Subgradient Descent

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October 18, 2017

Motivation and Review: Support Vector Machines

The Classification Problem

- Output space $\mathcal{Y} = \{-1, 1\}$ Action space $\mathcal{A} = \mathbf{R}$
- **Real-valued prediction function $f : \mathcal{X} \to \mathbf{R}$**
- The value $f(x)$ is called the **score** for the input x.
- Intuitively, magnitude of the score represents the **confidence of our prediction**.
- Typical convention:

$$
\begin{aligned}
f(x) > 0 &\implies \text{Predict } 1 \\
f(x) < 0 &\implies \text{Predict } -1
\end{aligned}
$$

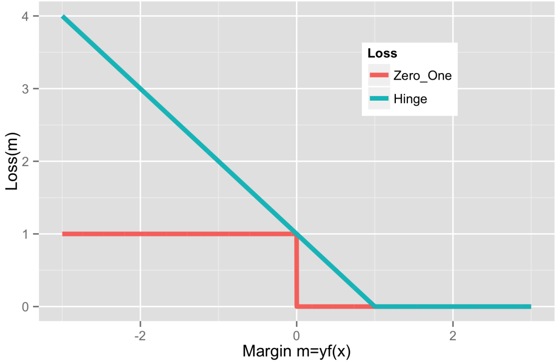
(But we can choose other thresholds...)

The Margin

- The **margin** (or **functional margin**) for predicted score $\hat{y}$ and true class $y \in \{-1, 1\}$ is $y\hat{y}$.
- The margin often looks like $yf(x)$, where $f(x)$ is our score function.
- The margin is a measure of how **correct** we are.
- We want to **maximize the margin**.

[Margin-Based] Classification Losses

SVM/Hinge loss: $\ell_{\text{Hinge}} = \max\{1-m, 0\} = (1-m)_+$



Not differentiable at $m=1$. We have a **"margin error"** when $m<1$.

[Soft Margin] Linear Support Vector Machine (No Intercept)

- Hypothesis space $\mathcal{F} = \left\{ f(x) = w^T x \mid w \in \mathbf{R}^d \right\}$.
- Loss $\ell(m) = \max(1, m)$
- ℓ_2 regularization

$$\min_{w \in \mathbf{R}^d} \sum_{i=1}^{n} \max\left(0, 1 - y_i w^T x_i\right) + \lambda \|w\|_2^2$$

SVM Optimization Problem (no intercept)

- SVM objective function:

$$J(w) = \frac{1}{n}\sum_{i=1}^{n} \max\left(0, 1 - y_i\left[w^T x_i\right]\right) + \lambda\|w\|^2.$$

- Not differentiable... but let's think about gradient descent anyway.
- Derivative of hinge loss $\ell(m) = \max(0, 1-m)$:

$$\ell'(m) = \begin{cases} 0 & m > 1 \\ -1 & m < 1 \\ \text{undefined} & m = 1 \end{cases}$$

“Gradient” of SVM Objective

- We need gradient with respect to parameter vector $w \in \mathbf{R}^d$:

$$
\begin{aligned}
\nabla_w \ell\left(y_i w^T x_i\right) &= \ell'\left(y_i w^T x_i\right) y_i x_i \text{ (chain rule)} \\
&= \left(\begin{cases} 0 & y_i w^T x_i > 1 \\ -1 & y_i w^T x_i < 1 \\ \text{undefined} & y_i w^T x_i = 1 \end{cases}\right) y_i x_i \text{ (expanded } m \text{ in } \ell'(m)\text{)} \\
&= \begin{cases} 0 & y_i w^T x_i > 1 \\ -y_i x_i & y_i w^T x_i < 1 \\ \text{undefined} & y_i w^T x_i = 1 \end{cases}
\end{aligned}
$$

"Gradient" of SVM Objective

$$\nabla_w \ell\left(y_i w^T x_i\right) = \begin{cases} 0 & y_i w^T x_i > 1 \\ -y_i x_i & y_i w^T x_i < 1 \\ \text{undefined} & y_i w^T x_i = 1 \end{cases}$$

