Convexity, Local and Global Optimality, etc.

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Directional Derivative: Simplified Expression

Define $g(h) = f(\mathbf{x} + \mathbf{v}h)$. Now:

- $g'(0) = \lim_{h \to 0} \frac{g(0+h)-g(0)}{h} = \lim_{h \to 0} \frac{f(\mathbf{x}+h\mathbf{v})-f(\mathbf{x})}{h}$, which is the expression for the directional derivative defined in equation 1. Thus, $g'(0) = D_{\mathbf{v}}f(\mathbf{x})$.
- By definition of the chain rule for partial differentiation, we get another expression for $g^\prime(0)$ as

$$g'(0) = \sum_{k=1}^{n} \frac{\partial f(\mathbf{x})}{\partial x_k} v_k$$

Therefore,
$$g'(0) = D_{\mathbf{v}}f(\mathbf{x}) = \sum_{k=1}^{n} \frac{\partial f(\mathbf{x})}{\partial x_{k}} v_{k}$$

Homeworks:

Consider the polynomial $f(x, y, z) = x^2 y + z \sin xy$ and the unit vector $\mathbf{v}^T = \frac{1}{\sqrt{3}} [1, 1, 1]^T$. Consider the point $p_0 = (0, 1, 3)$. Compute the directional derivative of f at p_0 in the direction of \mathbf{v} .

find the rate of change of $f(x, y, z) = e^{xyz}$ at $p_0 = (1, 2, 3)$ in the direction from $p_1 = (1, 2, 3)$ to $p_2 = (-4, 6, -1)$.

The Gradient Vector and Directional Derivative

We can see that the right hand side of (2) can be realized as the dot product of two vectors, viz., \[\frac{\partial f(\mathbf{x})}{\partial x_1}, \frac{\partial f(\mathbf{x})}{\partial x_2}, \ldots, \frac{\partial f(\mathbf{x})}{\partial x_n} \] T and v.
Let us denote \[\frac{\partial f(\mathbf{x})}{\partial x_1}, \frac{\partial f(\mathbf{x})}{\partial x_n} \]. Then we assign a name to this special vector:

Definition

[Gradient Vector]: If *f* is differentiable function of $\mathbf{x} \in \Re^n$, then the gradient of $f(\mathbf{x})$ is the vector function $\nabla f(\mathbf{x})$, defined as:

$$abla f(\mathbf{x}) = \begin{bmatrix} f_{x_1}(\mathbf{x}), & f_{x_2}(\mathbf{x}), \dots, & f_{x_n}(\mathbf{x}) \end{bmatrix}$$

The directional derivative of a function f at a point \mathbf{x} in the direction of a unit vector \mathbf{v} can be now written as

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$$D_{\mathbf{v}}f(\mathbf{x}) = \nabla^T f(\mathbf{x}).\mathbf{v} \tag{3}$$

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• Consider the polynomial $f(x, y, z) = x^2y + z \sin xy$ and the unit vector $\mathbf{v}^T = \frac{1}{\sqrt{3}}[1, 1, 1]^T$. Consider the point $p_0 = (0, 1, 3)$. We will compute the directional derivative of f at p_0 in the direction of \mathbf{v} .

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- To do this, we first compute the gradient of f in general: $\nabla f = [2xy + yz \cos xy, x^2 + xz \cos xy, \sin xy]^T$.

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- To do this, we first compute the gradient of *f* in general: $\nabla f = \left[2xy + yz\cos xy, \ x^2 + xz\cos xy, \ \sin xy\right]^T.$
- Evaluating the gradient at a specific point p_0 , $\nabla f(0, 1, 3) = [3, 0, 0]^T$. The directional derivative at p_0 in the direction \mathbf{v} is $D_{\mathbf{v}}f(0, 1, 3) = [3, 0, 0] \cdot \frac{1}{\sqrt{3}}[1, 1, 1]^T = \sqrt{3}$.
- This directional derivative is the rate of change of f at p_0 in the direction \mathbf{v} ; it is positive indicating that the function f increases at p_0 in the direction \mathbf{v} .

