often under some constraints:

- $\|\vec{\theta}\|_2 \leq 1$, $\|\vec{\theta}\|_1 \leq 1$.
- $A\vec{\theta} \leq \vec{b}$, $\vec{\theta}^T A\vec{\theta} \geq 0$.
- $\sum_{i=1}^d \vec{\theta}(i) \leq c$. 
Modern machine learning centers around continuous optimization.

**Typical Set Up: (supervised machine learning)**

- Have a **model**, which is a function mapping inputs to predictions (neural network, linear function, low-degree polynomial etc).
- The model is parameterized by a **parameter vector** (weights in a neural network, coefficients in a linear function or polynomial).
- Want to **train** this model on input data, by picking a parameter vector such that the model does a good job mapping inputs to predictions on your training data.

This training step is typically formulated as a continuous optimization problem.
Example 1: Linear Regression, e.g., predicting house prices based on $d$ features (sq. footage, average price of houses in neighborhood...)

Model: $\mathbf{M} \vec{\theta} : \mathbb{R}^d \rightarrow \mathbb{R}$ with $\mathbf{M} \vec{\theta}(\vec{x}) = \vec{\theta}(1) \cdot \vec{x}(1) + ... + \vec{\theta}(d) \cdot \vec{x}(d)$.

Parameter Vector: $\vec{\theta} \in \mathbb{R}^d$ (the regression coefficients)

Optimization Problem: Given data points (training points) $\vec{x}_1, ..., \vec{x}_n$ (the rows of data matrix $X \in \mathbb{R}^{n \times d}$) and labels $y_1, ..., y_n \in \mathbb{R}$, find $\vec{\theta}^*$ minimizing the loss function:

$$L_X, y(\vec{\theta}) = L(\vec{\theta}, X, \vec{y}) = \sum_{i=1}^{n} \ell(\mathbf{M} \vec{\theta}(\vec{x}_i), y_i)$$

where $\ell$ is some measurement of how far $\mathbf{M} \vec{\theta}(\vec{x}_i)$ is from $y_i$.

- $\ell(\mathbf{M} \vec{\theta}(\vec{x}_i), y_i) = (\mathbf{M} \vec{\theta}(\vec{x}_i) - y_i)^2$ (least squares regression)
- $y_i \in \{-1, 1\}$ and $\ell(\mathbf{M} \vec{\theta}(\vec{x}_i), y_i) = \ln(1 + \exp(-y_i \mathbf{M} \vec{\theta}(\vec{x}_i)))$ (logistic regression)
Example 1: Linear Regression, e.g., predicting house prices based on \( d \) features (sq. footage, average price of houses in neighborhood . . . )

Model: \( M_{\theta}: \mathbb{R}^d \rightarrow \mathbb{R} \) with \( M_{\theta}(\vec{x}) \overset{\text{def}}{=} \vec{\theta}(1) \cdot \vec{x}(1) + \ldots + \vec{\theta}(d) \cdot \vec{x}(d) \).
Example 1: Linear Regression, e.g., predicting house prices based on $d$ features (sq. footage, average price of houses in neighborhood . . .)

Model: $M_{\vec{\theta}} : \mathbb{R}^d \rightarrow \mathbb{R}$ with $M_{\vec{\theta}}(\vec{x}) \overset{\text{def}}{=} \vec{\theta}(1) \cdot \vec{x}(1) + \ldots + \vec{\theta}(d) \cdot \vec{x}(d)$. 
Example 1: Linear Regression, e.g., predicting house prices based on $d$ features (sq. footage, average price of houses in neighborhood...) 

Model: $M_{\vec{\theta}} : \mathbb{R}^d \rightarrow \mathbb{R}$ with $M_{\vec{\theta}}(\vec{x}) \overset{\text{def}}{=} \vec{\theta}(1) \cdot \vec{x}(1) + \ldots + \vec{\theta}(d) \cdot \vec{x}(d)$.

