

# Psych 253

## Advanced Statistical Modeling

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### Review of Differential Calculus

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$$= \lim_{\Delta x \rightarrow 0} \frac{2\Delta x \cdot x + (\Delta x)^2}{\Delta x} = \lim_{\Delta x \rightarrow 0} 2x + \Delta x = \boxed{2x}$$

(cancel leading term)                      (divide out  $\Delta x$ )                      (take limit)

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$$= \lim_{\Delta x \rightarrow 0} \frac{x^n + nx^{n-1} \cdot (\Delta x) + \sum_{i=2}^n \binom{n}{i} x^{n-i} (\Delta x)^i - x^n}{\Delta x}$$

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NB: these three steps, in this specific computation, represent Newton's most important mathematical contributions, shifting the course of history after ever

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# Interpretation as Local Slope

$F'(x)$  is the slope of the line that is tangent to the graph of  $F(x)$  at  $x$ :

Suppose that line is:

$$y = mx + b$$

Then:

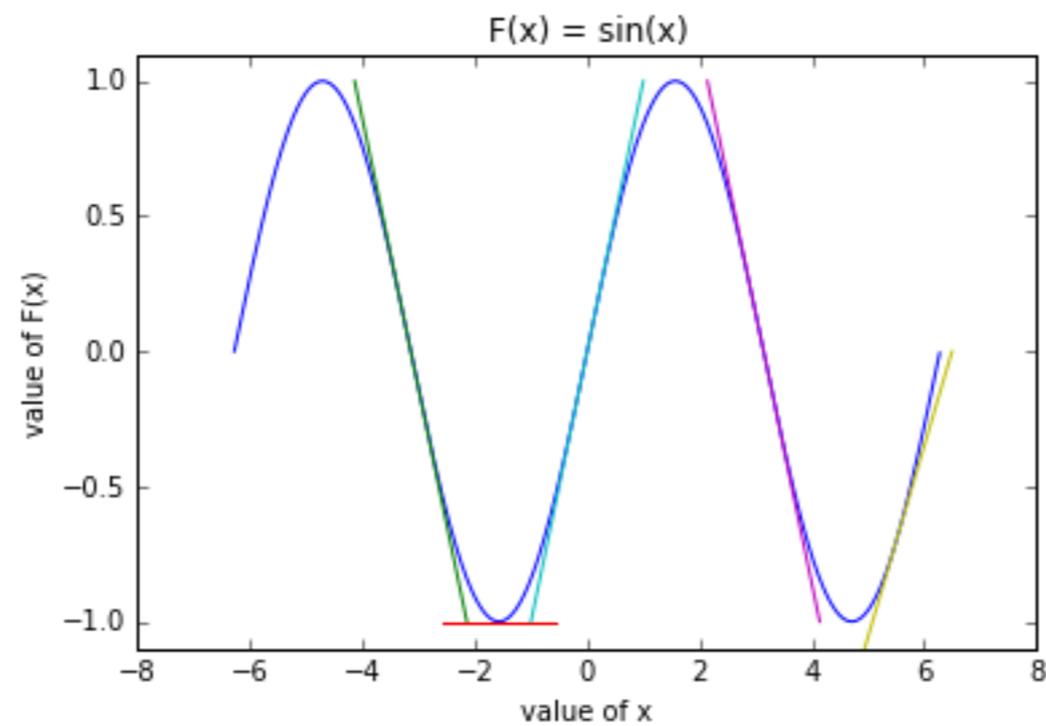
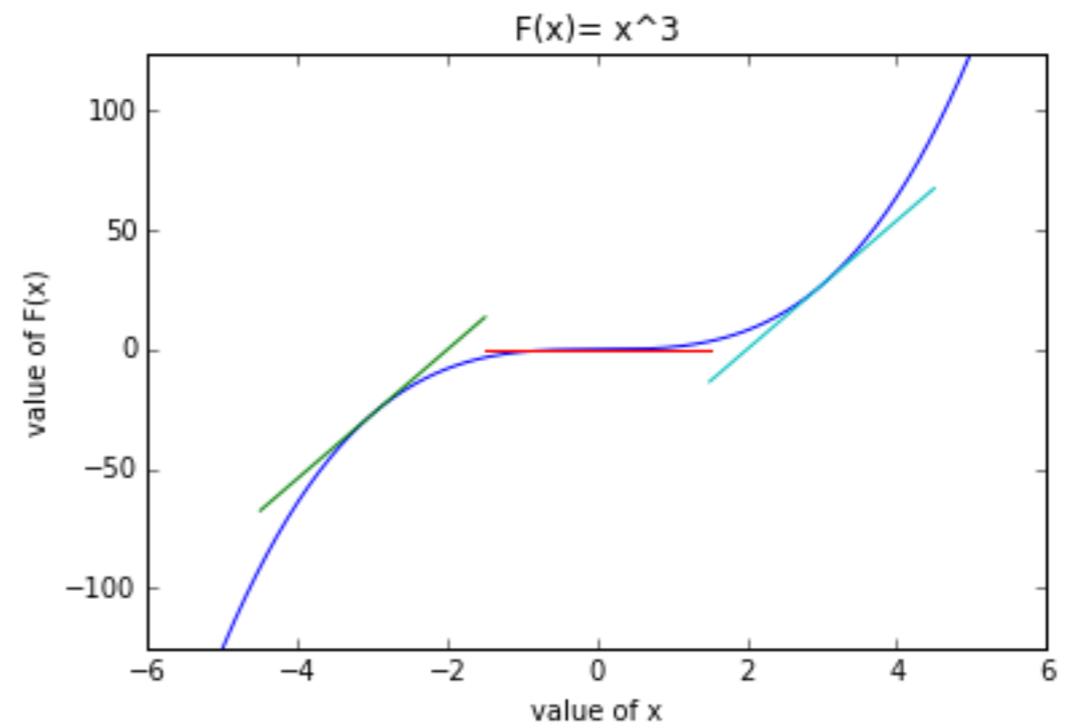
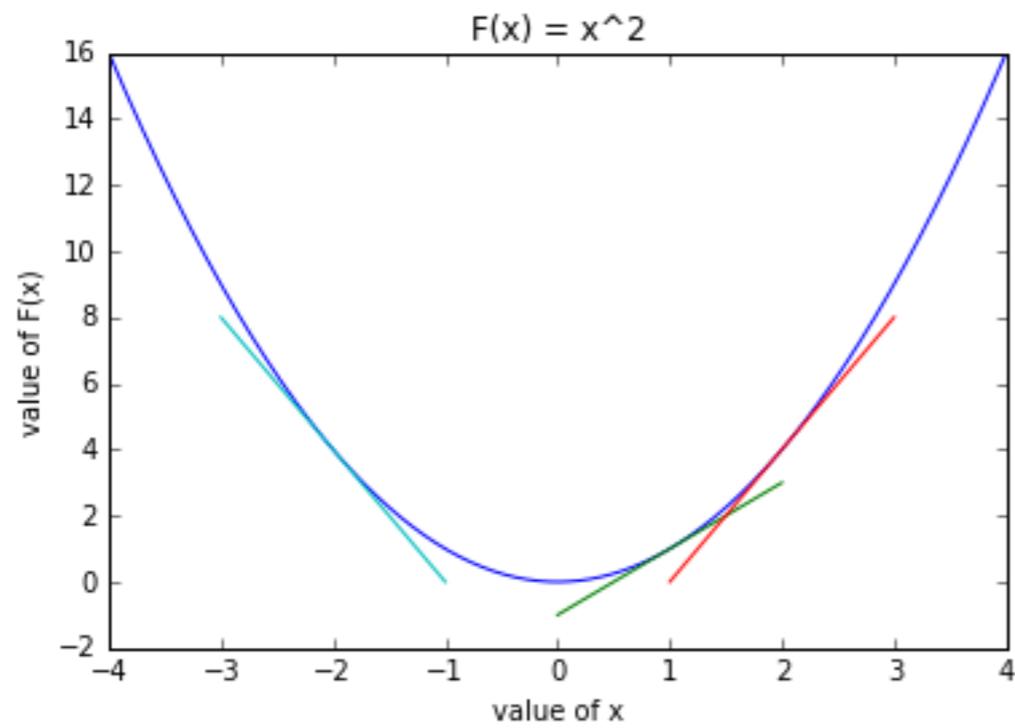
$$F(x) = F'(x)x + b$$

So:

$$b = F(x) - F'(x)x$$

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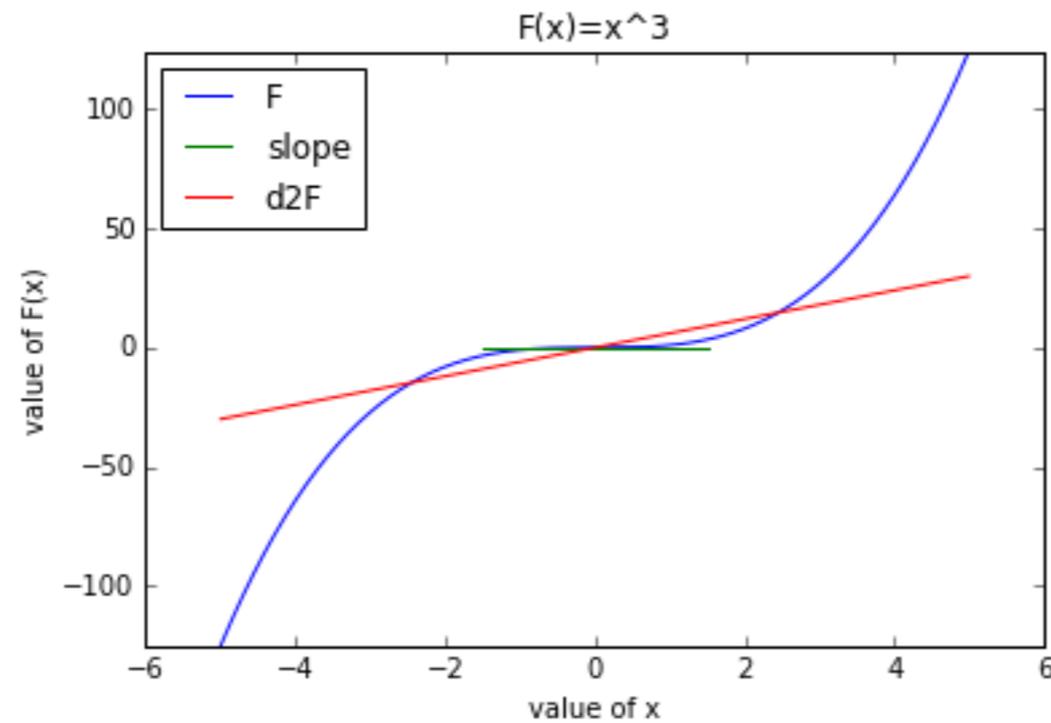
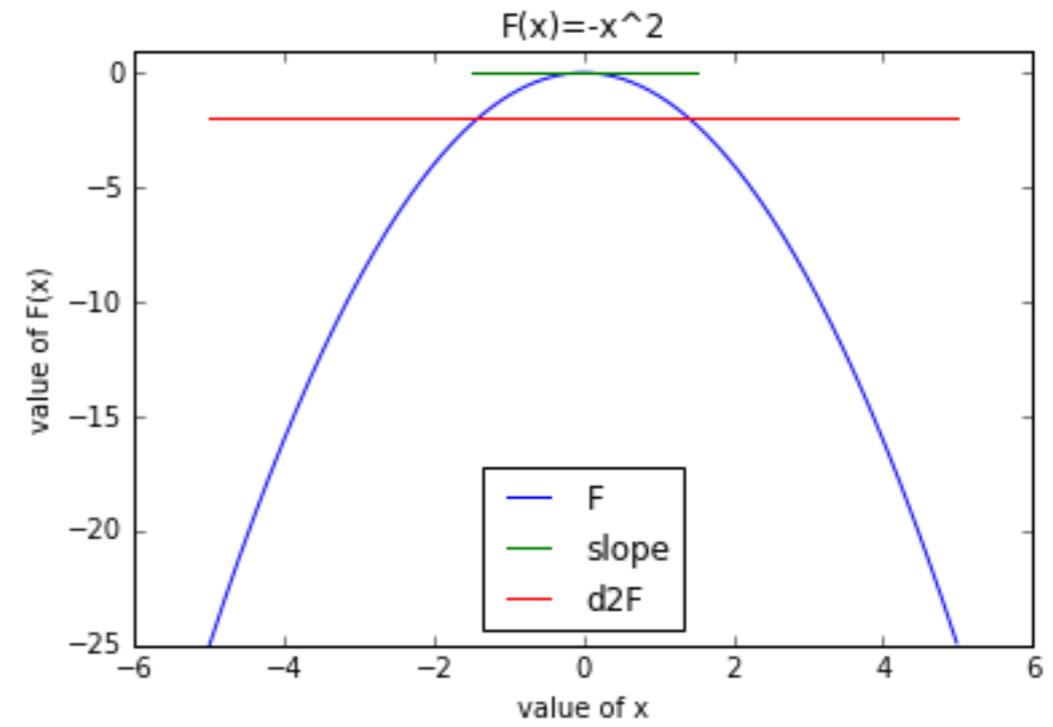
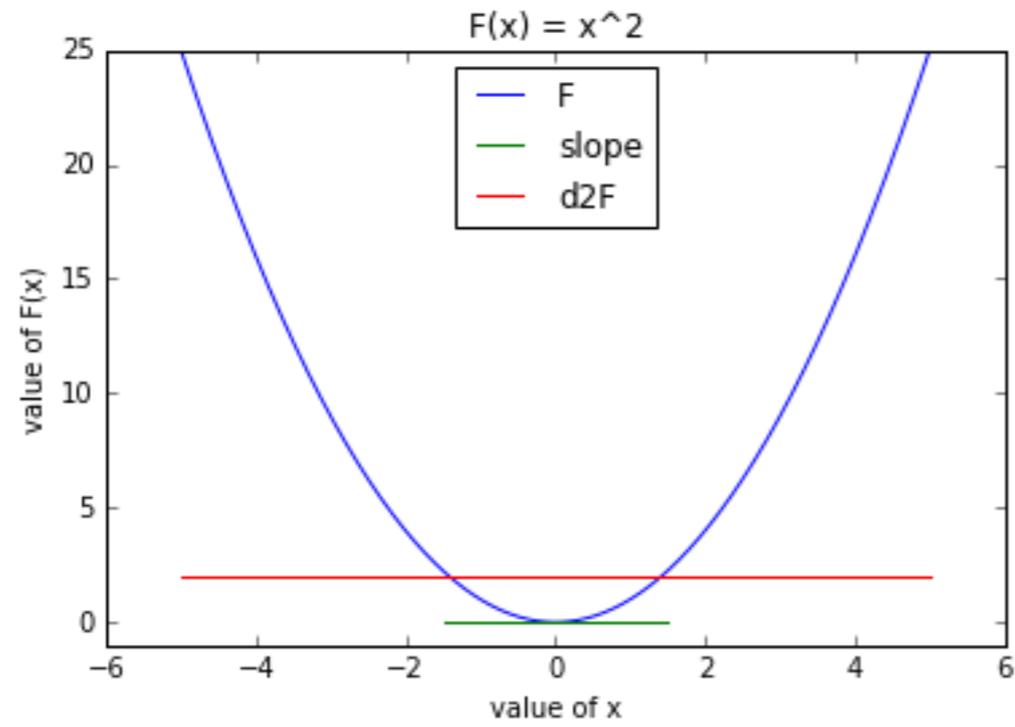
# Higher Derivatives