So

$$\begin{aligned}
\nabla_w J(w) &= \nabla_w \left(\frac{1}{n} \sum_{i=1}^{n} \ell\left(y_i w^T x_i\right) + \lambda \|w\|^2 \right) \\
&= \frac{1}{n} \sum_{i=1}^{n} \nabla_w \ell\left(y_i w^T x_i\right) + 2\lambda w \\
&= \begin{cases} \frac{1}{n} \sum_{i: y_i w^T x_i < 1} \left(-y_i x_i\right) + 2\lambda w & \text{all } y_i w^T x_i \neq 1 \\ \text{undefined} & \text{otherwise} \end{cases}
\end{aligned}$$

Gradient Descent on SVM Objective?

- The gradient of the SVM objective is

$$\nabla_w J(w) = \frac{1}{n} \sum_{i: y_i w^T x_i < 1} (-y_i x_i) + 2\lambda w$$

when $y_i w^T x_i \neq 1$ for all i, and **otherwise is undefined**.

Suppose we tried gradient descent on $J(w)$:

- If we start with a random w, will we ever hit $y_i w^T x_i = 1$?
- If we did, could we perturb the step size by ε to miss such a point?
- Does it even make sense to check $y_i w^T x_i = 1$ with floating point numbers?

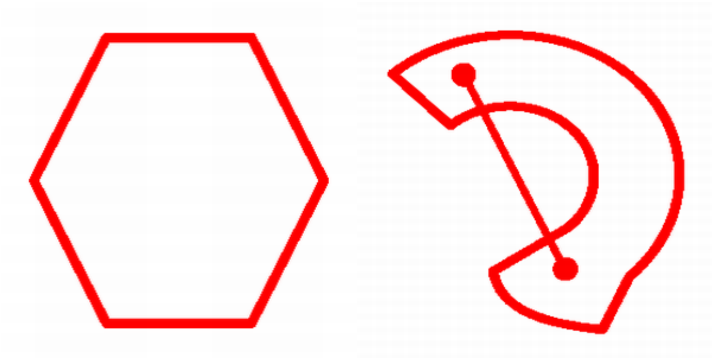
Gradient Descent on SVM Objective?

- If we blindly apply gradient descent from a random starting point
  - seems unlikely that we'll hit a point where the gradient is undefined.
- Still, doesn't mean that gradient descent will work if objective not differentiable!
- Theory of subgradients and subgradient descent will clear up any uncertainty.

Convexity and Sublevel Sets

Definition

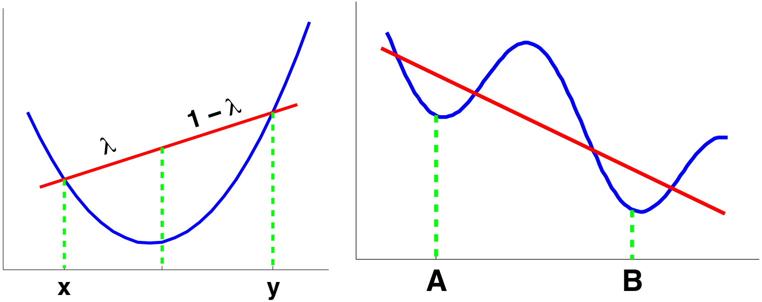
A set C is **convex** if the line segment between any two points in C lies in C.



KPM Fig. 7.4

Definition

A function $f : \mathbf{R}^d \to \mathbf{R}$ is **convex** if the line segment connecting any two points on the graph of f lies above the graph. f is **concave** if $-f$ is convex.



KPM Fig. 7.5

Convex Optimization Problem: Standard Form

$$
\begin{array}{ll}
\text{minimize} & f_0(x) \\
\text{subject to} & f_i(x) \leqslant 0, \;\; i = 1, \ldots, m
\end{array}
$$

where $f_0, \ldots, f_m$ are convex functions.