Parameter Vector: $\vec{\theta} \in \mathbb{R}^d$ (the regression coefficients)
Example 1: Linear Regression, e.g., predicting house prices based on \( d \) features (sq. footage, average price of houses in neighborhood . . . )

Model: \( M_{\vec{\theta}} : \mathbb{R}^d \rightarrow \mathbb{R} \) with \( M_{\vec{\theta}}(\vec{x}) \overset{\text{def}}{=} \vec{\theta}(1) \cdot \vec{x}(1) + \ldots + \vec{\theta}(d) \cdot \vec{x}(d) \).

Parameter Vector: \( \vec{\theta} \in \mathbb{R}^d \) (the regression coefficients)

Optimization Problem: Given data points (training points) \( \vec{x}_1, \ldots, \vec{x}_n \) (the rows of data matrix \( \mathbf{X} \in \mathbb{R}^{n \times d} \)) and labels \( y_1, \ldots, y_n \in \mathbb{R} \), find \( \vec{\theta}_* \) minimizing the loss function:

\[
L(\vec{\theta}, \mathbf{X}, \vec{y}) = \sum_{i=1}^{n} \ell(M_{\vec{\theta}}(\vec{x}_i), y_i)
\]

where \( \ell \) is some measurement of how far \( M_{\vec{\theta}}(\vec{x}_i) \) is from \( y_i \).
Example 1: Linear Regression, e.g., predicting house prices based on $d$ features (sq. footage, average price of houses in neighborhood...)

Model: $M_{\vec{\theta}} : \mathbb{R}^d \to \mathbb{R}$ with $M_{\vec{\theta}}(\vec{x}) \overset{\text{def}}{=} \vec{\theta}(1) \cdot \vec{x}(1) + \ldots + \vec{\theta}(d) \cdot \vec{x}(d)$.

Parameter Vector: $\vec{\theta} \in \mathbb{R}^d$ (the regression coefficients)

Optimization Problem: Given data points (training points) $\vec{x}_1, \ldots, \vec{x}_n$ (the rows of data matrix $X \in \mathbb{R}^{n \times d}$) and labels $y_1, \ldots, y_n \in \mathbb{R}$, find $\vec{\theta}_*$ minimizing the loss function:

$$L(\vec{\theta}, X, \vec{y}) = \sum_{i=1}^{n} \ell(M_{\vec{\theta}}(\vec{x}_i), y_i)$$

where $\ell$ is some measurement of how far $M_{\vec{\theta}}(\vec{x}_i)$ is from $y_i$.

- $\ell(M_{\vec{\theta}}(\vec{x}_i), y_i) = (M_{\vec{\theta}}(\vec{x}_i) - y_i)^2$ (least squares regression)

- $y_i \in \{-1, 1\}$ and $\ell(M_{\vec{\theta}}(\vec{x}_i), y_i) = \ln (1 + \exp(-y_i M_{\vec{\theta}}(\vec{x}_i)))$ (logistic regression)
Example 1: Linear Regression, e.g., predicting house prices based on $d$ features (sq. footage, average price of houses in neighborhood...)

Model: $M_{\theta^*} : \mathbb{R}^d \to \mathbb{R}$ with $M_{\theta^*}(\bar{x}) \overset{\text{def}}{=} \theta(1) \cdot \bar{x}(1) + \ldots + \theta(d) \cdot \bar{x}(d)$.

Parameter Vector: $\theta \in \mathbb{R}^d$ (the regression coefficients)

Optimization Problem: Given data points (training points) $\bar{x}_1, \ldots, \bar{x}_n$ (the rows of data matrix $X \in \mathbb{R}^{n \times d}$) and labels $y_1, \ldots, y_n \in \mathbb{R}$, find $\theta^*$ minimizing the loss function:

$$L_{X,y}(\theta) = L(\theta, X, \bar{y}) = \sum_{i=1}^{n} \ell(M_{\theta^*}(\bar{x}_i), y_i)$$

where $\ell$ is some measurement of how far $M_{\theta^*}(\bar{x}_i)$ is from $y_i$.

- $\ell(M_{\theta^*}(\bar{x}_i), y_i) = (M_{\theta^*}(\bar{x}_i) - y_i)^2$ (least squares regression)
- $y_i \in \{-1, 1\}$ and $\ell(M_{\theta^*}(\bar{x}_i), y_i) = \ln (1 + \exp(-y_i M_{\theta^*}(\bar{x}_i)))$ (logistic regression)
Example 2: Neural Networks

Model: $M_{\vec{\theta}}: \mathbb{R}^d \rightarrow \mathbb{R}$. $M_{\vec{\theta}}(\vec{x}) = \langle \vec{w}_{out}, \sigma(W_2\sigma(W_1\vec{x})) \rangle$.