The  $n$ th derivative is the derivative of the  $(n-1)$ st derivative:

$$F^{(n)}(x) = \frac{d^n F}{dx^n} = \frac{d}{dx} (F^{(n-1)}(x))$$

# Higher Derivatives

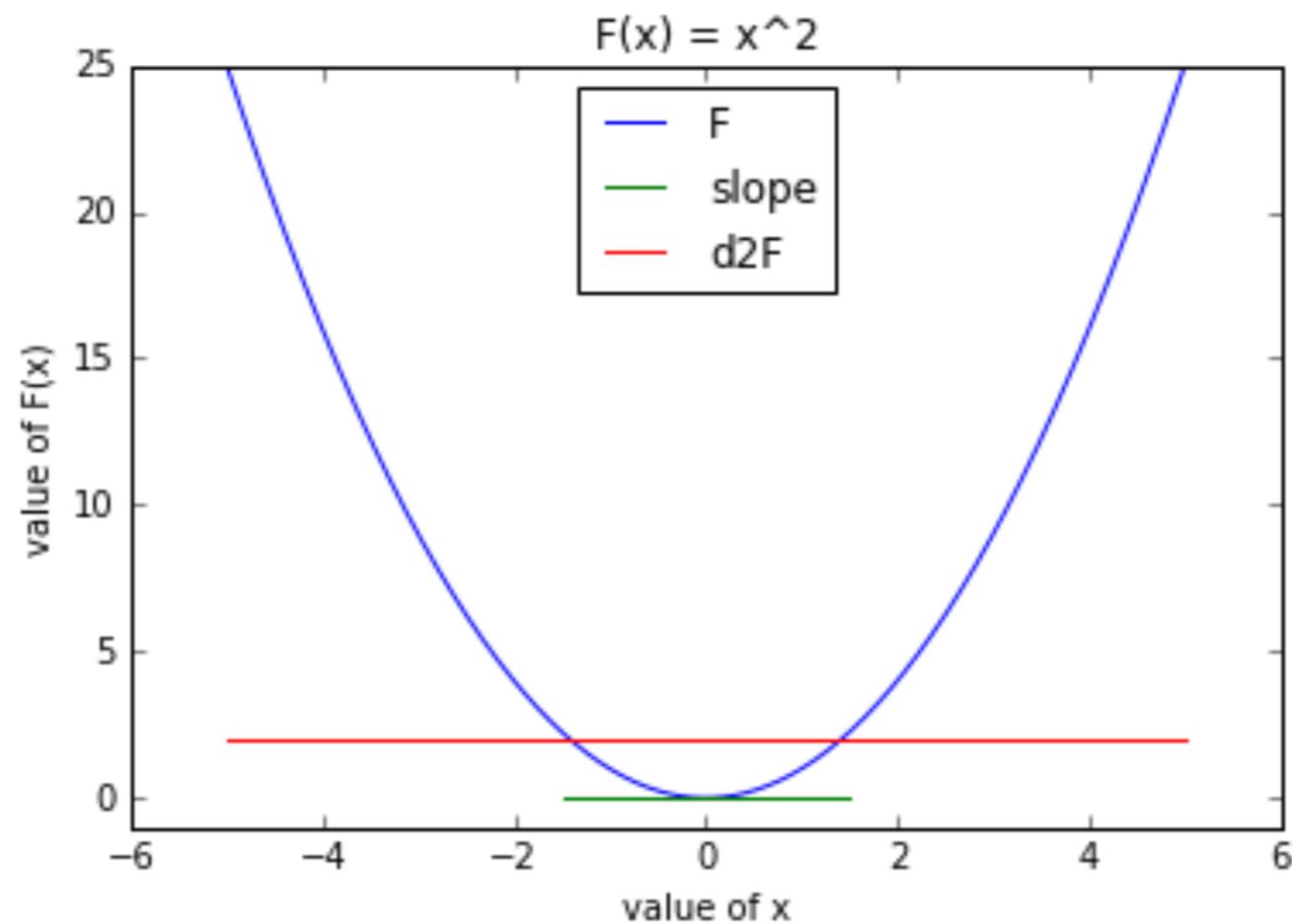
E.g., second derivatives:



# Critical Points and Local Optima

Critical points are those  $\mathbf{x}^*$  such that:

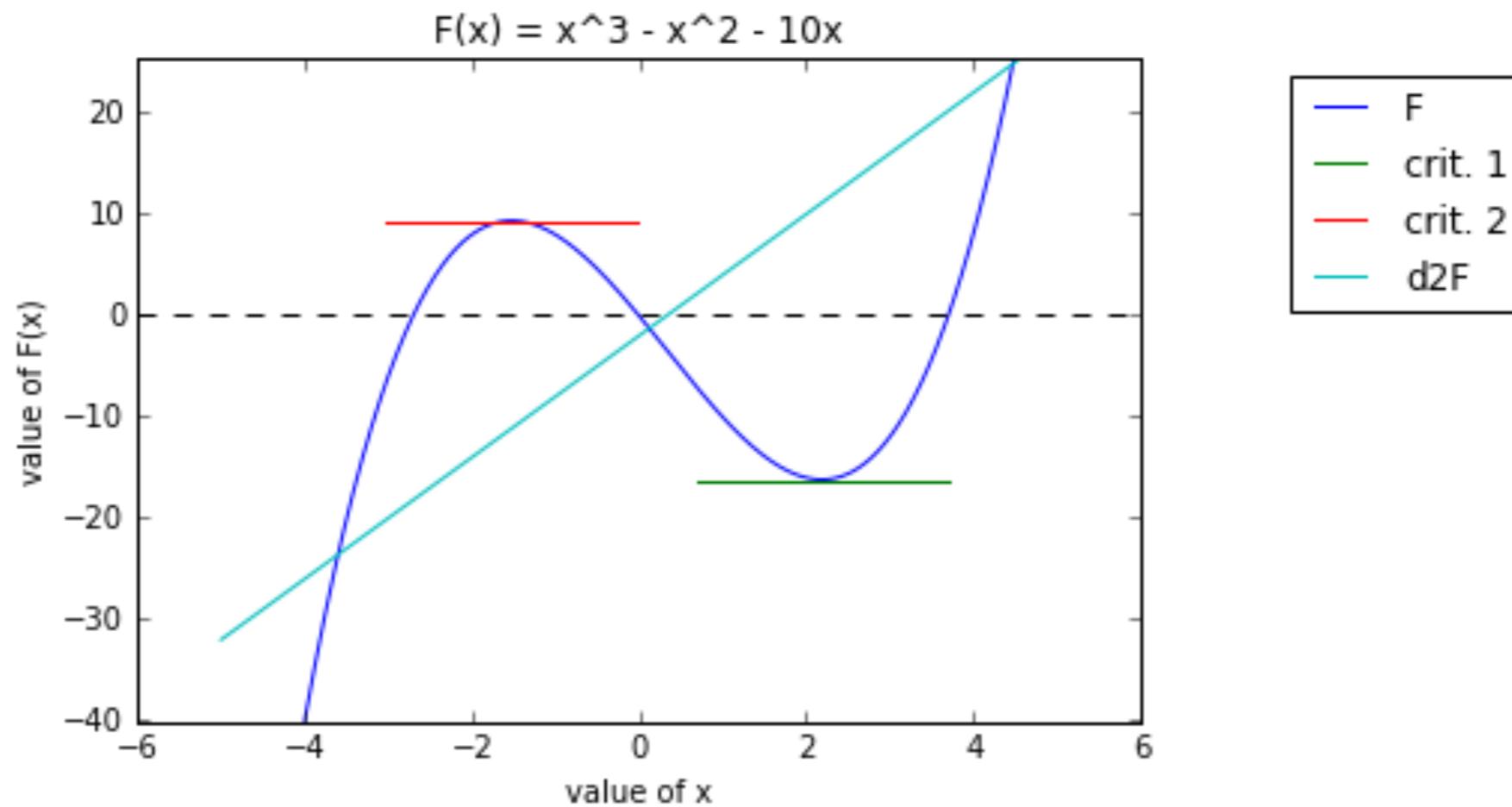
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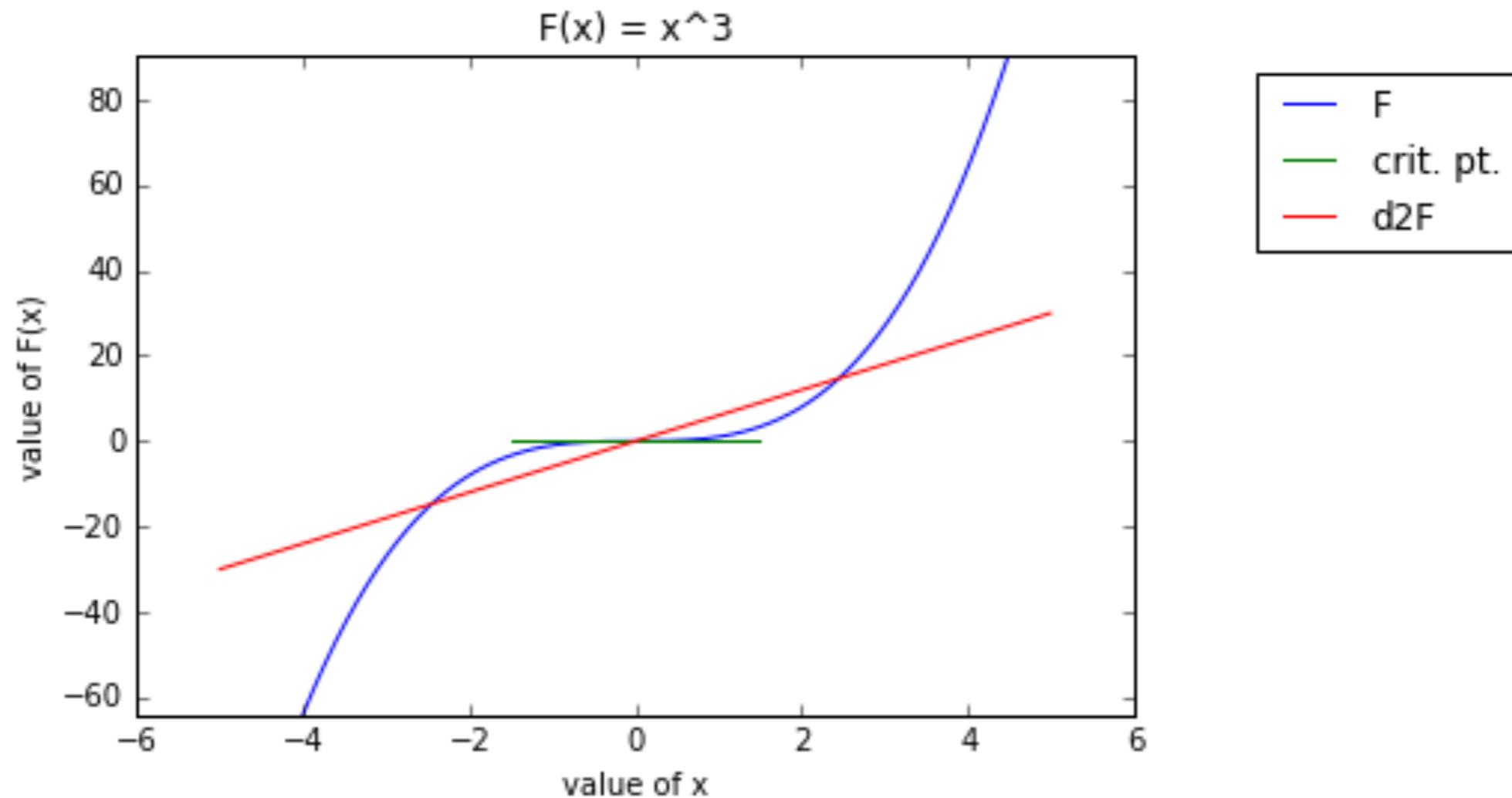
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Second derivative test:

$$\text{critical point } x^* = \left\{ \begin{array}{ll} \text{local maximum,} & \text{if } d^2 F/dx^2 < 0 \\ \text{local minimum,} & \text{if } d^2 F/dx^2 > 0 \\ \text{saddle point (maybe),} & \text{if } d^2 F/dx^2 = 0 \end{array} \right\}$$

# Taylor Series

Let's say we wanted to approximate a function  **$F$**  around a point  **$x_0$**  as a series in  **$\Delta x$** :

$$F(x_0 + \Delta x) = a_0 + a_1 \Delta x + a_2 [\Delta x]^2 + a_3 [\Delta x]^3 + \dots$$

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$$F(x_0 + \Delta x) = \overset{\text{constant term}}{a_0} + a_1 \Delta x + a_2 [\Delta x]^2 + a_3 [\Delta x]^3 + \dots$$

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$$\begin{aligned} F(x_0 + \Delta x) &= \overset{\text{constant term}}{\boxed{a_0}} + \underset{\text{linear term}}{\boxed{a_1 \Delta x}} + \overset{\text{quadratic term}}{\boxed{a_2 [\Delta x]^2}} + \underset{\text{cubic term}}{\boxed{a_3 [\Delta x]^3}} + \dots \\ &= \sum_{i=0}^{\infty} a_i [\Delta x]^i \end{aligned}$$

First of all:  $\Delta x = 0 \rightarrow a_0 = F(x_0)$

Then:  $\frac{dF}{d\Delta x}(x_0 + \Delta x) = a_1 + 2a_2\Delta x + \dots = \sum_{i=1}^{\infty} i \cdot a_i [\Delta x]^{i-1}$

So:  $\Delta x = 0 \rightarrow a_1 = \left. \frac{dF}{dx} \right|_{x=x_0}$

# Taylor Series

But if 
$$\frac{dF}{d\Delta x}(x_0 + \Delta x) = a_1 + 2a_2\Delta x + \dots = \sum_{i=1}^{\infty} i \cdot a_i [\Delta x]^{i-1}$$

then 
$$\frac{d^2 F}{d\Delta x^2}(x_0 + \Delta x) = 2a_2 + 6a_3\Delta x + \dots = \sum_{i=2}^{\infty} i \cdot (i - 1) \cdot a_i [\Delta x]^{i-2}$$

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thus again, 
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$$k \cdot (k - 1) \dots 2 \cdot 1 \cdot a_k = \frac{d^k F}{dx^k} \Big|_{x=x_0}$$

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Or:

$$k \cdot (k - 1) \dots 2 \cdot 1 \cdot a_k = \frac{d^k F}{dx^k} \Big|_{x=x_0}$$

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$$= \sum_{k=0}^{\infty} a_k [\Delta x]^k$$

$$= \sum_{k=0}^{\infty} \frac{1}{k!} \left. \frac{d^k F}{dx^k} \right|_{x=x_0} \cdot [\Delta x]^k$$

Taylor Series Approximation

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So now we need to calculate these two limits

# Taylor Series

We'll use the Taylor Series concept to calculate the first limit.

# Taylor Series

Cosine's Taylor series around 0 is:

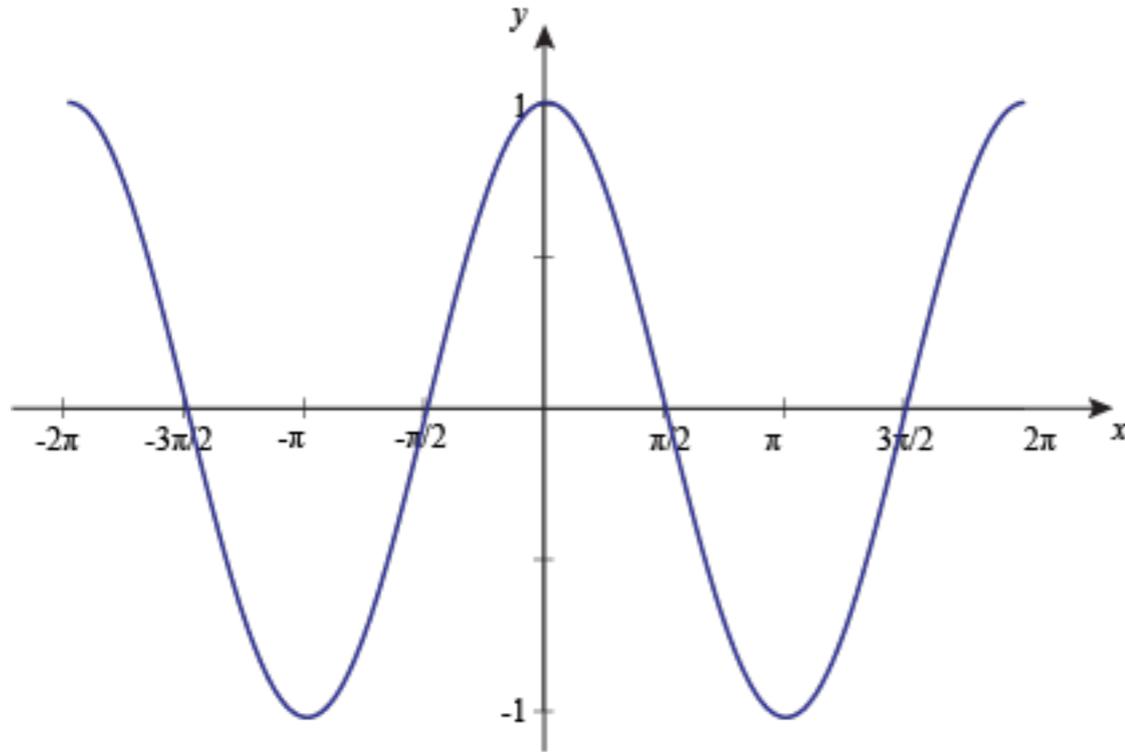
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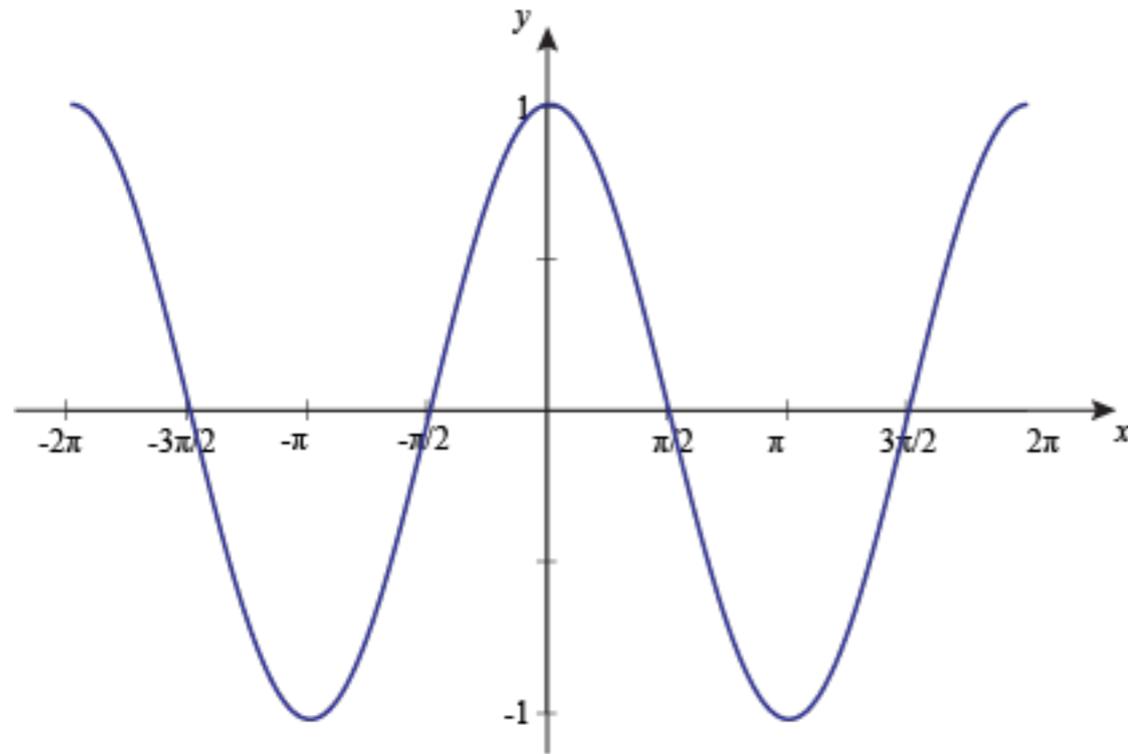
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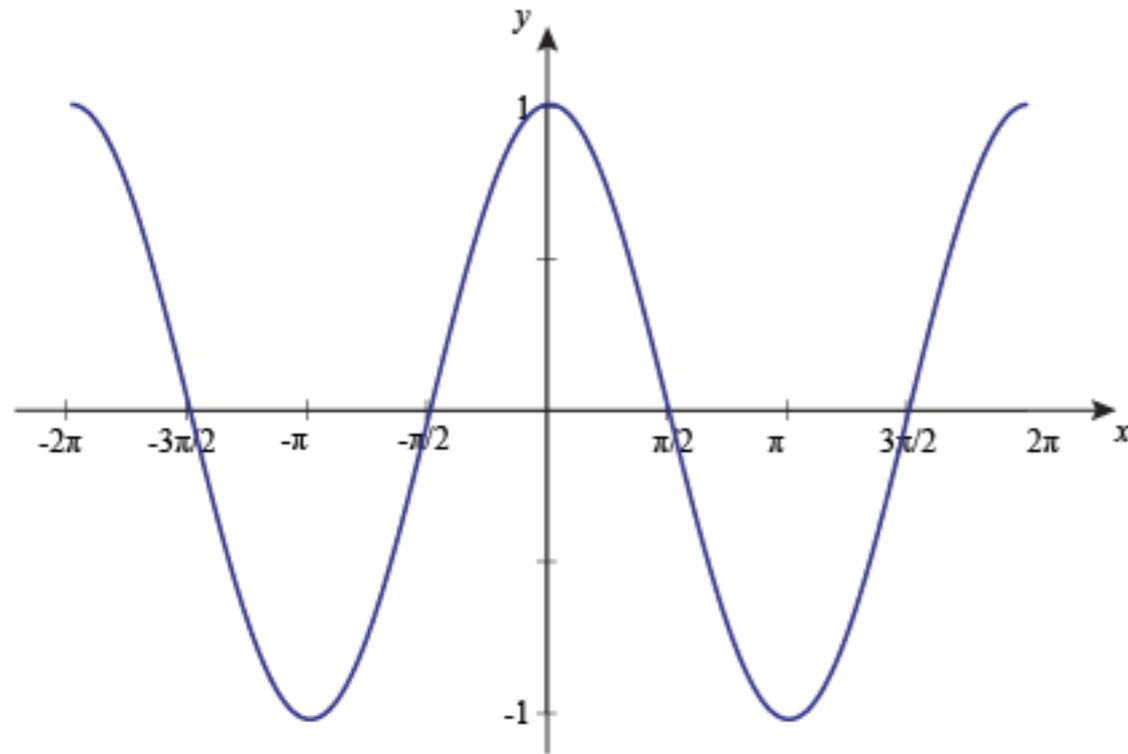
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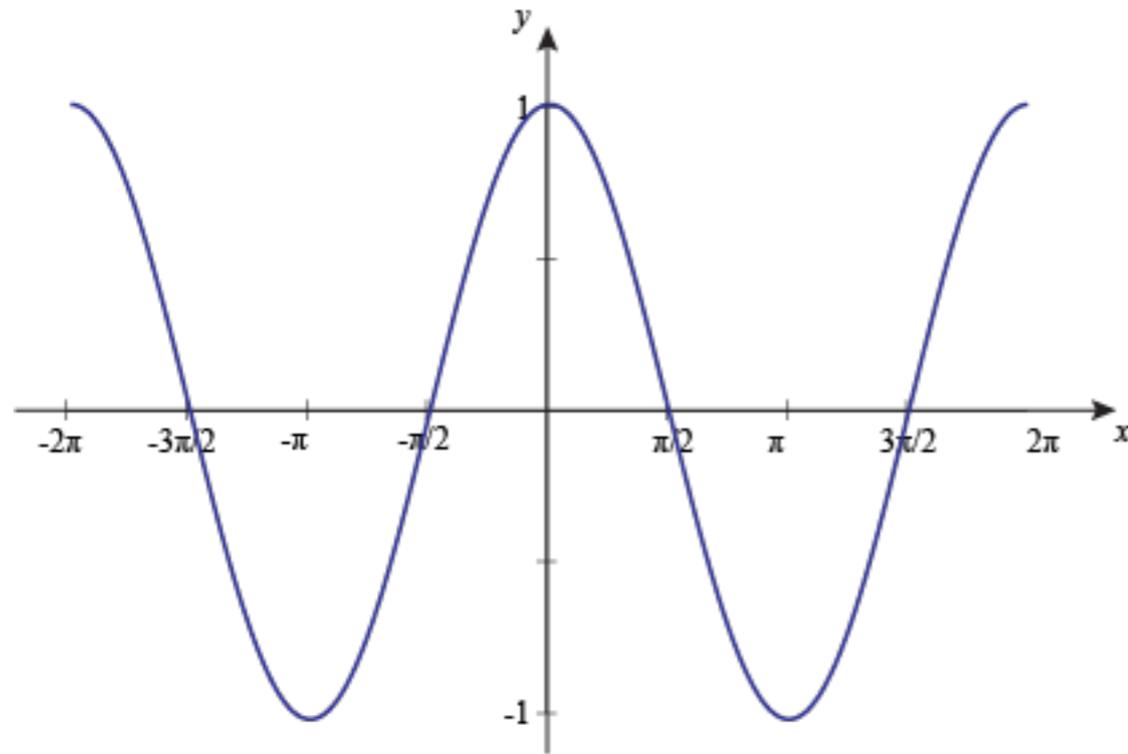
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Actually:

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So cosine's Taylor series is:

$$\cos(\Delta x) = 1 + a_2 \cos''(0)(\Delta x)^2 + \dots$$

# Taylor Series

Since

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we have:

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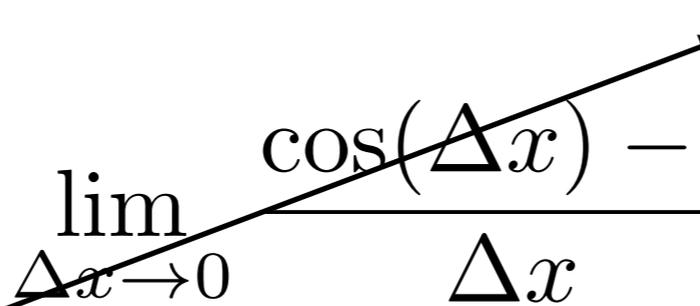
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So

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Observation: note that we didn't need to know cosine's full Taylor series for this calculation — just that cosine's being an even fn meant that its first order term disappeared ... this is one reason **why** Taylor series are useful

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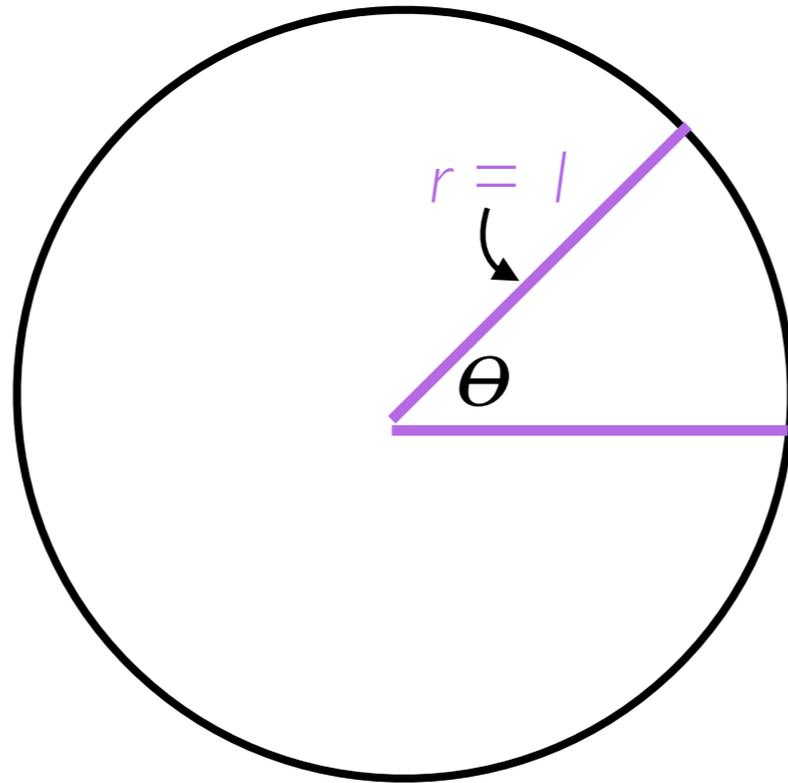
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$$= \cos(x) \lim_{\Delta x \rightarrow 0} \frac{\sin(\Delta x)}{\Delta x} = \sin'(0)$$

Ok, but what is **this** limit?