• As another example, let us find the rate of change of $f(x, y, z) = e^{xyz}$ at $p_0 = (1, 2, 3)$ in the direction from $p_1 = (1, 2, 3)$ to $p_2 = (-4, 6, -1)$.

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- We first construct a unit vector from p_1 to p_2 ; $\mathbf{v} = \frac{1}{\sqrt{57}}[-5, 4, -4]$.
- The gradient of f in general is $\nabla f = [yze^{xyz}, xze^{xyz}, xye^{xyz}] = e^{xyz}[yz, xz, xy].$
- Evaluating the gradient at a specific point p_0 , $\nabla f(1,2,3) = e^6 [6,3,2]^T$. The directional derivative at p_0 in the direction \mathbf{v} is $D_{\mathbf{u}}f(1,2,3) = e^6 [6,3,2] \cdot \frac{1}{\sqrt{57}} [-5,4,-4]^T = \frac{e^6 26}{\sqrt{57}}$.
- This directional derivative is negative, indicating that the function *f* decreases at *p*₀ in the direction from *p*₁ to *p*₂.

More on the Gradient Vector

- All our ideas about first and second derivative in the case of a single variable carry over to the directional derivative.
- What does the gradient ∇f(x) tell you about the function f(x)? While there exist infinitely many direction vectors v at any point x, there is a unique gradient vector ∇f(x).
- Since we expressed $D_{\mathbf{v}}f(\mathbf{x})$ as the dot product of $\nabla f(\mathbf{x})$ with \mathbf{v} , we can study $\nabla f(\mathbf{x})$ independently.

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Claim

Suppose f is a differentiable function of $\mathbf{x} \in \Re^n$. The maximum value of the directional derivative $D_{\mathbf{v}}f(\mathbf{x})$ is $||\nabla f(\mathbf{x})|$ and it is so when \mathbf{v} has the same direction as the gradient vector $\nabla f(\mathbf{x})$.

Proof: Directional derivative is a dot product of gradient and direction which can be upper bounded using Cauchy Shwarz inequality More on the Gradient Vector (contd.)

Proof:

- The cauchy schwartz inequality when applied in the eucledian space gives us $|\mathbf{x}^T \mathbf{y}| \le ||\mathbf{x}|| ||\mathbf{y}||$ for any $\mathbf{x}, \mathbf{y} \in \Re^n$, with equality holding *iff* \mathbf{x} and \mathbf{y} are linearly dependent.
- The inequality gives upper and lower bounds on the dot product between two vectors; $-||\mathbf{x}||||\mathbf{y}|| \leq \mathbf{x}^T \mathbf{y} \leq ||\mathbf{x}||||\mathbf{y}||.$
- Applying these bounds to the right hand side of (3) and using the fact that $||\mathbf{v}||=1$, we
 - ^{get} Upper and lower bounds for directional derivative at x. Are these upper and lower bounds attainable?

ANS: Yes. In or against direction of gradient of f at x!

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- Applying these bounds to the right hand side of (3) and using the fact that $||\mathbf{v}|| = 1$, we get

$$-||\nabla f(\mathbf{x})|| \le D_{\mathbf{v}}f(\mathbf{x}) = \nabla^{T}f(\mathbf{x}).\mathbf{v} \le ||\nabla f(\mathbf{x})||$$

with equality holding *iff* $\mathbf{v} = k \nabla f(\mathbf{x})$ for some $k \ge 0$.

• Since $||\mathbf{v}|| = 1$, equality can hold iff $\mathbf{v} = \frac{\nabla f(\mathbf{x})}{||\nabla f(\mathbf{x})||}$.

More on the Gradient Vector (contd.)

- Thus, the maximum rate of change of f at a point \mathbf{x} is given by the norm $||\nabla f(\mathbf{x})|$ of the gradient vector at \mathbf{x} .
- And the direction in which the rate of change of f is maximum is given by the unit vector $\frac{\nabla f(\mathbf{x})}{||\nabla f(\mathbf{x})|}$.
- An associated fact is that the minimum value of the directional derivative $D_{\mathbf{v}}f(\mathbf{x})$ is $-||\nabla f(\mathbf{x})||$ and it is attained when \mathbf{v} has the opposite direction of the gradient vector, *i.e.*, $-\frac{\nabla f(\mathbf{x})}{||\nabla f(\mathbf{x})||}$.
- The method of steepest descent uses this result to iteratively choose a new value of \mathbf{x} by traversing in the direction of $-\nabla f(\mathbf{x})$, especially while minimizing the value of some complex function.