Parameter Vector: $\vec{\theta} \in \mathbb{R}^{(# edges)}$ (the weights on every edge)

Optimization Problem: Given data points $\vec{x}_1, \ldots, \vec{x}_n$ and labels $z_1, \ldots, z_n \in \mathbb{R}$, find $\vec{\theta}^*$ minimizing the loss function:

$$L_{\vec{x}, \vec{y}}(\vec{\theta}) = \sum_{i=1}^{n} \ell(M_{\vec{\theta}}(\vec{x}_i), z_i)$$
\[ L_{x,\overline{y}}(\overrightarrow{\theta}) = \sum_{i=1}^{n} \ell(M_{\overrightarrow{\theta}}(\overrightarrow{x}_i), y_i) \]

- **Supervised** means we have labels \( y_1, \ldots, y_n \) for the training points.
- Solving the final optimization problem has many different names: likelihood maximization, empirical risk minimization, minimizing training loss, etc.
- Continuous optimization is also very common in unsupervised learning. (PCA, spectral clustering, etc.)
- **Generalization** tries to explain why minimizing the loss \( L_{x,\overline{y}}(\overrightarrow{\theta}) \) on the *training points* minimizes the loss on future *test points*. I.e., makes us have good predictions on future inputs.
Choice of optimization algorithm for minimizing $f(\vec{\theta})$ will depend on many things:

- The form of $f$ (in ML, depends on the model & loss function).
- Any constraints on $\vec{\theta}$ (e.g., $||\vec{\theta}|| < c$).
- Computational constraints, such as memory constraints.

\[
L_{X, \bar{y}}(\vec{\theta}) = \sum_{i=1}^{n} \ell(M_{\vec{\theta}}(\vec{x}_i), y_i)
\]
**Next few classes:** Gradient descent (and some important variants)

- An extremely simple greedy iterative method, that can be applied to almost any continuous function we care about optimizing.

- Often not the ‘best’ choice for any given function, but it is the approach of choice in ML since it is simple, general, and often works very well.

- At each step, tries to move towards the lowest nearby point in the function that is can – in the opposite direction of the gradient.
Let $\vec{e}_i \in \mathbb{R}^d$ denote the $i^{th}$ standard basis vector,

$$\vec{e}_i = [0, 0, 1, 0, 0, \ldots, 0] \quad \text{1 at position } i$$
Let $\vec{e}_i \in \mathbb{R}^d$ denote the $i^{th}$ standard basis vector,

$$\vec{e}_i = [0, 0, 1, 0, 0, \ldots, 0] \quad \text{1 at position } i$$

Partial Derivative:

$$\frac{\partial f}{\partial \vec{\theta}(i)} = \lim_{\epsilon \to 0} \frac{f(\vec{\theta} + \epsilon \cdot \vec{e}_i) - f(\vec{\theta})}{\epsilon}.$$
Let $\vec{e}_i \in \mathbb{R}^d$ denote the $i^{th}$ standard basis vector,

$$\vec{e}_i = [0, 0, 1, 0, 0, \ldots, 0]_1$$

at position $i$.

**Partial Derivative:**

$$\frac{\partial f}{\partial \theta(i)} = \lim_{\epsilon \to 0} \frac{f(\vec{\theta} + \epsilon \cdot \vec{e}_i) - f(\vec{\theta})}{\epsilon}.$$

**Directional Derivative:** For unit vector $\vec{v}$:

$$D_{\vec{v}} f(\vec{\theta}) = \lim_{\epsilon \to 0} \frac{f(\vec{\theta} + \epsilon \vec{v}) - f(\vec{\theta})}{\epsilon}.$$
**Gradient:** Just a ‘list’ of the partial derivatives.

\[ \vec{\nabla} f(\vec{\theta}) = \begin{bmatrix} \frac{\partial f}{\partial \theta(1)} \\ \frac{\partial f}{\partial \theta(2)} \\ \vdots \\ \frac{\partial f}{\partial \theta(d)} \end{bmatrix} \]
Gradient: Just a ‘list’ of the partial derivatives.