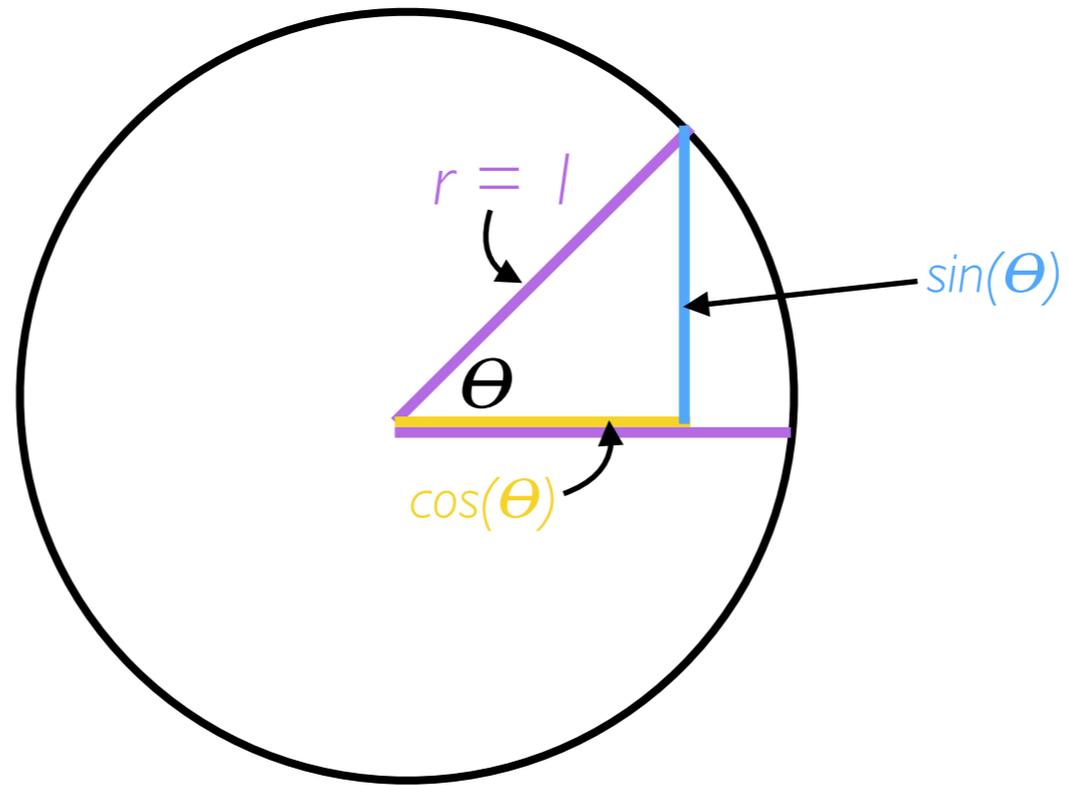
# Taylor Series

Assume circle is radius 1



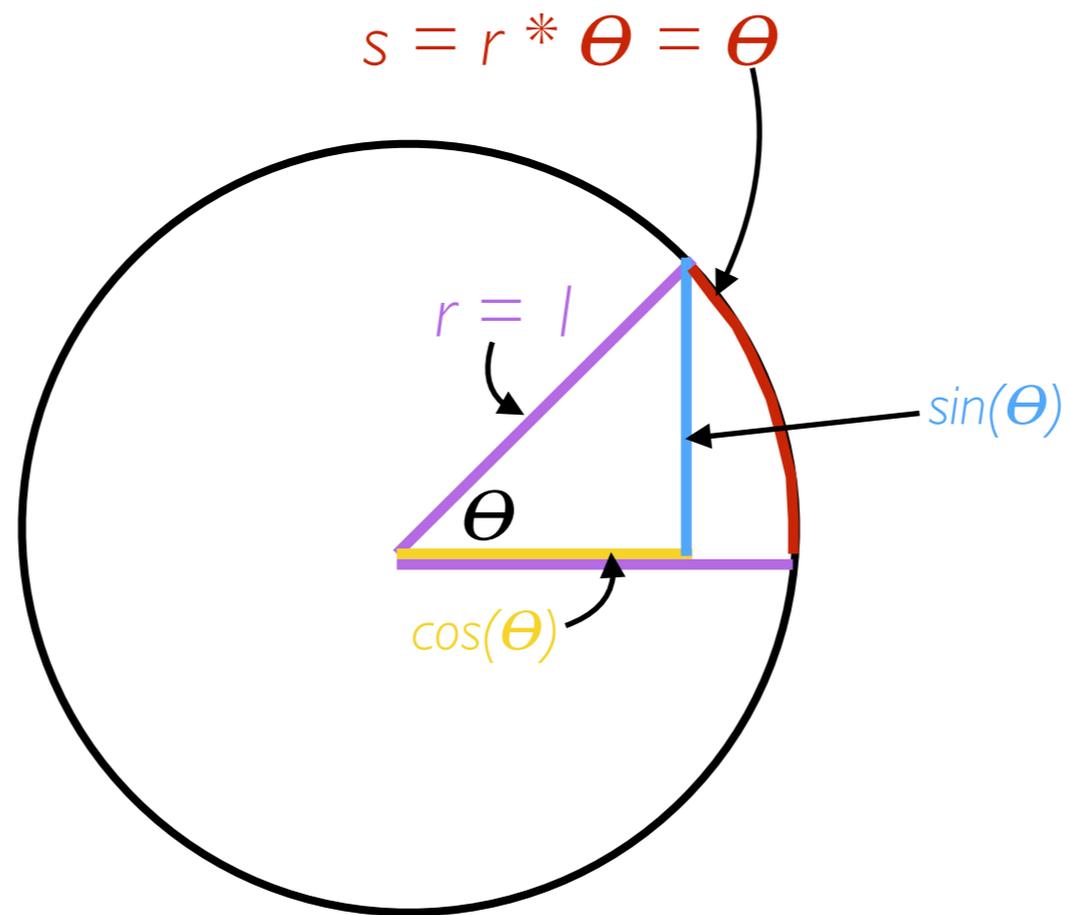
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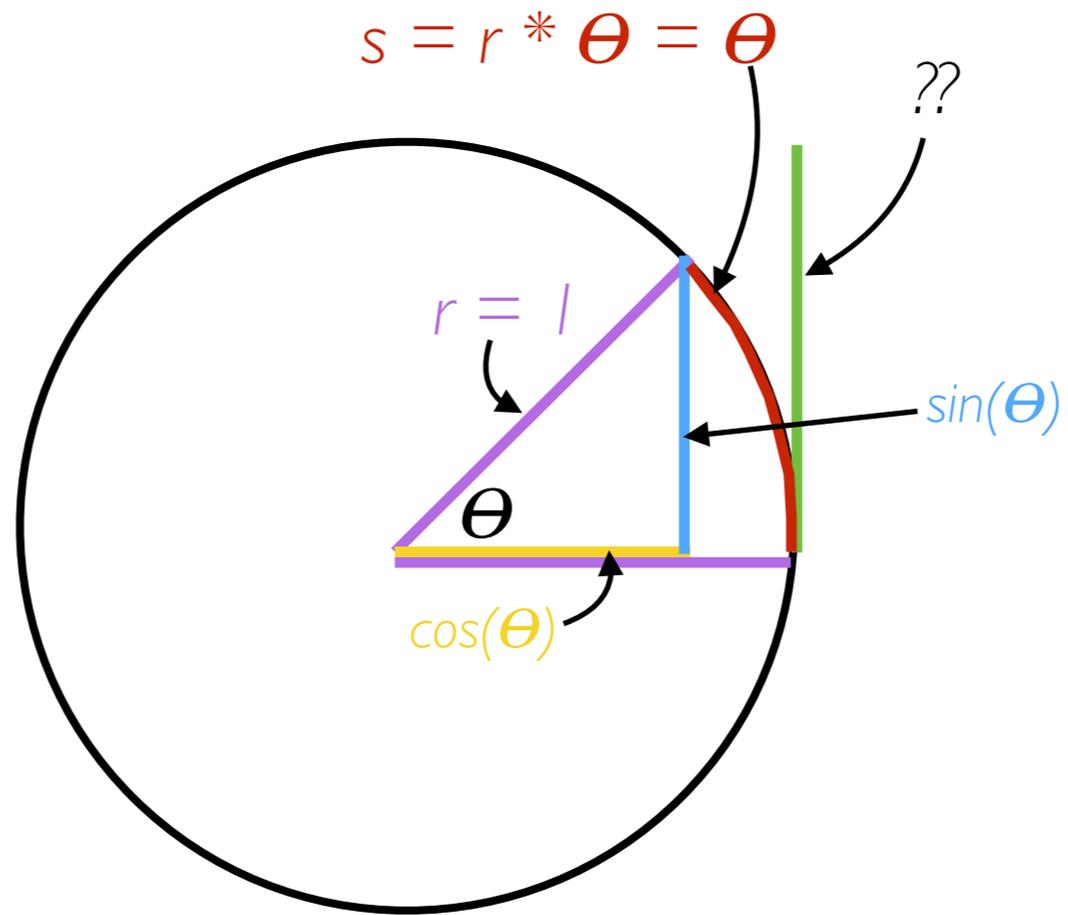
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Assume circle is radius 1



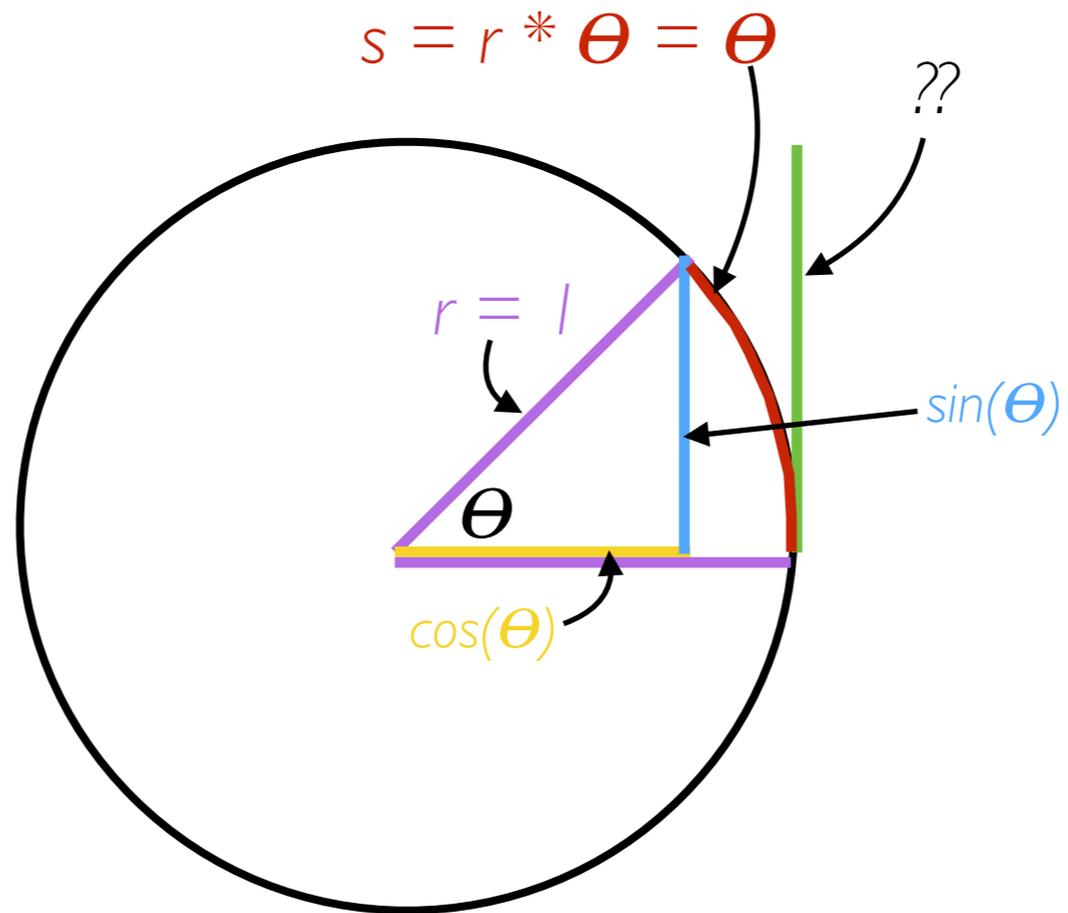
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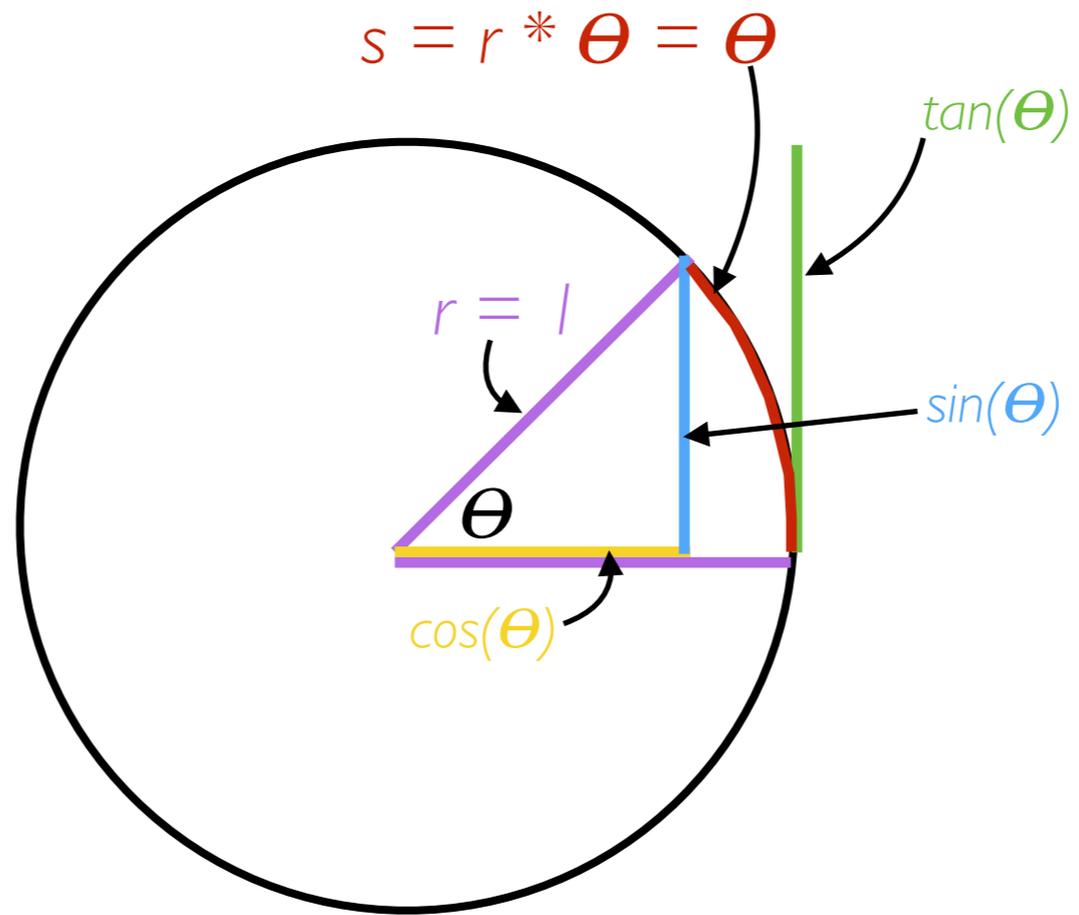


$$\frac{\sin(\theta)}{\cos(\theta)} = \text{ratio of blue to yellow} = \text{ratio of green to } r = \text{green}$$