Visualizing the Gradient Vector

Consider the function $f(x_1, x_2) = x_1 e^{x_2}$. The Figure below shows 10 level curves for this function, corresponding to $f(x_1, x_2) = c$ for c = 1, 2, ..., 10.



will be useful and discussed for constrained optimization

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The idea behind a level curve is that as you change x along any level curve, the function value remains unchanged, but as you move x across level curves, the function value changes.



Vanishing of the Directional Derivative

What if $D_{\mathbf{v}}f(\mathbf{x})$ turns out to be 0?

Level curves for $x^2 + y^2$



Vanishing of the Directional Derivative

What if $D_{\mathbf{v}}f(\mathbf{x})$ turns out to be 0? We then expect that $\nabla f(\mathbf{x})$ and \mathbf{v} are othogonal.

Definition

Level Surface/Set: The level surface/set of $\mathit{f}(\mathbf{x})$ at \mathbf{x}^* is



$$\{\mathbf{x}|\mathit{f}(\mathbf{x})=\mathit{f}(\mathbf{x}^*)\}$$

(4)

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$$\{\mathbf{x}|f(\mathbf{x})=f(\mathbf{x}^*)\}$$

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There is a useful result in this regard.

Claim

Let $f: \mathcal{D} \to \Re$ with $\mathcal{D} \subseteq \Re^n$ be a differentiable function. The gradient ∇f evaluated at \mathbf{x}^* is orthogonal to the tangent hyperplane (tangent line in case n = 2) to the level surface of f passing through \mathbf{x}^* .

and lying on the level set, has gradient orthogonal to tangent line $\frac{22}{86}$

Proof: Let \mathcal{K} be the range of f and let $k \in \mathcal{K}$ such that $f(\mathbf{x}^*) = k$.

- Consider the level surface $f(\mathbf{x}) = k$. Let $\mathbf{r}(t) = [x_1(t), x_2(t), \dots, x_n(t)]$ be a curve on the level surface, parametrized by $t \in \Re$, with $\mathbf{r}(0) = \mathbf{x}^*$.
- Then, f(x(t), y(t), z(t)) = k. Applying the chain rule

For this example in 3d, df/dt = dot product of gradient of f with the vector of derivatives of xi wrt t

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- Then, f(x(t), y(t), z(t)) = k. Applying the chain rule

$$\frac{df(\mathbf{r}(t))}{dt} = \sum_{i=1}^{n} \frac{\partial f}{\partial x_i} \frac{dx_i(t)}{dt} = \nabla^T f(\mathbf{x}(t)) \frac{d\mathbf{r}(t)}{dt} = 0$$

• For t = 0, the equations become

Vanishing of the Directional Derivative & Level Surfaces: Proof (Not rigorous)

Proof: Let \mathcal{K} be the range of f and let $k \in \mathcal{K}$ such that $f(\mathbf{x}^*) = k$.

- Consider the level surface $f(\mathbf{x}) = k$. Let $\mathbf{r}(t) = [x_1(t), x_2(t), \dots, x_n(t)]$ be a curve on the level surface, parametrized by $t \in \Re$, with $\mathbf{r}(0) = \mathbf{x}^*$.
- Then, f(x(t), y(t), z(t)) = k. Applying the chain rule

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• For t = 0, the equations become

$$\nabla^{\mathsf{T}} f(\mathbf{x}^*) \frac{d\mathbf{r}(0)}{dt} = 0$$

• Now, $\frac{d\mathbf{r}(t)}{dt}$ represents any tangent vector to the curve through $\mathbf{r}(t)$ which lies completely on the level surface.