Question: Is the $\leqslant$ in the constraint just a convention? Could we also have used $\geqslant$ or $=$?

Level Sets and Sublevel Sets

Let $f : \mathbf{R}^d \to \mathbf{R}$ be a function. Then we have the following definitions:

Definition

A **level set** or **contour line** for the value c is the set of points $x \in \mathbf{R}^d$ for which $f(x) = c$.

Definition

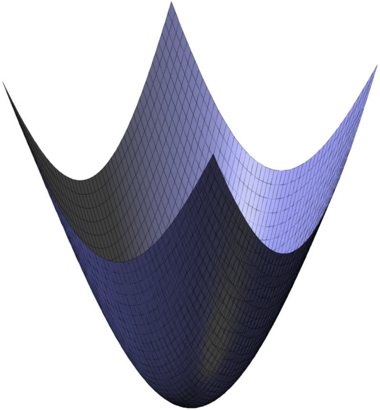
A **sublevel** set for the value c is the set of points $x \in \mathbf{R}^d$ for which $f(x) \leqslant c$.

Theorem

If $f : \mathbf{R}^d \to \mathbf{R}$ is ***convex****, then the* ***sublevel sets are convex****.*

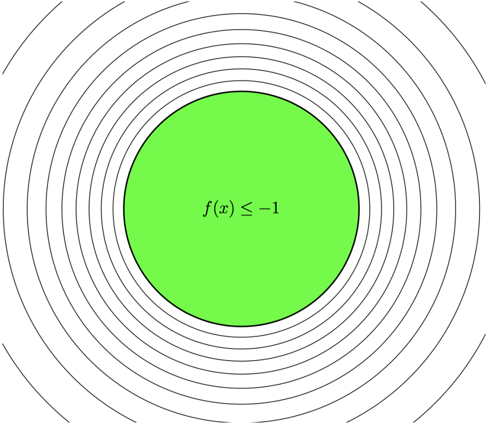
(Proof straight from definitions.)

Convex Function



Plot courtesy of Brett Bernstein.

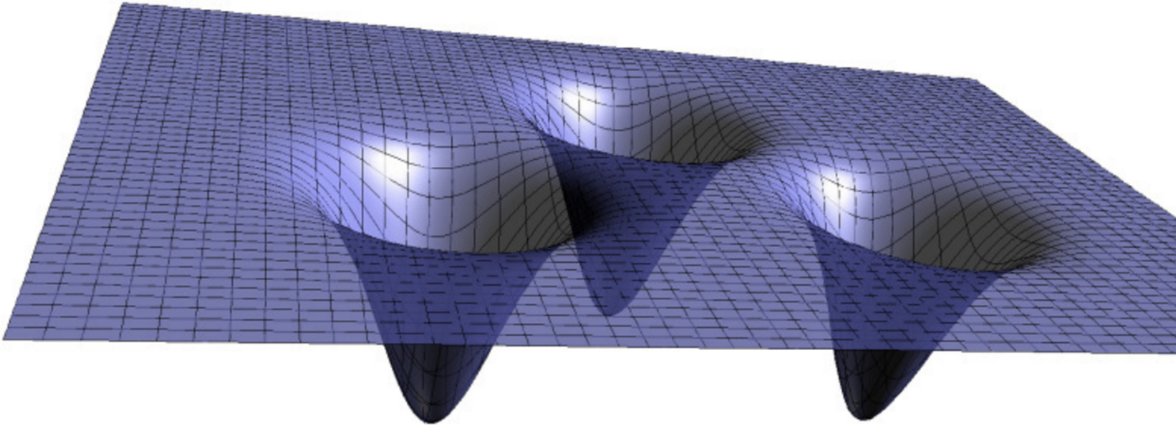
Contour Plot Convex Function: Sublevel Set



Is the sublevel set $\{x \mid f(x) \leqslant 1\}$ convex?