$$\parallel$$
$$\tan(\theta)$$

# Taylor Series

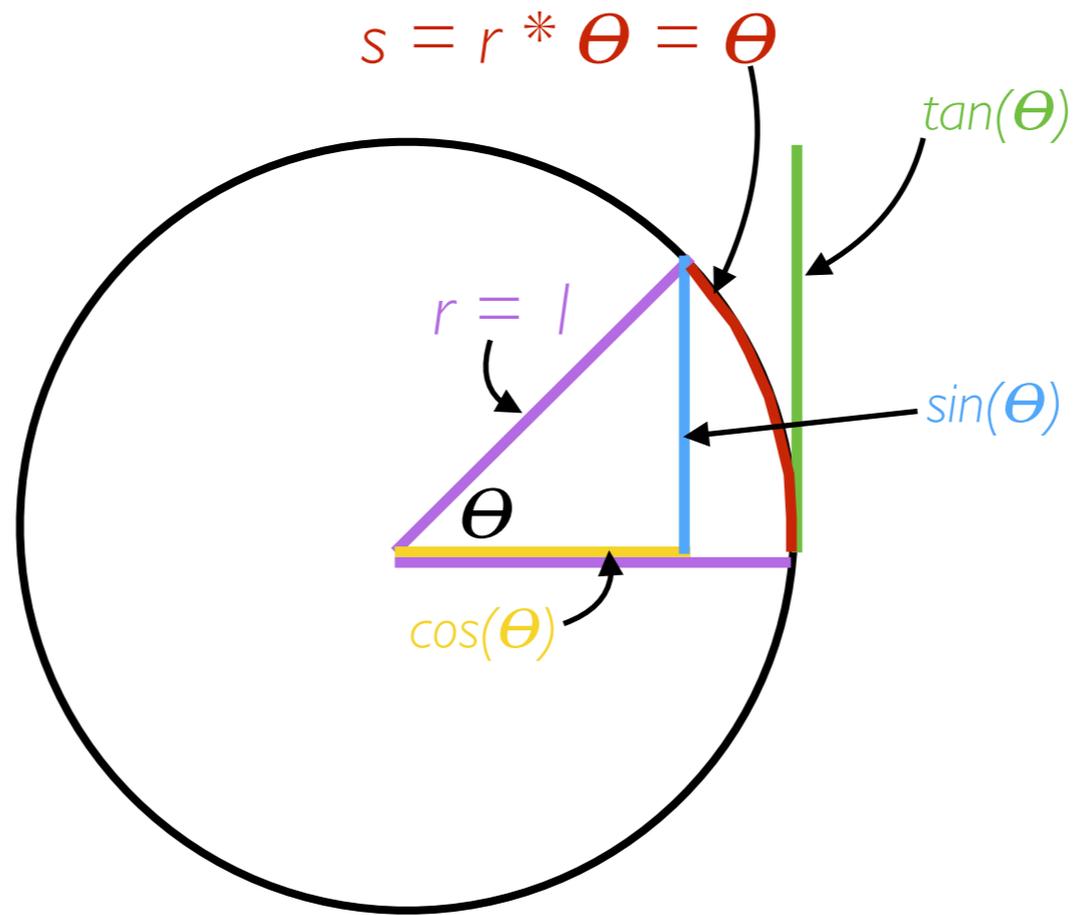
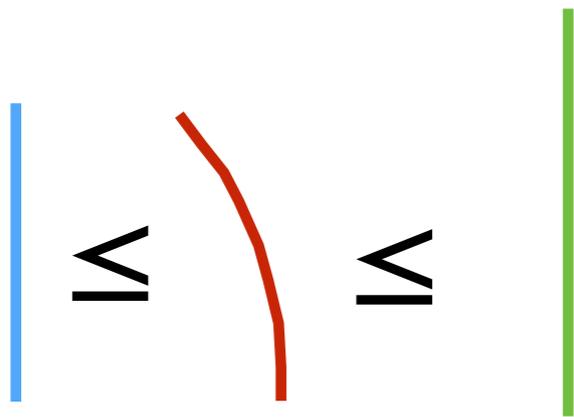
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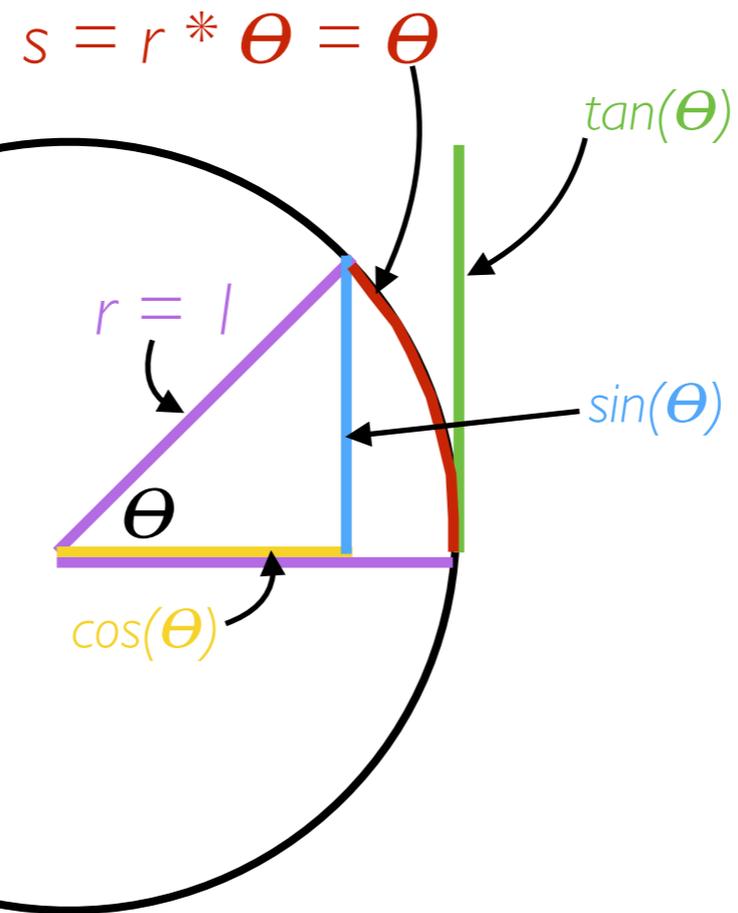
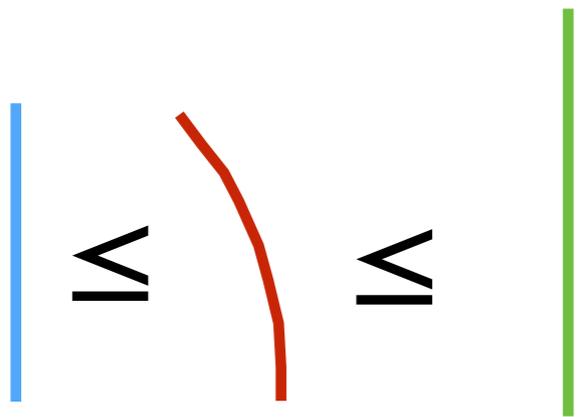
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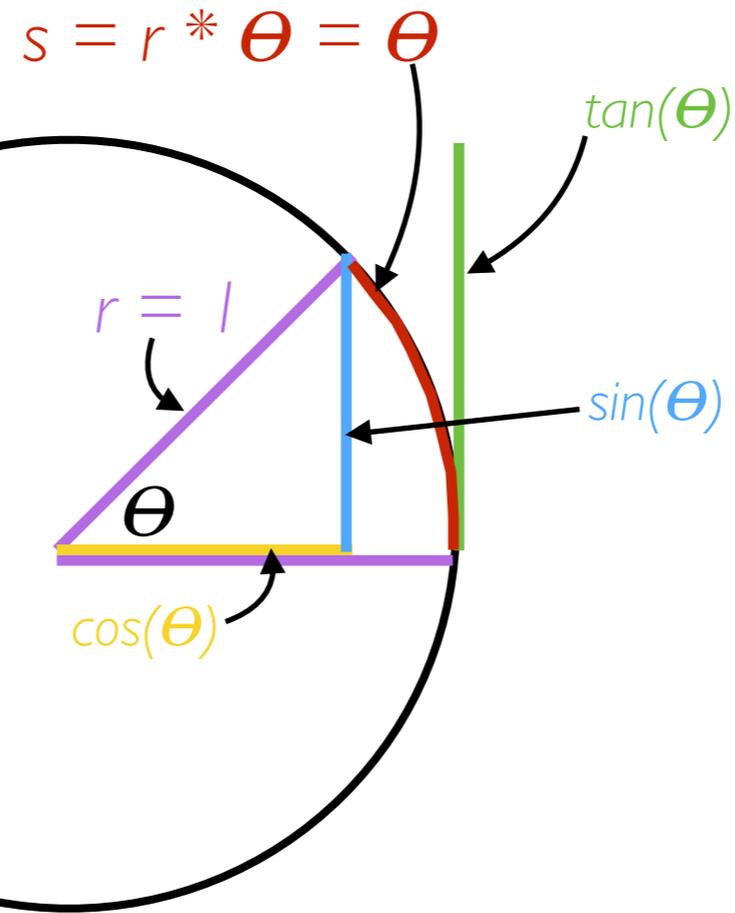
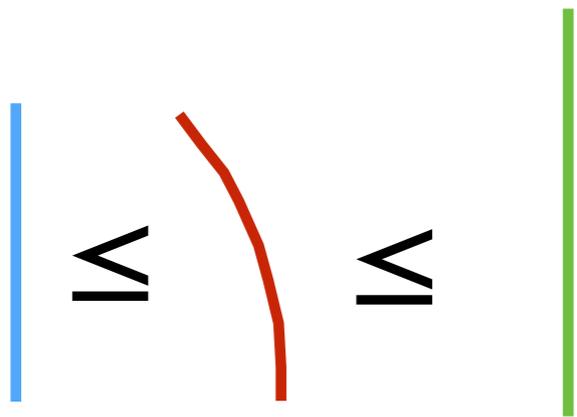
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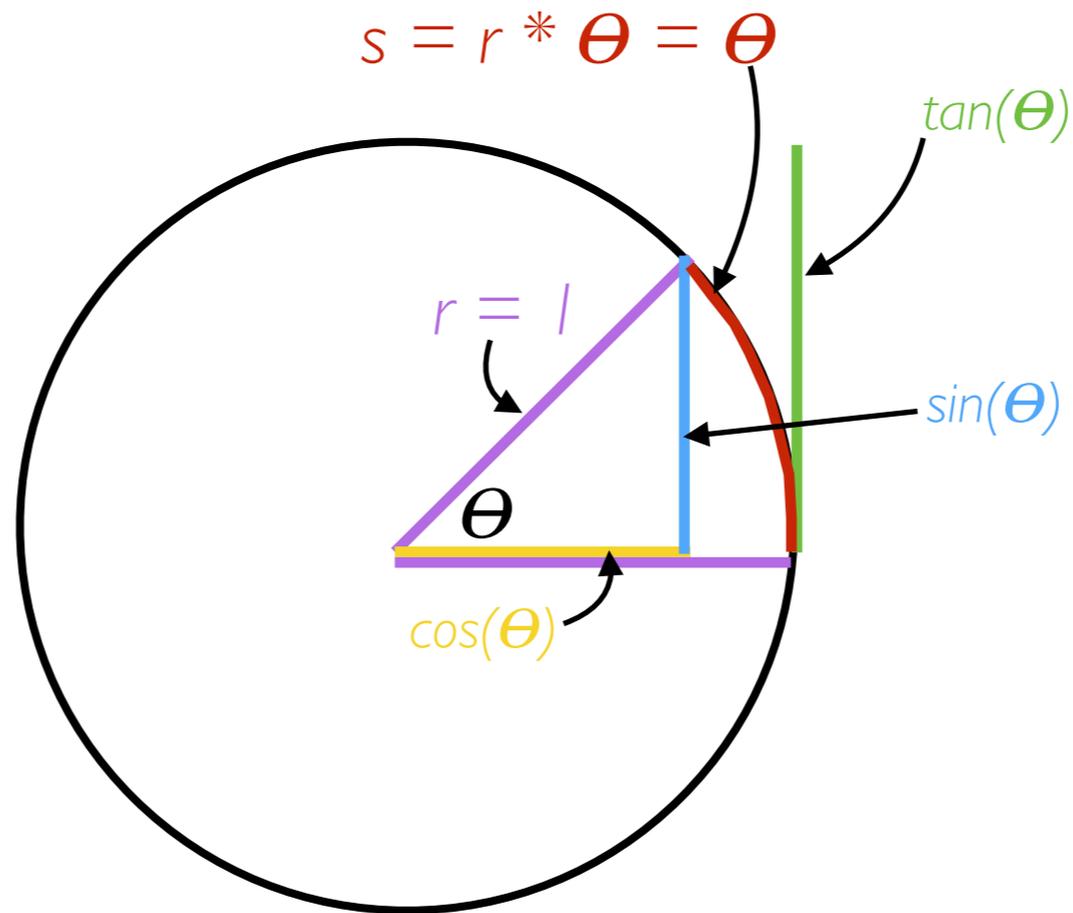
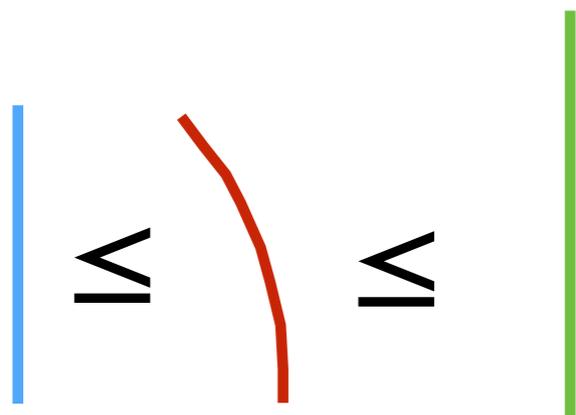
Thus:

$$1 \leq \frac{\theta}{\sin(\theta)} \leq \frac{\tan(\theta)}{\cos(\theta)} = \frac{1}{\cos(\theta)}$$

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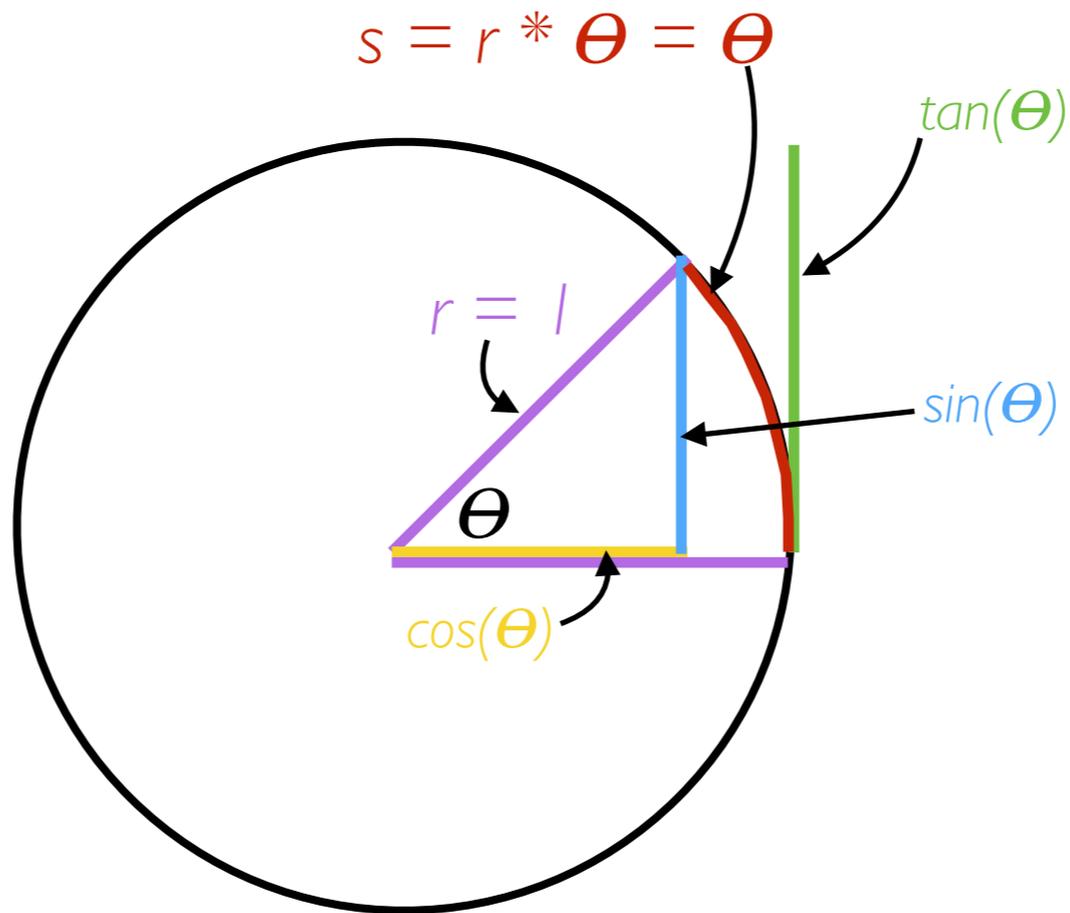
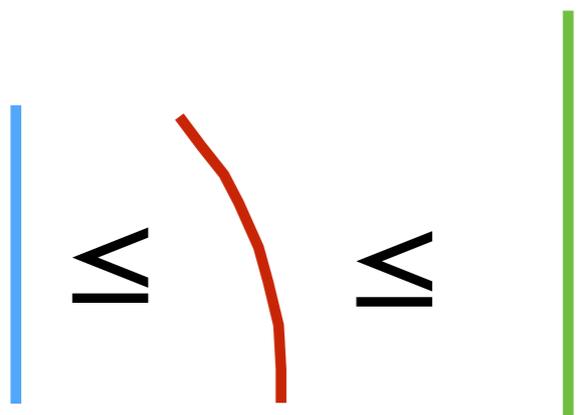
When  $\theta \rightarrow 0$ ,  $\cos(\theta) \rightarrow 1$ , so:

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BEAUTIFUL!!!

# Taylor Series

[Tangential Observation: this calculation of this  **$\sin(x)/x$**  limit much “more specific” mathematically than the  **$(\cos(x) - 1) / x$**  limit, because the latter just depended on  **$\cos(x)$**  being an even function — any even function would have had a similar Taylor series. However, to get  **$\sin(x)/x$**  right, we really needed to understand the specifics of trigonometry.]



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Anyway, we finally have:

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Similarly we can show:

$$\sin''(x) = \cos'(x) = -\sin(x)$$

Thus:

$$\sin^{(3)}(x) = -\cos(x)$$

And:

$$\sin^{(4)}(x) = \sin(x)$$

# Taylor Series

With that in mind we can calculate full Taylor series' for sine and cosine (around 0):

$$\sin(x) = \sin(0) + \sin'(0)x + \frac{1}{2} \sin^{(2)}(0)x^2 + \dots$$

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And similarly:

$$\cos(x) = \sum_{i=0}^{\infty} \frac{(-1)^i}{(2i)!} x^{2i}$$

# Chain Rule

Assume we have a function that's a composition of functions:

$$h(x) = g(f(x))$$

Then the chain rule says:

$$\frac{dh}{dx}(x) = \frac{dg}{dx}(f(x)) \cdot \frac{df}{dx}(x) = g'(f(x)) \cdot f'(x)$$

# Chain Rule

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Now apply the same reasoning to  $\mathbf{g}$  and treating  $\mathbf{f}'(\mathbf{x})\Delta\mathbf{x}$  as the “new  $\Delta\mathbf{x}$ ” and  $f(x)$  as the “new  $\mathbf{x}$ ”:

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Really, the proof of the Chain Rule is essentially a nested set of two Taylor Series approximations, one for  $\mathbf{f}$  and the other for  $\mathbf{g}$ .