The tangent plane is the plane containing all such tangent vectors across all such r(t

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$$\nabla^T f(\mathbf{x}^*) \frac{d\mathbf{r}(0)}{dt} = 0$$

- That is, the tangent line to any curve at x^{*} on the level surface containing x^{*}, is orthogonal to ∇f(x^{*}).
- Since the tangent hyperplane to a surface at any point is the hyperplane containing all tangent vectors to curves on the surface passing through the point, the gradient $\nabla f(\mathbf{x}^*)$ is perpendicular to the tangent hyperplane to the level surface passing through that point \mathbf{x}^* .
- The equation of the tangent hyperplane is given by

Hyperplane(x*,gradient of f at x*)

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- Since the tangent hyperplane to a surface at any point is the hyperplane containing all tangent vectors to curves on the surface passing through the point, the gradient $\nabla f(\mathbf{x}^*)$ is perpendicular to the tangent hyperplane to the level surface passing through that point \mathbf{x}^* .
- The equation of the tangent hyperplane is given by $(\mathbf{x} \mathbf{x}^*)^T \nabla f(\mathbf{x}^*) = 0$

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- Recall that the normal to a plane can be found by taking the cross product of any two vectors lying within the plane. Thus, the gradient vector $\nabla f(\mathbf{x}^*)$ at any point \mathbf{x}^* on the level surface of a function f(.) is normal to the tangent hyperplane (or tangent line in the case of two variables) to the surface at the same point.
- The same gradient vector ∇f(x*) at a point x* can also be conveniently computed as the vector of partial derivatives of the function at that point.
- We will illustrate this geometric understanding through some examples.

• Consider the same plot as earlier with a gradient vector at (2,0) as shown below. The gradient vector $\begin{bmatrix} 1, 2 \end{bmatrix}^T$ is perpendicular to the tangent hyperplane to the level curve $x_1 e^{x_2} = 2$ at (2,0). The equation of the tangent hyperplane is $(x_1 - 2) + 2(x_2 - 0) = 0$ and it turns out to be a tangent line.



The level surfaces for $f(x_1, x_2, x_3) = x_1^2 + x_2^2 + x_3^2$ are shown in the Figure below. The gradient at (1, 1, 1) is orthogonal to the tangent hyperplane to the level surface $f(x_1, x_2, x_3) = x_1^2 + x_2^2 + x_3^2 = 3$ at (1, 1, 1). The gradient vector at (1, 1, 1) is $[2, 2, 2]^T$ and the tanget hyperplane has the equation $2(x_1 - 1) + 2(x_2 - 1) + 2(x_3 - 1) = 0$, which is a plane in 3D.



On the other hand, the dotted line in the Figure below is not orthogonal to the level surface, since it does not coincide with the gradient.



• Let $f(x_1, x_1, x_3) = x_1^2 x_2^3 x_3^4$ and consider the point $\mathbf{x}^0 = (1, 2, 1)$. We will find the equation of the tangent plane to the level surface through \mathbf{x}^0 .

Compute gradient at x0

- Let $f(x_1, x, x_3) = x_1^2 x_2^3 x_3^4$ and consider the point $\mathbf{x}^0 = (1, 2, 1)$. We will find the equation of the tangent plane to the level surface through \mathbf{x}^0 .
- The level surface through \mathbf{x}^0 is determined by setting f equal to its value evaluated at \mathbf{x}^0 ; that is, the level surface will have the equation $x_1^2 x_2^3 x_3^4 = 1^2 2^3 1^4 = 8$.
- The gradient vector (normal to tangent plane) at (1, 2, 1) is $\nabla f(x_1, x_2, x_3) \Big|_{(1,2,1)} = [2x_1x_2^3x_3^4, 3x_1^2x_2^2x_3^4, 4x_1^2x_2^3x_3^3]^T \Big|_{(1,2,1)} = [16, 12, 32]^T.$
- The equation of the tangent plane at \mathbf{x}^0 , given the normal vector $\nabla f(\mathbf{x}^0)$ can be easily written down: $\nabla f(\mathbf{x}^0)^T [\mathbf{x} \mathbf{x}^0] = 0$ which turns out to be $16(x_1 1) + 12(x_2 2) + 32(x_3 1) = 0$, a plane in 3D.