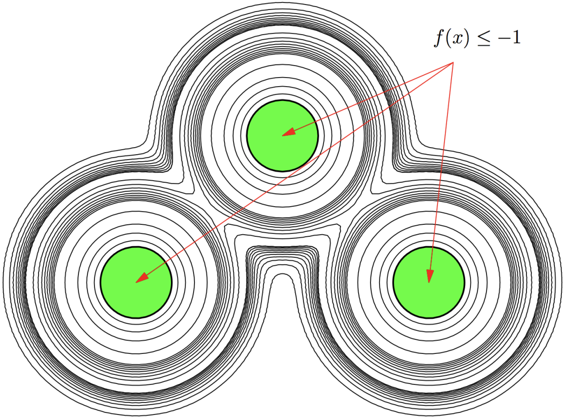
Plot courtesy of Brett Bernstein.

Nonconvex Function



Plot courtesy of Brett Bernstein.

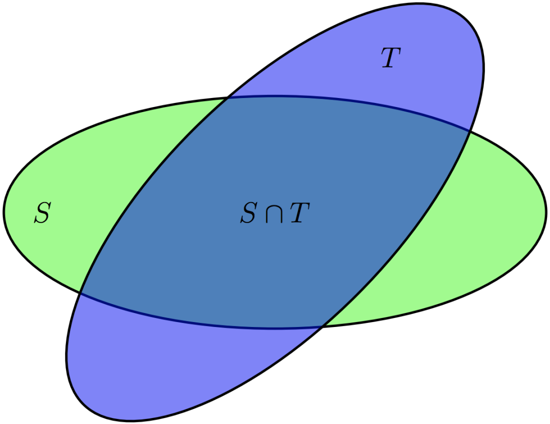
Contour Plot Nonconvex Function: Sublevel Set



Is the sublevel set $\{x \mid f(x) \leqslant 1\}$ convex?

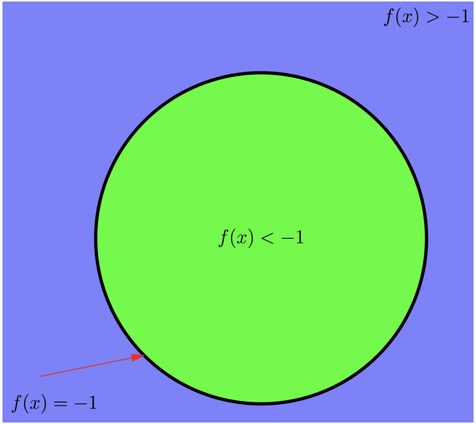
Plot courtesy of Brett Bernstein.

Fact: Intersection of Convex Sets is Convex



Plot courtesy of Brett Bernstein.

Level and Superlevel Sets



Level sets and superlevel sets of convex functions are **not** generally convex.

Plot courtesy of Brett Bernstein.

Convex Optimization Problem: Standard Form

$$
\begin{array}{ll}
\text{minimize} & f_0(x) \\
\text{subject to} & f_i(x) \leqslant 0, \quad i = 1, \ldots, m
\end{array}
$$

where $f_0, \ldots, f_m$ are convex functions.

- What can we say about each constraint set $\{x \mid f_i(x) \leqslant 0\}$? (convex)
- What can we say about the feasible set $\{x \mid f_i(x) \leqslant 0, i = 1, \ldots, m\}$? (convex)

Convex Optimization Problem: Implicit Form

Convex Optimization Problem: Implicit Form

$$
\begin{array}{ll}
\text{minimize} & f(x) \\
\text{subject to} & x \in C
\end{array}
$$

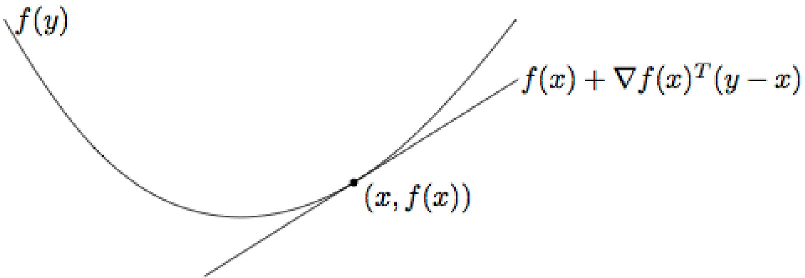
where f is a convex function and C is a convex set.
An alternative "generic" convex optimization problem.