$$\vec{\nabla} f(\vec{\theta}) = \left[ \begin{array}{c} \frac{\partial f}{\partial \theta(1)} \\ \frac{\partial f}{\partial \theta(2)} \\ \vdots \\ \frac{\partial f}{\partial \theta(d)} \end{array} \right]$$

Directional Derivative in Terms of the Gradient:

$$D_{\vec{v}} f(\vec{\theta}) = \langle \vec{v}, \vec{\nabla} f(\vec{\theta}) \rangle.$$
Often the functions we are trying to optimize are very complex (e.g., a neural network). We will assume access to:

**Function Evaluation**: Can compute $f(\vec{\theta})$ for any $\vec{\theta}$.

**Gradient Evaluation**: Can compute $\vec{\nabla} f(\vec{\theta})$ for any $\vec{\theta}$.
Often the functions we are trying to optimize are very complex (e.g., a neural network). We will assume access to:

**Function Evaluation**: Can compute $f(\vec{\theta})$ for any $\vec{\theta}$.

**Gradient Evaluation**: Can compute $\vec{\nabla} f(\vec{\theta})$ for any $\vec{\theta}$.

In neural networks:

- Function evaluation is called a **forward pass** (propogate an input through the network).
- Gradient evaluation is called a **backward pass** (compute the gradient via chain rule, using backpropagation).
Gradient descent is a greedy iterative optimization algorithm: Starting at $\theta^{(0)}$, in each iteration let $\theta^{(i)} = \theta^{(i-1)} + \eta \vec{v}$, where $\eta$ is a (small) ‘step size’ and $\vec{v}$ is a direction chosen to minimize $f(\theta^{(i-1)} + \eta \vec{v})$. 
Gradient descent is a greedy iterative optimization algorithm: Starting at $\vec{\theta}^{(0)}$, in each iteration let $\vec{\theta}^{(i)} = \vec{\theta}^{(i-1)} + \eta \vec{v}$, where $\eta$ is a (small) ‘step size’ and $\vec{v}$ is a direction chosen to minimize $f(\vec{\theta}^{(i-1)} + \eta \vec{v})$.

$$D_{\vec{v}} f(\vec{\theta}) = \lim_{\epsilon \to 0} \frac{f(\vec{\theta} + \epsilon \vec{v}) - f(\vec{\theta})}{\epsilon}.$$
Gradient descent is a greedy iterative optimization algorithm: Starting at $\vec{\theta}^{(0)}$, in each iteration let $\vec{\theta}^{(i)} = \vec{\theta}^{(i-1)} + \eta \vec{v}$, where $\eta$ is a (small) ‘step size’ and $\vec{v}$ is a direction chosen to minimize $f(\vec{\theta}^{(i-1)} + \eta \vec{v})$.

$$D_{\vec{v}} f(\vec{\theta}^{(i-1)}) = \lim_{\epsilon \to 0} \frac{f(\vec{\theta}^{(i-1)} + \epsilon \vec{v}) - f(\vec{\theta}^{(i-1)})}{\epsilon}.$$
Gradient descent is a greedy iterative optimization algorithm: Starting at \( \theta^{(0)} \), in each iteration let \( \theta^{(i)} = \theta^{(i-1)} + \eta \vec{v} \), where \( \eta \) is a (small) ‘step size’ and \( \vec{v} \) is a direction chosen to minimize \( f(\theta^{(i-1)} + \eta \vec{v}) \).

\[
D_{\vec{v}} f(\theta^{(i-1)}) = \lim_{\epsilon \to 0} \frac{f(\theta^{(i-1)} + \epsilon \vec{v}) - f(\theta^{(i-1)})}{\epsilon}.
\]

So for small \( \eta \):

\[
f(\theta^{(i)}) - f(\theta^{(i-1)}) = f(\theta^{(i-1)} + \eta \vec{v}) - f(\theta^{(i-1)})
\]
Gradient descent is a greedy iterative optimization algorithm: Starting at $\vartheta(0)$, in each iteration let $\vartheta(i) = \vartheta(i-1) + \eta \vec{v}$, where $\eta$ is a (small) ‘step size’ and $\vec{v}$ is a direction chosen to minimize $f(\vartheta(i-1) + \eta \vec{v})$.