# Multi-variable Functions

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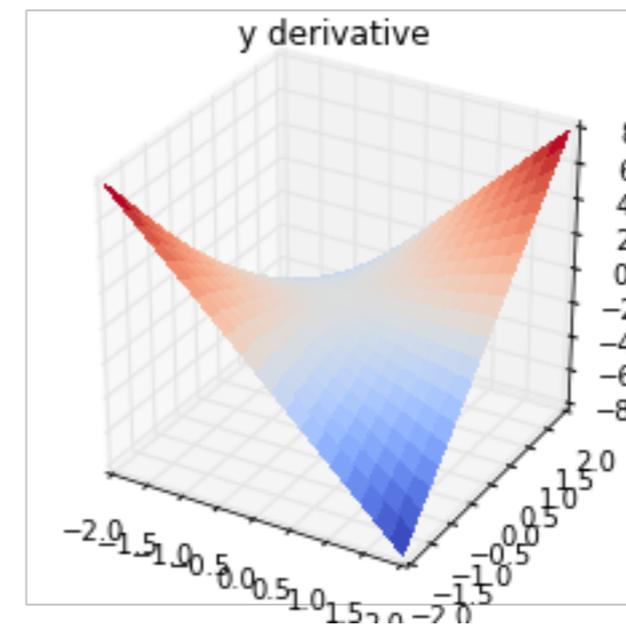
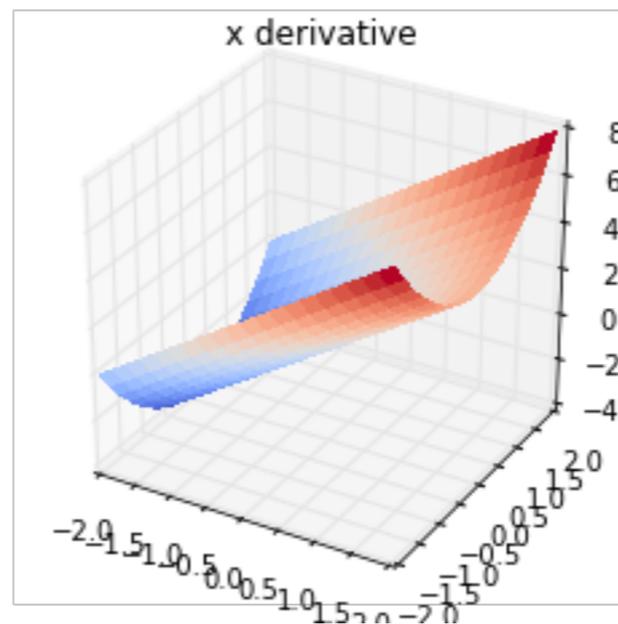
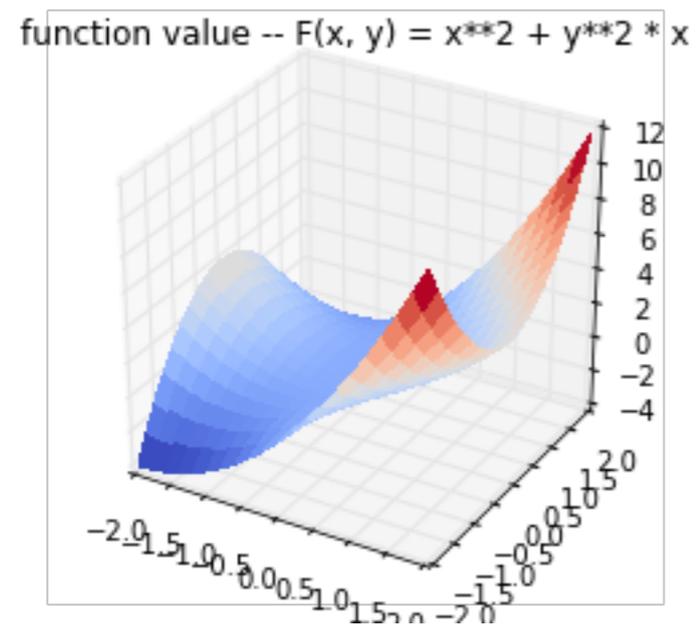
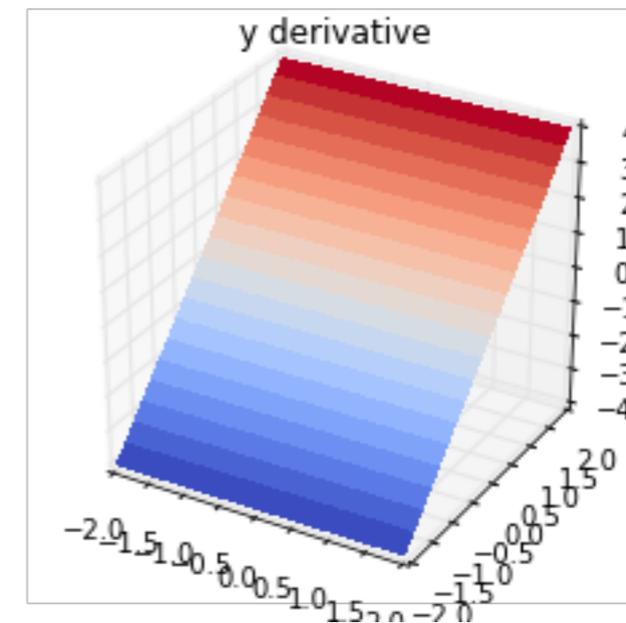
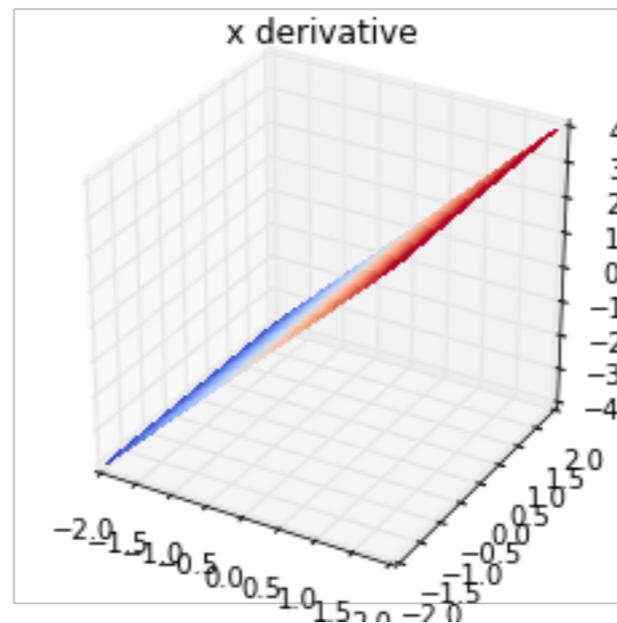
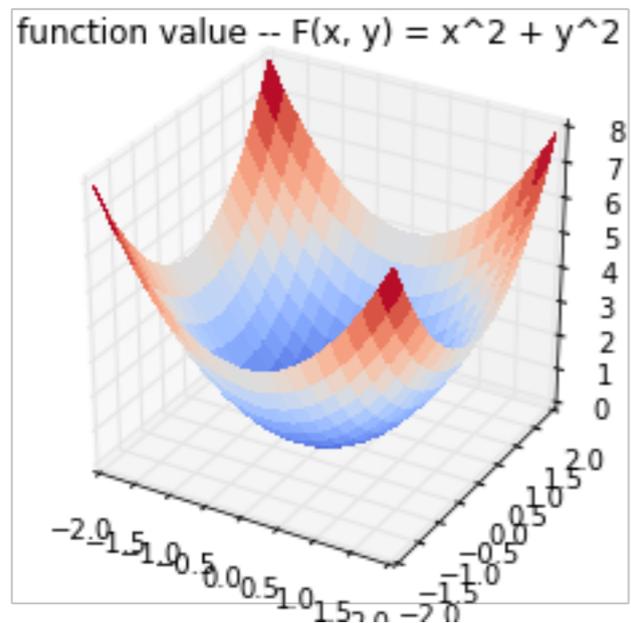
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Partial derivative is w.r.t.  $\mathbf{x}$  is just derivative of the function holding  $\mathbf{y}$  constant

... and vice versa for partial derivative w.r.t.  $\mathbf{y}$

# Multi-variable Functions



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We can also calculate second partial derivatives:

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# Multi-variable Functions

Let  $\mathbf{F}(x_1, x_2, \dots, x_n)$  be a real-valued function of  $\mathbf{n}$  variables.

The “gradient of  $\mathbf{F}$ ” is the  $\mathbf{n}$ -vector-valued function:

$$\nabla F(\vec{x}) = \left[ \frac{\partial F}{\partial x_1}(\vec{x}), \dots, \frac{\partial F}{\partial x_n}(\vec{x}) \right]$$

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the “hessian”  
matrix

$$H[f] = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \frac{\partial^2 f}{\partial x_1 \partial x_3} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2 \partial x_2} & \frac{\partial^2 f}{\partial x_2 \partial x_3} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \frac{\partial^2 f}{\partial x_n \partial x_3} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{bmatrix}$$

shape =  
 $(\mathbf{n}, \mathbf{n})$

# Multi-variable Functions

function itself (“0th”-derivative):

$$F : \mathbb{R}^n \longrightarrow \mathbb{R}$$

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$$H[F] : \mathbb{R}^n \longrightarrow \mathbb{R}^{n \times n}$$

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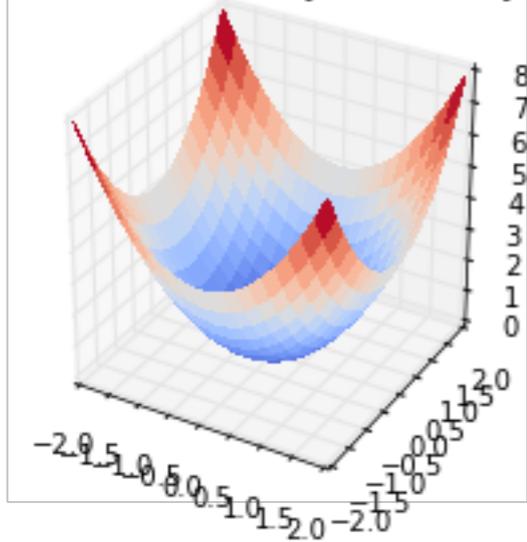
can be generalized to  
k-tensor-valued function for k-th  
derivative ... but third derivatives  
and higher essentially never  
used...

$$\nabla F : \mathbb{R}^n \longrightarrow \mathbb{R}^n$$

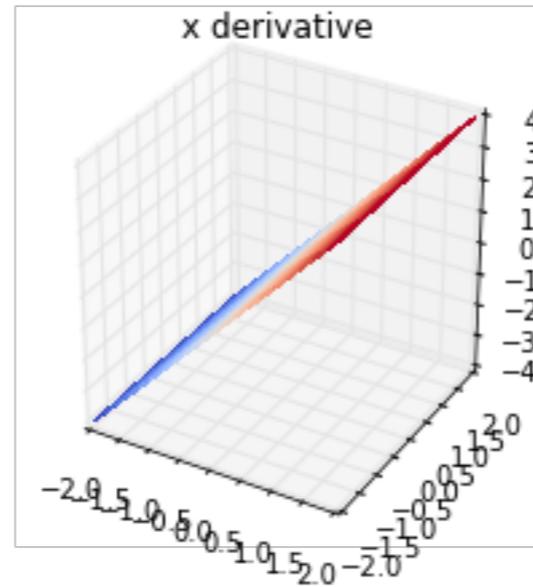
$$H[F] : \mathbb{R}^n \longrightarrow \mathbb{R}^{n \times n}$$

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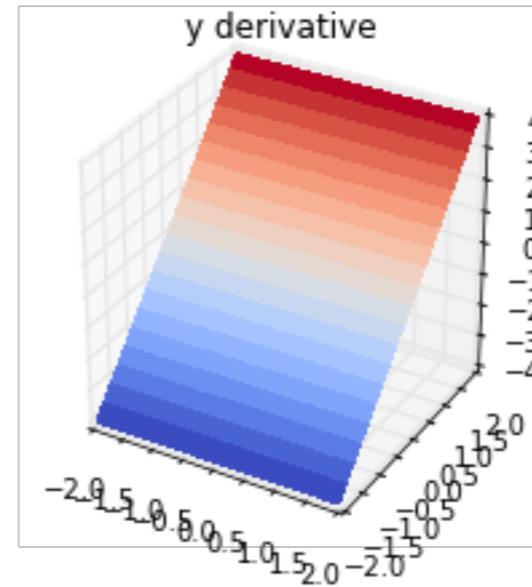
function value --  $F(x, y) = x^{**2} + y^{**2}$



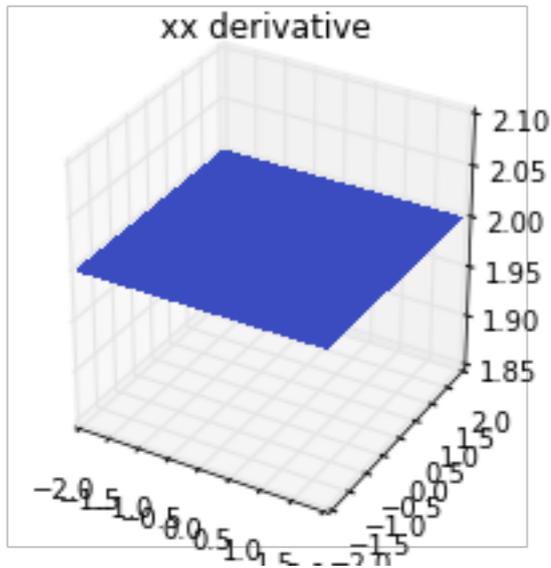
x derivative



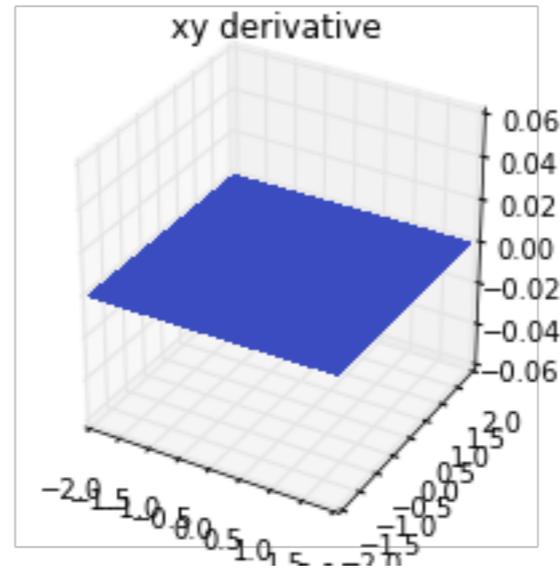
y derivative



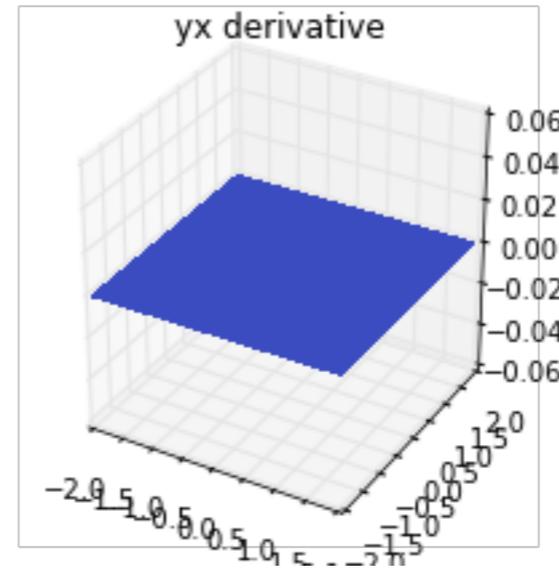
xx derivative



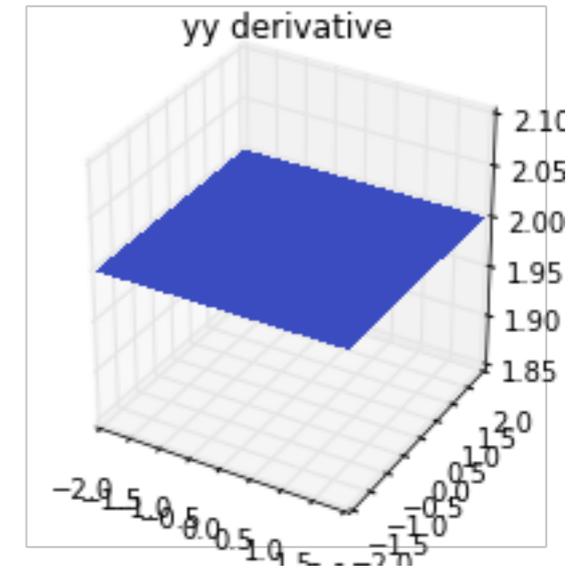
xy derivative



yx derivative

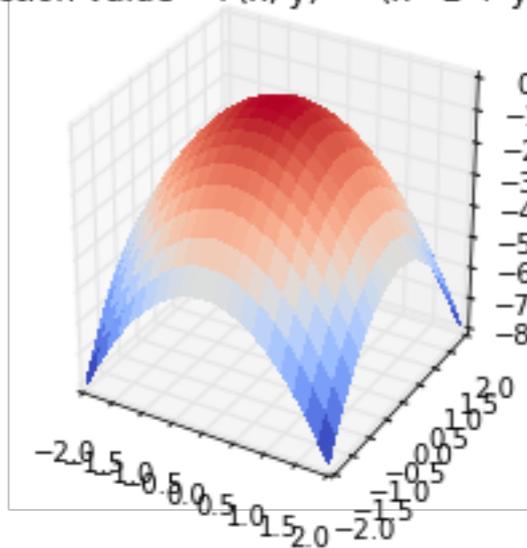


yy derivative

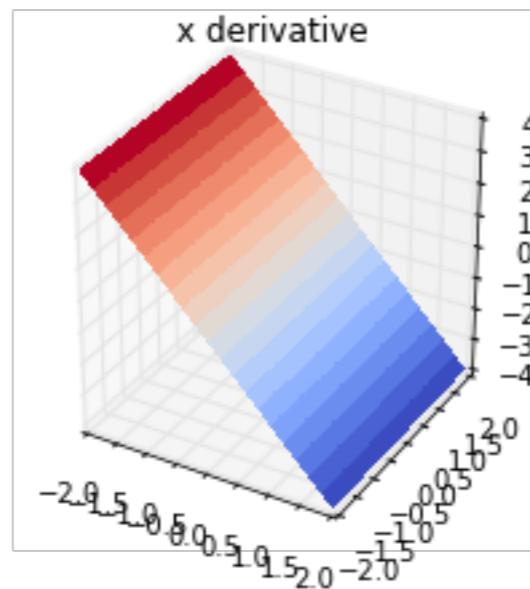


# Multi-variable Functions

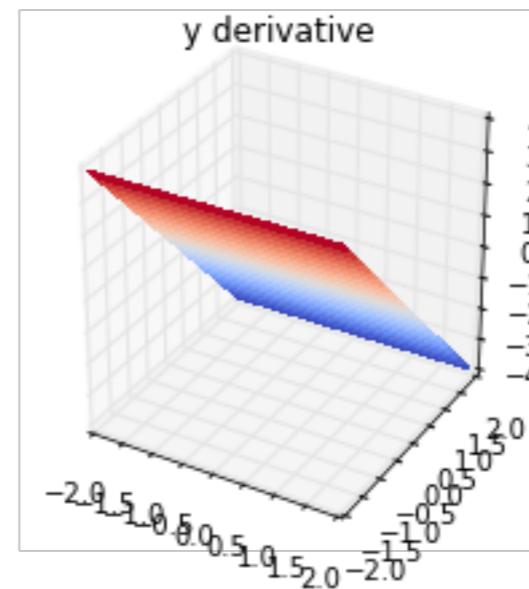
function value --  $F(x, y) = -(x^2 + y^2)$