Convex and Differentiable Functions

First-Order Approximation

- Suppose $f : \mathbf{R}^d \to \mathbf{R}$ is **differentiable.**
- Predict $f(y)$ given $f(x)$ and $\nabla f(x)$?
- Linear (i.e. "**first order**") approximation:

$$f(y) \approx f(x) + \nabla f(x)^T (y - x)$$



Boyd & Vandenberghe Fig. 3.2

First-Order Condition for Convex, Differentiable Function

- Suppose $f : \mathbf{R}^d \to \mathbf{R}$ is **convex** and **differentiable.**
- Then for any $x, y \in \mathbf{R}^d$
$$f(y) \geqslant f(x) + \nabla f(x)^T (y - x)$$
- The linear approximation to f at x is a **global underestimator** of f:

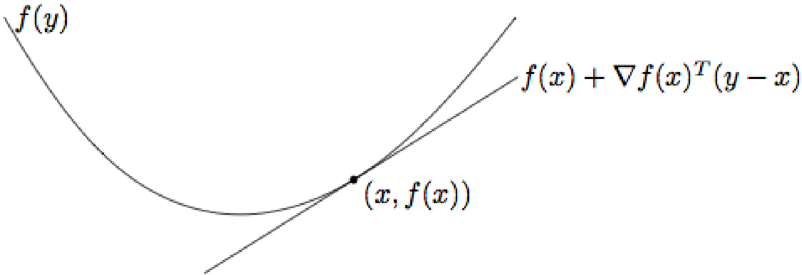


Figure from Boyd & Vandenberghe Fig. 3.2; Proof in Section 3.1.3

First-Order Condition for Convex, Differentiable Function

- Suppose $f : \mathbf{R}^d \to \mathbf{R}$ is **convex** and **differentiable**
- Then for any $x, y \in \mathbf{R}^d$

$$f(y) \geqslant f(x) + \nabla f(x)^T (y - x)$$

Corollary

If $\nabla f(x) = 0$ then x is a global minimizer of f.

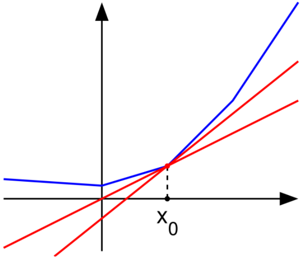
For convex functions, **local information gives global information.**

Subgradients

Definition

A vector $g \in \mathbf{R}^d$ is a **subgradient** of $f : \mathbf{R}^d \to \mathbf{R}$ at x if for all z,

$$f(z) \geqslant f(x) + g^T(z - x).$$



Blue is a graph of $f(x)$.
Each red line $x \mapsto f(x_0) + g^T(x - x_0)$ is a global lower bound on $f(x)$.

Subdifferential

Definitions

- f is **subdifferentiable** at x if $\exists$ at least one subgradient at x.
- The set of all subgradients at x is called the **subdifferential:** $\partial f(x)$

Basic Facts

- f is convex and differentiable $\implies \partial f(x) = \{\nabla f(x)\}$.
- Any point x, there can be 0, 1, or infinitely many subgradients.
- $\partial f(x) = \emptyset \implies f$ is not convex.