$$D_{\vec{v}} f(\vartheta(i-1)) = \lim_{\epsilon \to 0} \frac{f(\vartheta(i-1) + \epsilon \vec{v}) - f(\vartheta(i-1))}{\epsilon}.$$  

So for small $\eta$:

$$f(\vartheta(i)) - f(\vartheta(i-1)) = f(\vartheta(i-1) + \eta \vec{v}) - f(\vartheta(i-1)) \approx \eta \cdot D_{\vec{v}} f(\vartheta(i-1))$$
Gradient descent is a greedy iterative optimization algorithm: Starting at $\theta^{(0)}$, in each iteration let $\theta^{(i)} = \theta^{(i-1)} + \eta \nabla f$, where $\eta$ is a (small) ‘step size’ and $\nabla f$ is a direction chosen to minimize $f(\theta^{(i-1)} + \eta \nabla f)$.

$$D_{\nabla f} f(\theta^{(i-1)}) = \lim_{\epsilon \to 0} \frac{f(\theta^{(i-1)} + \epsilon \nabla f) - f(\theta^{(i-1)})}{\epsilon}.$$ 

So for small $\eta$:

$$f(\theta^{(i)}) - f(\theta^{(i-1)}) = f(\theta^{(i-1)} + \eta \nabla f) - f(\theta^{(i-1)}) \approx \eta \cdot D_{\nabla f} f(\theta^{(i-1)})$$

$$= \eta \cdot \langle \nabla f, \nabla f(\theta^{(i-1)}) \rangle.$$
Gradient descent is a greedy iterative optimization algorithm: Starting at $\theta^{(0)}$, in each iteration let $\theta^{(i)} = \theta^{(i-1)} + \eta \vec{v}$, where $\eta$ is a (small) ‘step size’ and $\vec{v}$ is a direction chosen to minimize $f(\theta^{(i-1)} + \eta \vec{v})$.

$$D_{\vec{v}} f(\theta^{(i-1)}) = \lim_{\epsilon \to 0} \frac{f(\theta^{(i-1)} + \epsilon \vec{v}) - f(\theta^{(i-1)})}{\epsilon}.$$  

So for small $\eta$:

$$f(\theta^{(i)}) - f(\theta^{(i-1)}) = f(\theta^{(i-1)} + \eta \vec{v}) - f(\theta^{(i-1)}) \approx \eta \cdot D_{\vec{v}} f(\theta^{(i-1)})$$

$$= \eta \cdot \langle \vec{v}, \nabla f(\theta^{(i-1)}) \rangle.$$

We want to choose $\vec{v}$ minimizing $\langle \vec{v}, \nabla f(\theta^{(i-1)}) \rangle$ – i.e., pointing in the direction of $\nabla f(\theta^{(i-1)})$ but with the opposite sign.
Gradient Descent

• Choose some initialization $\vec{\theta}^{(0)}$.
• For $i = 1, \ldots, t$
  • $\vec{\theta}^{(i)} = \vec{\theta}^{(i-1)} - \eta \nabla f(\vec{\theta}^{(i-1)})$
• Return $\vec{\theta}^{(t)}$, as an approximate minimizer of $f(\vec{\theta})$.

Step size $\eta$ is chosen ahead of time or adapted during the algorithm (details to come.)
Gradient Descent

• Choose some initialization $\vec{\theta}^{(0)}$.
• For $i = 1, \ldots, t$
  • $\vec{\theta}^{(i)} = \vec{\theta}^{(i-1)} - \eta \nabla f(\vec{\theta}^{(i-1)})$
• Return $\vec{\theta}^{(t)}$, as an approximate minimizer of $f(\vec{\theta})$.

Step size $\eta$ is chosen ahead of time or adapted during the algorithm (details to come.)

• For now assume $\eta$ stays the same in each iteration.
Gradient Descent Update: $\vec{\theta}_{i+1} = \vec{\theta}_i - \eta \nabla f(\vec{\theta}_i)$