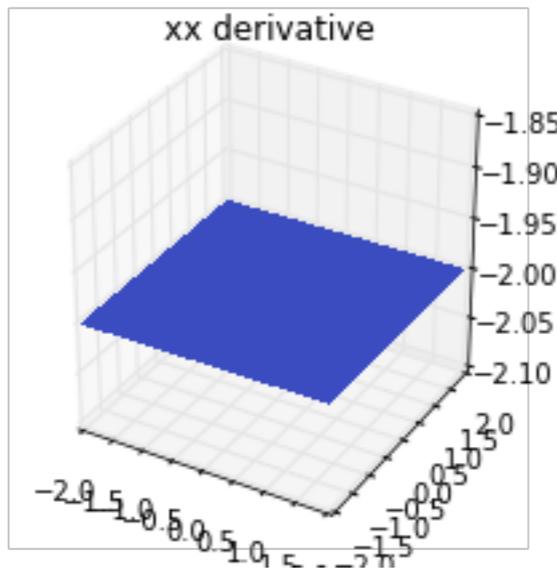
x derivative



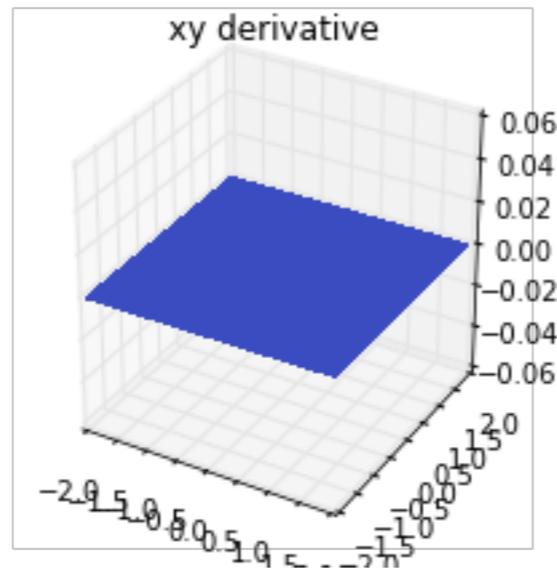
y derivative



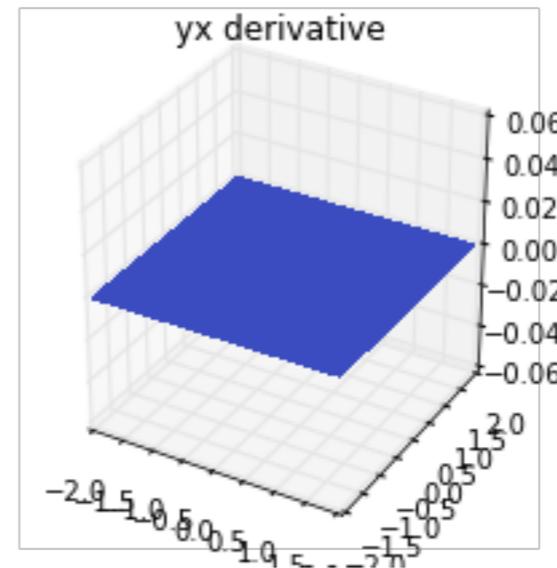
xx derivative



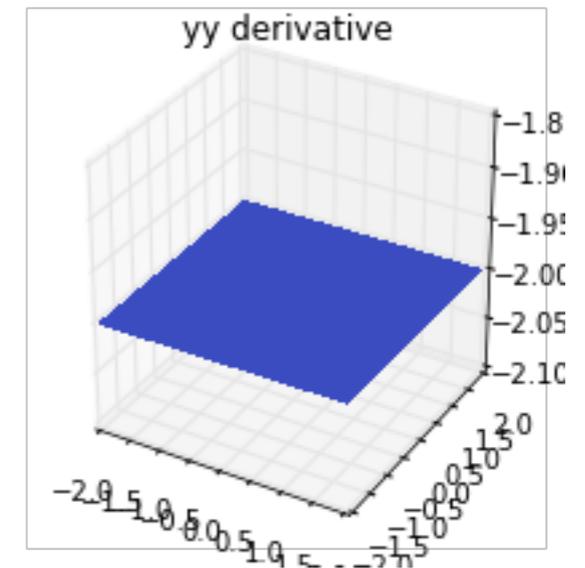
xy derivative



yx derivative

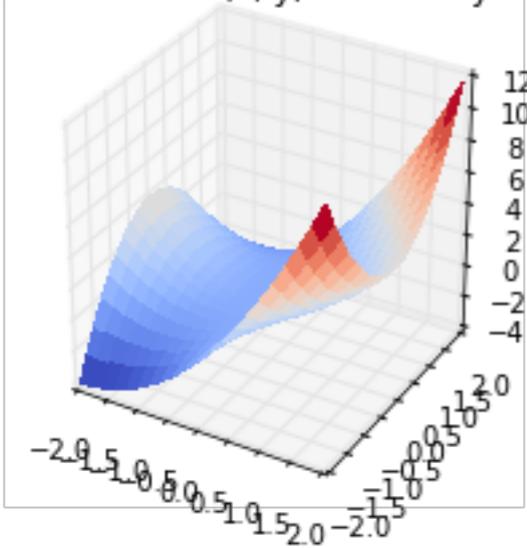


yy derivative

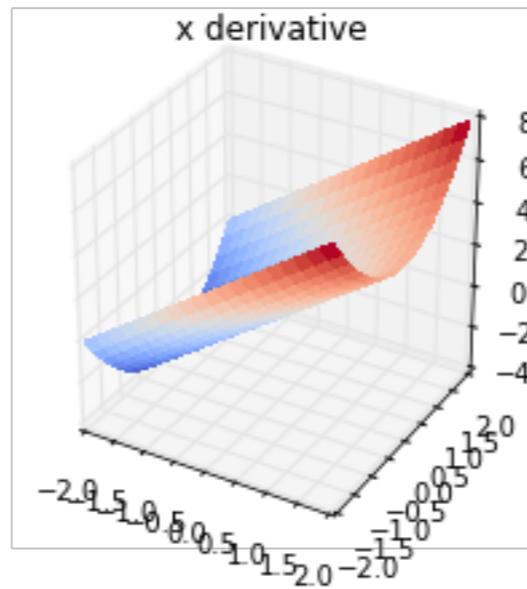


# Multi-variable Functions

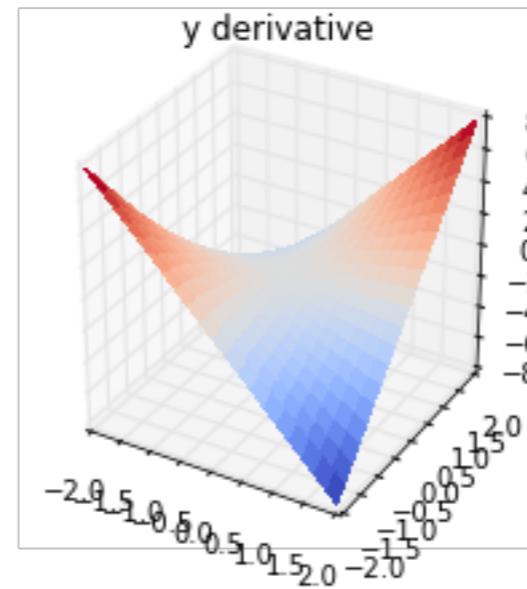
function value --  $F(x, y) = x^2 + y^2 * x$



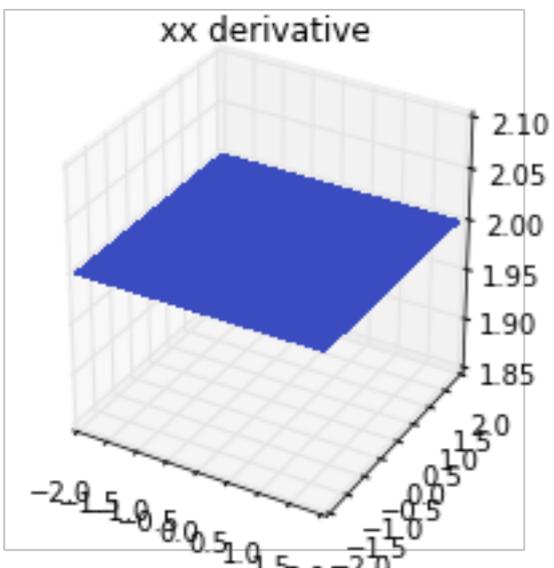
x derivative



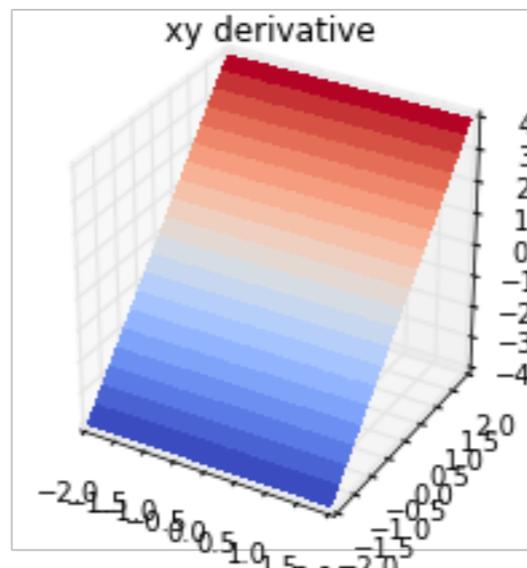
y derivative



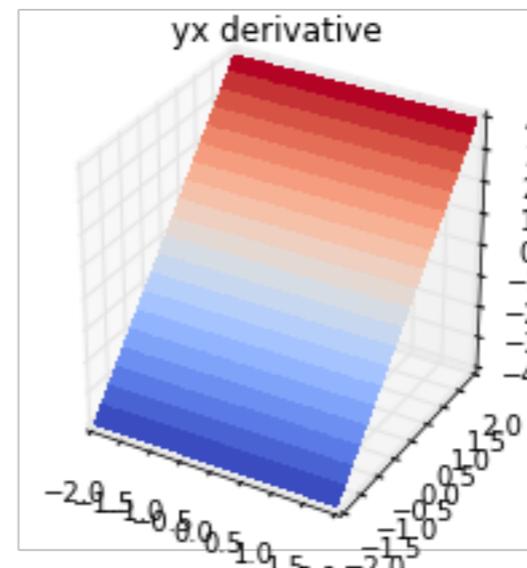
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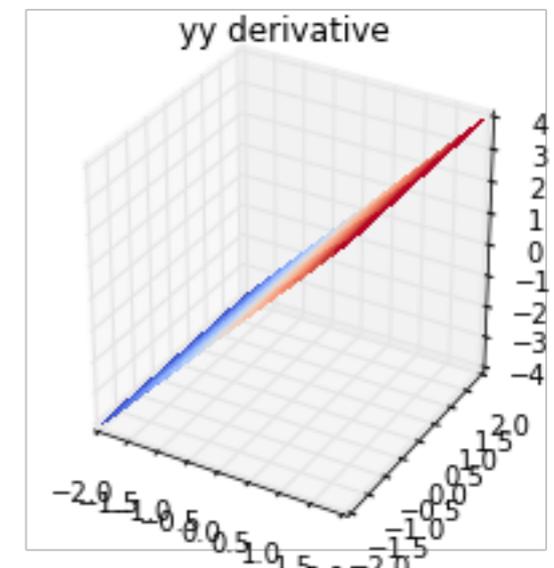
xy derivative



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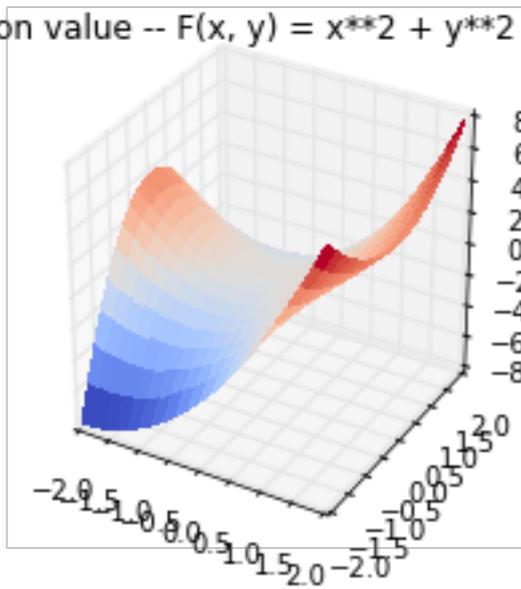


yy derivative

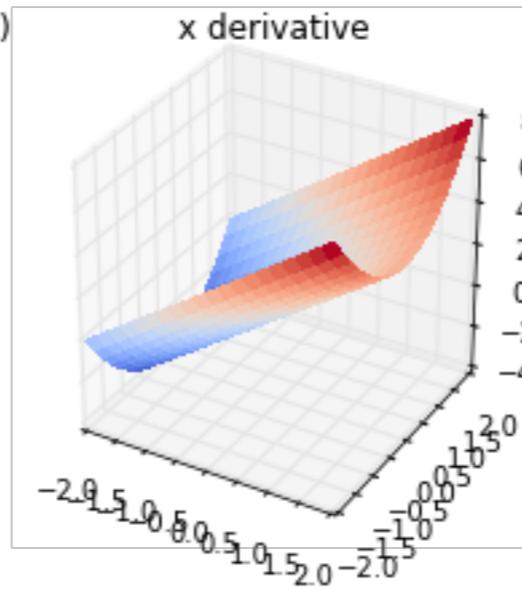


# Multi-variable Functions

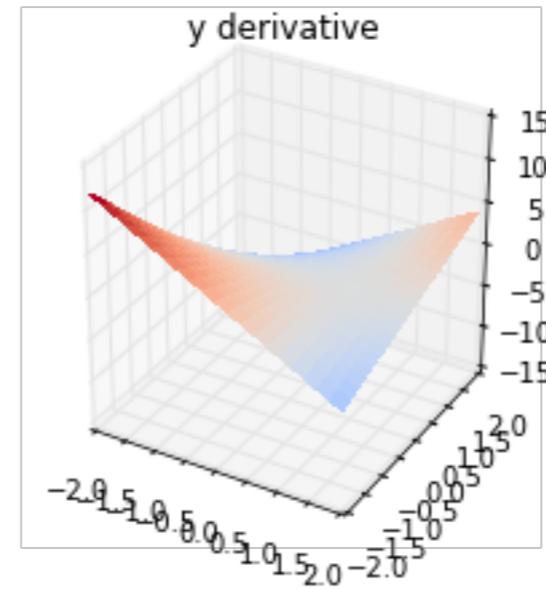
function value --  $F(x, y) = x^2 + y^2 * (x-1)$