Globla Optimality Condition

Definition

A vector $g \in \mathbf{R}^d$ is a **subgradient** of $f : \mathbf{R}^d \to \mathbf{R}$ at x if for all z,

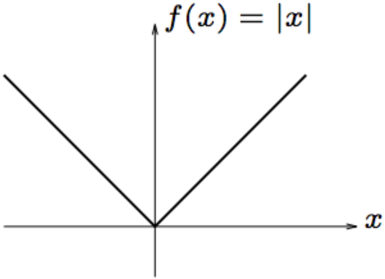
$$f(z) \geqslant f(x) + g^T(z - x).$$

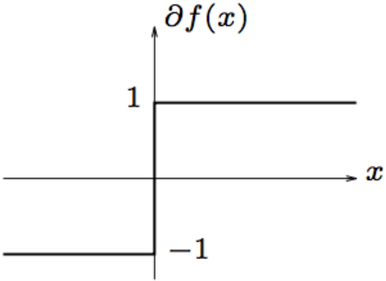
Corollary

*If $0 \in \partial f(x)$, then x is a **global minimizer** of f.*

Subdifferential of Absolute Value

- Consider $f(x) = |x|$

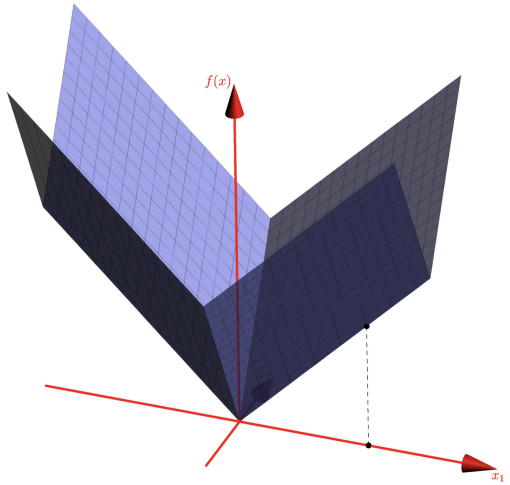




- Plot on right shows $\{(x, g) \mid x \in \mathbf{R},\ g \in \partial f(x)\}$

Boyd EE364b: Subgradients Slides

$f(x_1, x_2) = |x_1| + 2|x_2|$

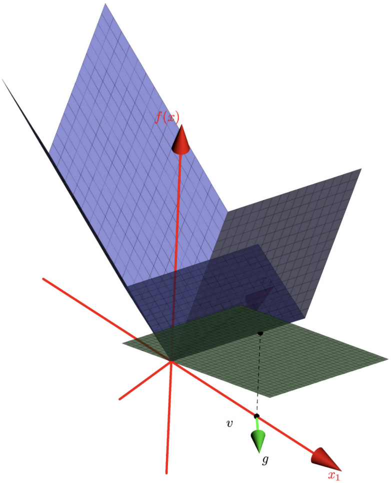


Plot courtesy of Brett Bernstein.

Subgradients of $f(x_1, x_2) = |x_1| + 2|x_2|$

- Let's find the subdifferential of $f(x_1, x_2) = |x_1| + 2|x_2|$ and $(3, 0)$.
- First coordinate of subgradient must be 1, from $|x_1|$ part (at $x_1 = 3$).
- Second coordinate of subgradient can be anything in $[-2, 2]$.
- So graph of $h(x_1, x_2) = f(3, 0) + g^T(x_1 - 3, x_2 - 0)$ is a global underestimate of $f(x_1, x_2)$, for any $g = (g_1, g_2)$, where $g_1 = 1$ and $g_2 \in [-2, 2]$.

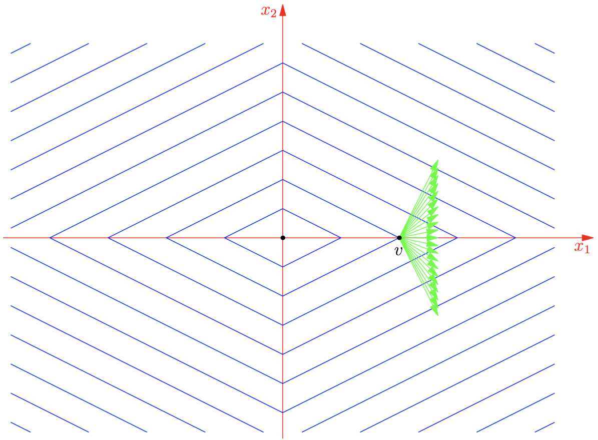
Underestimating Hyperplane to $f(x_1, x_2) = |x_1| + 2|x_2|$



Plot courtesy of Brett Bernstein.