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• Consider the function $f(x, y, z) = \frac{x}{y+z}$. The directional derivative of f in the direction of the vector $\mathbf{v} = \frac{1}{\sqrt{14}} [1, 2, 3]$ at the point $x^0 = (4, 1, 1)$ is

- Consider the function $f(x, y, z) = \frac{x}{y+z}$. The directional derivative of f in the direction of the vector $\mathbf{v} = \frac{1}{\sqrt{14}} [1, 2, 3]$ at the point $x^0 = (4, 1, 1)$ is $\nabla^T f \Big|_{(4,1,1)} \cdot \frac{1}{\sqrt{14}} [1, 2, 3]^T = \left[\frac{1}{y+z}, -\frac{x}{(y+z)^2}, -\frac{x}{(y+z)^2} \right] \Big|_{(4,1,1)} \cdot \frac{1}{\sqrt{14}} [1, 2, 3]^T = \left[\frac{1}{2}, -1, -1 \right] \cdot \frac{1}{\sqrt{14}} [1, 2, 3]^T = -\frac{9}{2\sqrt{14}}.$
- The directional derivative is negative, indicating that the function decreases along the direction of v. Based on an earlier result, we know that the maximum rate of change of a function at a point x is given by $||\nabla f(\mathbf{x})||$ and it is in the direction $\frac{\nabla f(\mathbf{x})}{||\nabla f(\mathbf{x})||}$.
- In the example under consideration, this maximum rate of change at \mathbf{x}^0 is $\frac{3}{2}$ and it is in the direction of the vector $\frac{2}{3} \left[\frac{1}{2}, -1, -1\right]$.

Let us find the maximum rate of change of the function $f(x, y, z) = x^2 y^3 z^4$ at the point $\mathbf{x}^0 = (1, 1, 1)$ and the direction in which it occurs. The gradient at \mathbf{x}^0 is

Let us find the maximum rate of change of the function $f(x, y, z) = x^2 y^3 z^4$ at the point $\mathbf{x}^0 = (1, 1, 1)$ and the direction in which it occurs. The gradient at \mathbf{x}^0 is $\nabla^T f\Big|_{(1,1,1)} = [2, 3, 4]$. The maximum rate of change at \mathbf{x}^0 is therefore $\sqrt{29}$ and the direction of the corresponding rate of change is $\frac{1}{\sqrt{29}}[2, 3, 4]$. The minimum rate of change is $-\sqrt{29}$ and the corresponding direction is $-\frac{1}{\sqrt{29}}[2, 3, 4]$.

Let us determine the equations of

(a) the tangent plane to the paraboloid $\mathcal{P}: x_1=x_2^2+x_3^2+2$ at (-1,1,0) and

(b) the normal line to the tangent plane.

To realize this as the level surface of a function of three variables, we define the function

f (such that P corresponds to one of its level sets)

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(a) the tangent plane to the paraboloid $\mathcal{P}: x_1 = x_2^2 + x_3^2 + 2$ at (-1, 1, 0) and (b) the normal line to the tangent plane.

To realize this as the level surface of a function of three variables, we define the function $f(x_1, x_2, x_3) = x_1 - x_2^2 - x_3^2$ and find that the paraboloid \mathcal{P} is the same as the level surface $f(x_1, x_2, x_3) = +2$. The normal to the tangent plane to \mathcal{P} at \mathbf{x}^0 is in the direction of the gradient vector $\nabla f(\mathbf{x}^0) = [1, -2, 0]^T$ and its parametric equation is $[x_1, x_2, x_3] = [-1 + t, 1 - 2t, 0]$.

The equation of the tangent plane is therefore $(x_1 + 1) - 2(x_2 - 1) = 0$.

Gradient and Convex Functions?

- How do we understand the behaviour of gradients for convex functions?
- While we have a lot to see in the coming sessions, here is a small peek through *sub-level* sets of a convex function

Definition

[Sublevel Sets]: Let $\mathcal{D} \subseteq \Re^n$ be a nonempty set and $f: \mathcal{D} \to \Re$. The set

$$L_{\alpha}(f) = \left\{ \mathbf{x} | \mathbf{x} \in \mathcal{D}, \ f(\mathbf{x}) \le \alpha \right\}$$

is called the α -sub-level set of *f*.

Now if a function f is convex, each of its sublevel set will be convex





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Now if a function f is convex, its α -sub-level set is a convex set.