Subdifferential on Contour Plot

$\partial f(3,0) = \{(1,b)^T \mid b \in [-2,2]\}$



Contour plot of $f(x_1,x_2) = |x_1| + 2|x_2|$, with set of subgradients at $(3,0)$. .

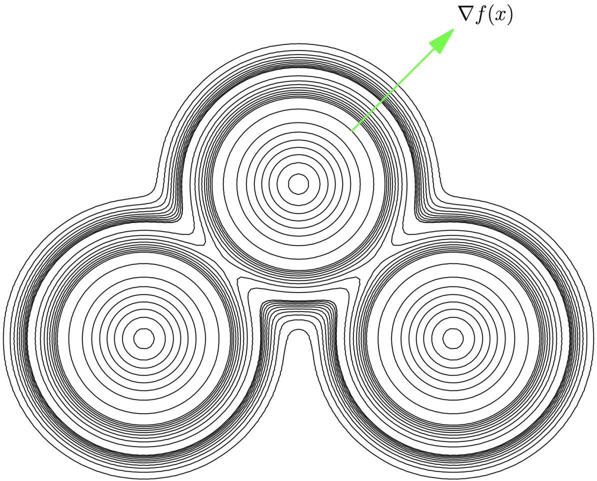
Contour Lines and Gradients

- For function $f : \mathbf{R}^d \to \mathbf{R}$,
  - **graph** of function lives in $\mathbf{R}^{d+1}$,
  - **gradient** and **subgradient** of f live in $\mathbf{R}^d$, and
  - **contours**, **level sets,** and **sublevel sets** are in $\mathbf{R}^d$.
- $f : \mathbf{R}^d \to \mathbf{R}$ continuously differentiable, $\nabla f(x_0) \neq 0$, then $\nabla f(x_0)$ normal to level set

$$S = \left\{ x \in \mathbf{R}^d \mid f(x) = f(x_0) \right\}.$$

- Proof sketch in notes.

Gradient orthogonal to sublevel sets



Plot courtesy of Brett Bernstein.

Contour Lines and Subgradients

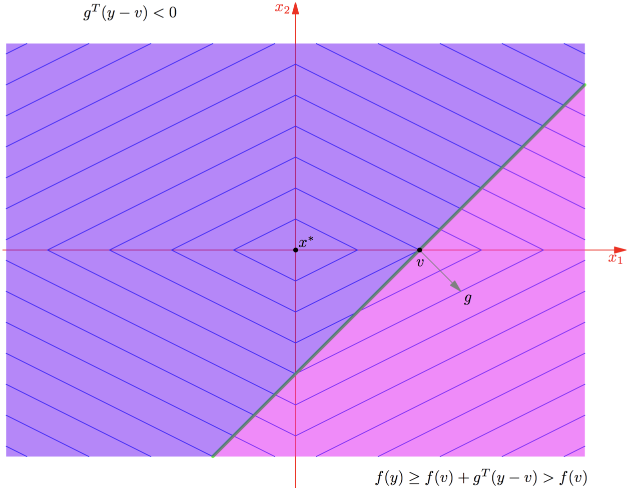
Let $f : \mathbf{R}^d \to \mathbf{R}$ have a subgradient g at x_0.

- Hyperplane H orthogonal to g at x_0 must **support** the level set $S = \left\{x \in \mathbf{R}^d \mid f(x) = f(x_0)\right\}$.
  - i.e H contains x_0 and all of S lies one one side of H.

Proof:

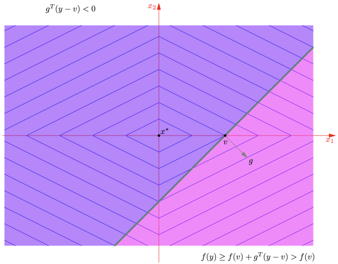
- For any y, we have $f(y) \geqslant f(x_0) + g^T(y - x_0)$. (def of subgradient)
- If y is strictly on side of H that g points in,
  - then $g^T(y - x_0) > 0$.
  - So $f(y) > f(x_0)$.
  - So y is not in the level set S.
- $\therefore$ All elements of S must be on H or on the $-g$ side of H.

Subgradient of $f(x_1, x_2) = |x_1| + 2|x_2|$



Plot courtesy of Brett Bernstein.

Subgradient of $f(x_1, x_2) = |x_1| + 2|x_2|$



- Points on g side of H have larger f-values than $f(x_0)$. (from proof)
- But points on $-g$ side may **not** have smaller f-values.
- So $-g$ may **not** be a descent direction. (shown in figure)

Plot courtesy of Brett Bernstein.

Subgradient Descent

Subgradient Descent

- Suppose f is convex, and we start optimizing at x_0.
- Repeat
  - Step in a negative subgradient direction:

$$x = x_0 - tg,$$

    where $t > 0$ is the step size and $g \in \partial f(x_0)$.

$-g$ not a descent direction – can this work?

Subgradient Gets Us Closer To Minimizer

Theorem

Suppose f is convex.

- *Let $x = x_0 - tg$, for $g \in \partial f(x_0)$.*
- *Let z be any point for which $f(z) < f(x_0)$.*
- *Then for small enough $t > 0$,*
$$\|x - z\|_2 < \|x_0 - z\|_2.$$

- Apply this with $z = x^* \in \arg\min_x f(x)$.

$\Longrightarrow$ **Negative subgradient step gets us closer to minimizer.**

Subgradient Gets Us Closer To Minimizer (Proof)

- Let $x = x_0 - tg$, for $g \in \partial f(x_0)$ and $t > 0$.
- Let z be any point for which $f(z) < f(x_0)$.
- Then

$$
\begin{aligned}
\|x - z\|_2^2 &= \|x_0 - tg - z\|_2^2 \\
&= \|x_0 - z\|_2^2 - 2tg^T(x_0 - z) + t^2\|g\|_2^2 \\
&\leqslant \|x_0 - z\|_2^2 - 2t\left[f(x_0) - f(z)\right] + t^2\|g\|_2^2
\end{aligned}
$$

- Consider $-2t\left[f(x_0) - f(z)\right] + t^2\|g\|_2^2$.
    - It's a convex quadratic (facing upwards).
    - Has zeros at $t = 0$ and $t = 2(f(x_0) - f(z))/\|g\|_2^2 > 0$.
    - Therefore, it's negative for any

$$
t \in \left(0, \frac{2(f(x_0) - f(z))}{\|g\|_2^2}\right).
$$

Based on Boyd EE364b: Subgradients Slides

Assume $f : \mathbf{R}^d \to \mathbf{R}$ is convex and

- f is Lipschitz continuous with constant $G > 0$:

$$|f(x) - f(y)| \leqslant G\|x - y\| \text{ for all } x, y$$

Theorem

For fixed step size t, subgradient method satisfies:

$$\lim_{k \to \infty} f(x_{best}^{(k)}) \leqslant f(x^*) + G^2 t/2$$

Based on https://www.cs.cmu.edu/~ggordon/10725-F12/slides/06-sg-method.pdf

Convergence Theorems for Decreasing Step Sizes

Assume $f : \mathbf{R}^d \to \mathbf{R}$ is convex and

- f is Lipschitz continuous with constant $G > 0$:

$$|f(x) - f(y)| \leqslant G\|x - y\| \text{ for all } x, y$$

Theorem

For step size respecting Robbins-Monro conditions,

$$\lim_{k \to \infty} f(x_{best}^{(k)}) = f(x^*)$$

Based on https://www.cs.cmu.edu/~ggordon/10725-F12/slides/06-sg-method.pdf