Convex Function \Rightarrow Convex Sub-level sets

Theorem

Let $\mathcal{D} \subseteq \Re^n$ be a nonempty convex set, and $f : \mathcal{D} \to \Re$ be a convex function. Then $L_{\alpha}(f)$ is a convex set for any $\alpha \in \Re$.

Proof: Consider $\mathbf{x}_1, \mathbf{x}_2 \in L_{\alpha}(f)$. Then by definition of the level set, $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{D}$, $f(\mathbf{x}_1) \leq \alpha$ and $f(\mathbf{x}_2) \leq \alpha$. From convexity of \mathcal{D} it follows that for all $\theta \in (0, 1)$, $\mathbf{x} = \theta \mathbf{x}_1 + (1 - \theta) \mathbf{x}_2 \in \mathcal{D}$. Moreover, since f is also convex,

$$f(\mathbf{x}) \le \theta f(\mathbf{x}_1) + (1-\theta)f(\mathbf{x}_2) \le \theta \alpha + (1-\theta)\alpha = \alpha$$

which implies that $\mathbf{x} \in L_{\alpha}(f)$. Thus, $L_{\alpha}(f)$ is a convex set.

The converse of this theorem does not hold. To illustrate this, consider the function $f(\mathbf{x}) = \frac{x_2}{1+2x_1^2}$. The <u>0-sublevel set of this function is $\{(x_1, x_2) \mid x_2 \leq 0\}$ </u>, which is convex. However, the function $f(\mathbf{x})$ itself is not convex.



0 level subset which is convex

$\mathsf{Convex}\ \mathsf{Function} \Rightarrow \mathsf{Convex}\ \mathsf{Sub-level}\ \mathsf{sets}$

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$$f(\mathbf{x}) \le \theta f(\mathbf{x}_1) + (1-\theta)f(\mathbf{x}_2) \le \theta \alpha + (1-\theta)\alpha = \alpha$$

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The converse of this theorem does not hold. To illustrate this, consider the function $f(\mathbf{x}) = \frac{x_2}{1+2x_1^2}$. The 0-sublevel set of this function is $\{(x_1, x_2) \mid x_2 \leq 0\}$, which is convex. However, the function $f(\mathbf{x})$ itself is not convex.

A function is called quasi-convex if all its sub-level sets are convex sets Eg: Negative of the normal distribution $-\frac{1}{\sigma\sqrt{2\pi}}exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$ is quasi-convex but not convex. [Homework]

Gradient, Convex Functions and Sub-level sets: A First Peek

We have already seen that

- The gradient $\nabla f(\mathbf{x}^*)$ at \mathbf{x}^* is normal to the tangent hyperplane to the level set $\{\mathbf{x}|f(\mathbf{x}) = f(\mathbf{x}^*)\}$ at \mathbf{x}^*
- The gradient $\nabla f(\mathbf{x}^*)$ at \mathbf{x}^* points in direction of increasing values of f(.) at \mathbf{x}^* Now, if $f(\mathbf{x})$ is also convex

Gradient, Convex Functions and Sub-level sets: A First Peek

We have already seen that

- The gradient $\nabla f(\mathbf{x}^*)$ at \mathbf{x}^* is normal to the tangent hyperplane to the level set $\{\mathbf{x}|f(\mathbf{x}) = f(\mathbf{x}^*)\}$ at \mathbf{x}^*
- The gradient $\nabla f(\mathbf{x}^*)$ at \mathbf{x}^* points in direction of increasing values of f(.) at \mathbf{x}^*

Now, if $f(\mathbf{x})$ is also convex

- The gradient $\nabla f(\mathbf{x}^*)$ at \mathbf{x}^* is normal to the tangent hyperplane to the sub-level set $\{\mathbf{x}|f(\mathbf{x}) \leq f(\mathbf{x}^*)\}$ at \mathbf{x}^*
- The tangent hyperplane defined by $\nabla f(\mathbf{x}^*)$ at \mathbf{x}^* is a supporting hyperplane to the convex set $\{\mathbf{x} | f(\mathbf{x}) \leq f(\mathbf{x}^*)\}$ at \mathbf{x}^*