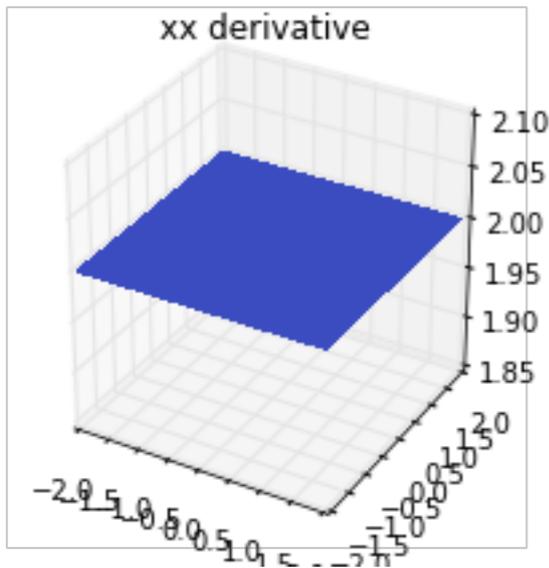
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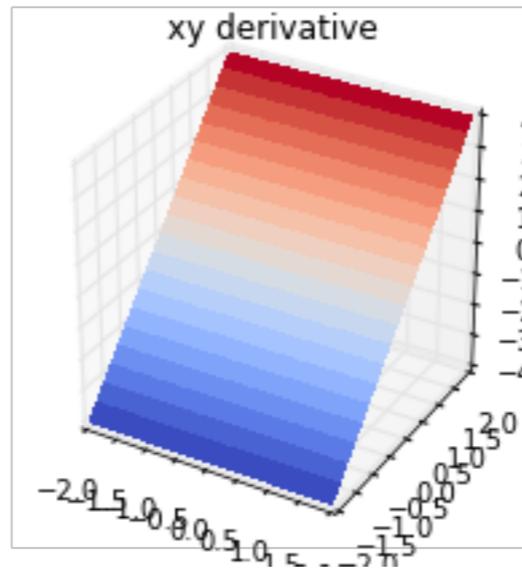
y derivative



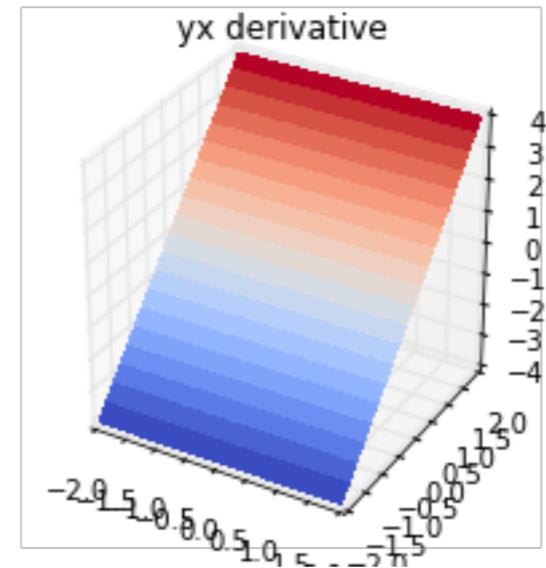
xx derivative



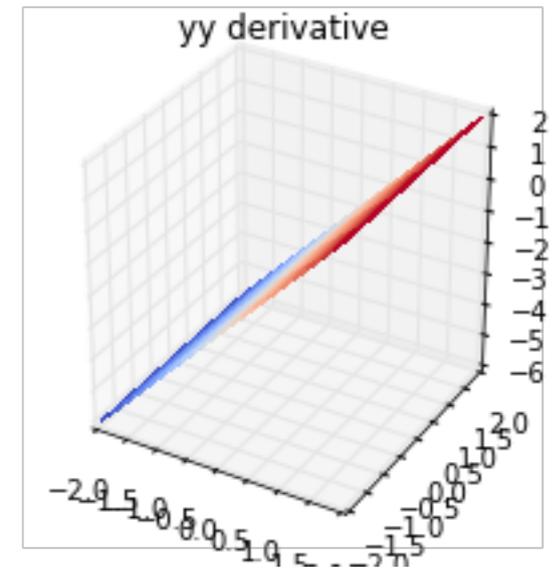
xy derivative



yx derivative



yy derivative



# Multi-variable Functions

In one dimension, critical points are those  $\mathbf{x}^*$  such that:

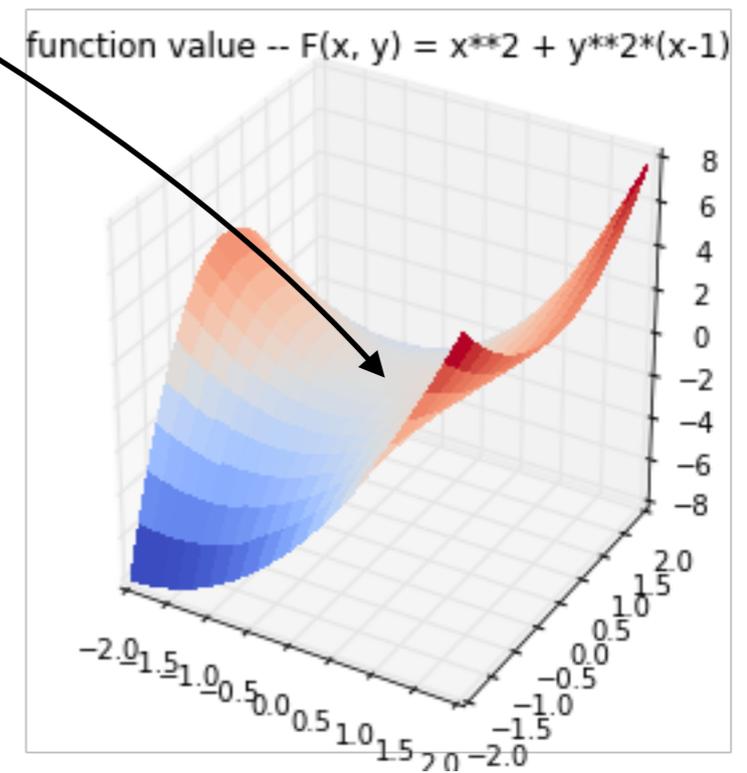
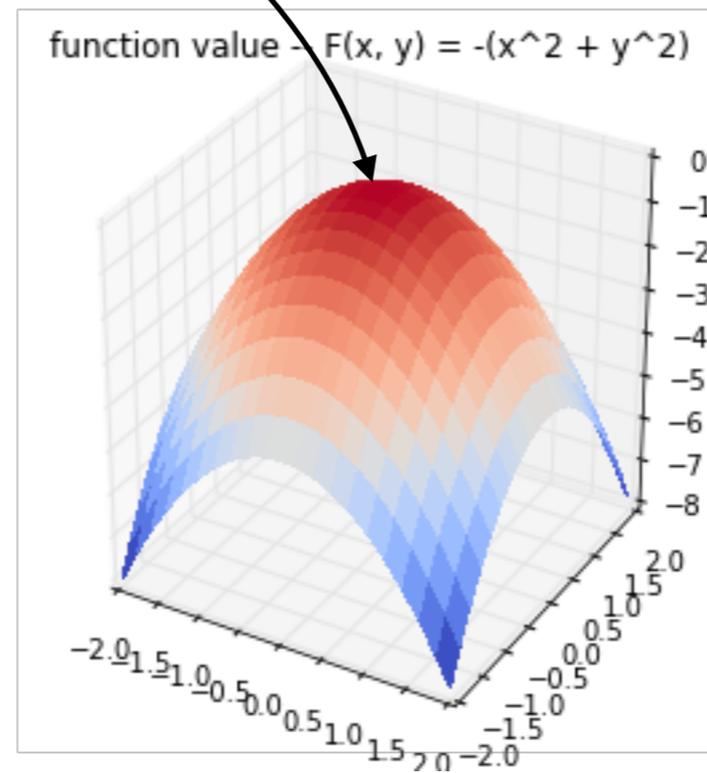
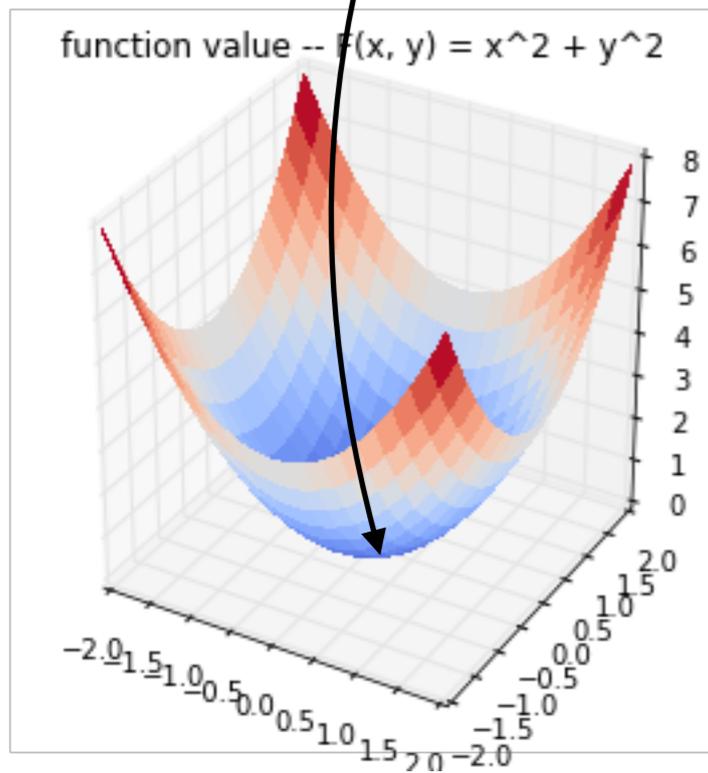
$$\left. \frac{dF}{dx} \right|_{x=x^*} = 0$$

In multiple dimensions, critical points are those  $\mathbf{x}^*$  such that:

$$\nabla F(\vec{x}^*) = \left[ \frac{\partial F}{\partial x_1}(\vec{x}^*), \dots, \frac{\partial F}{\partial x_n}(\vec{x}^*) \right] = [0, \dots, 0] = \vec{0}$$

# Multi-variable Functions

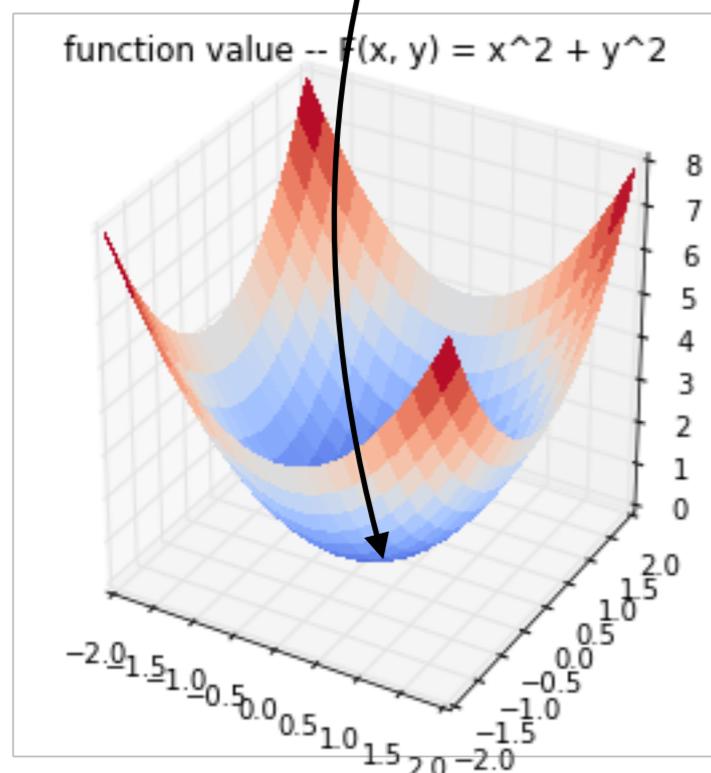
Critical point



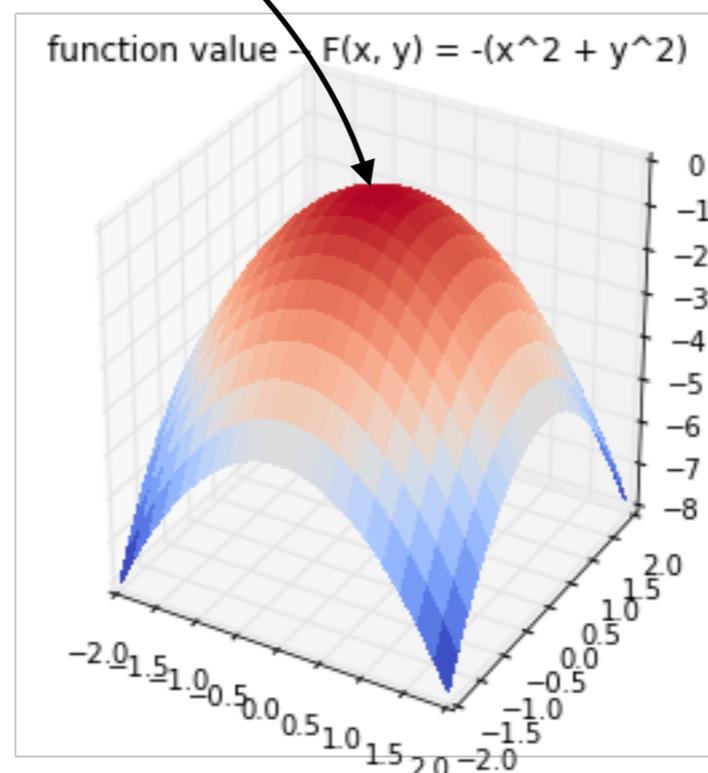
# Multi-variable Functions

Critical point

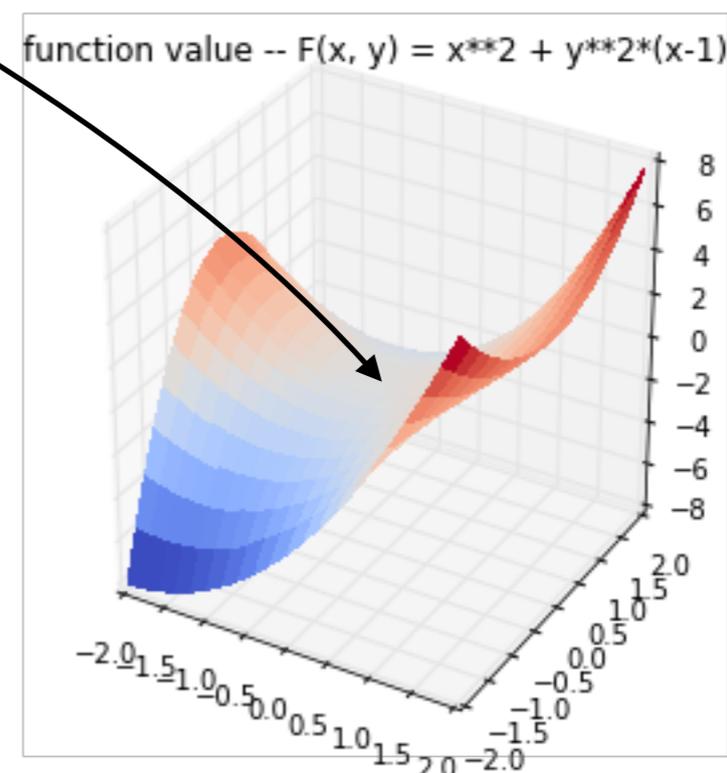
But what's the difference?



Hessian determinant  
positive



Hessian determinant  
positive



Hessian determinant  
negative

# Multi-variable Functions

Imagine you have a path through variable space as a function of a single variable (like time):

$$\vec{x}(t) = (x_1(t), x_2(t), \dots, x_n(t))$$

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is a one-variable real-valued function.

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What's its derivative?

$$\frac{df}{dt} = \lim_{\Delta t \rightarrow 0} \frac{\vec{F}(x_1(t + \Delta t), \dots, x_n(t + \Delta t)) - F(x_1(t), \dots, x_n(t))}{\Delta t}$$

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*applying definitions of derivatives, nested first to  $F(x)$  (partial derivative) and then to  $x(t)$*

$$= \lim_{\Delta t \rightarrow 0} \frac{\frac{\partial F}{\partial x_1}(x_1(t), x_2(t + \Delta t), \dots, x_n(t + \Delta t))x_1'(t)\Delta t + F(x_1(t), x_2(t + \Delta t), \dots, x_n(t + \Delta t)) - f(t)}{\Delta t}$$

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taking the limit in the first term

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applying same reasoning to **x2**

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dot product of two  $n$  vectors, yielding a scalar

# Multi-variable Functions

Imagine you have a path through variable space as a function of a single variable (like time):

$$\vec{x}(t) = (x_1(t), x_2(t), \dots, x_n(t))$$

Then

$$f(t) = \vec{F}(\vec{x}(t))$$

is a one-variable real-valued function. What's its derivative?

Answer:

$$\frac{df}{dt} = \frac{\partial F}{\partial x_1} \cdot \frac{dx_1(t)}{dt} + \dots + \frac{\partial F}{\partial x_n} \cdot \frac{dx_n(t)}{dt} = \nabla F(x(t)) \cdot \frac{d\vec{x}(t)}{dt}$$

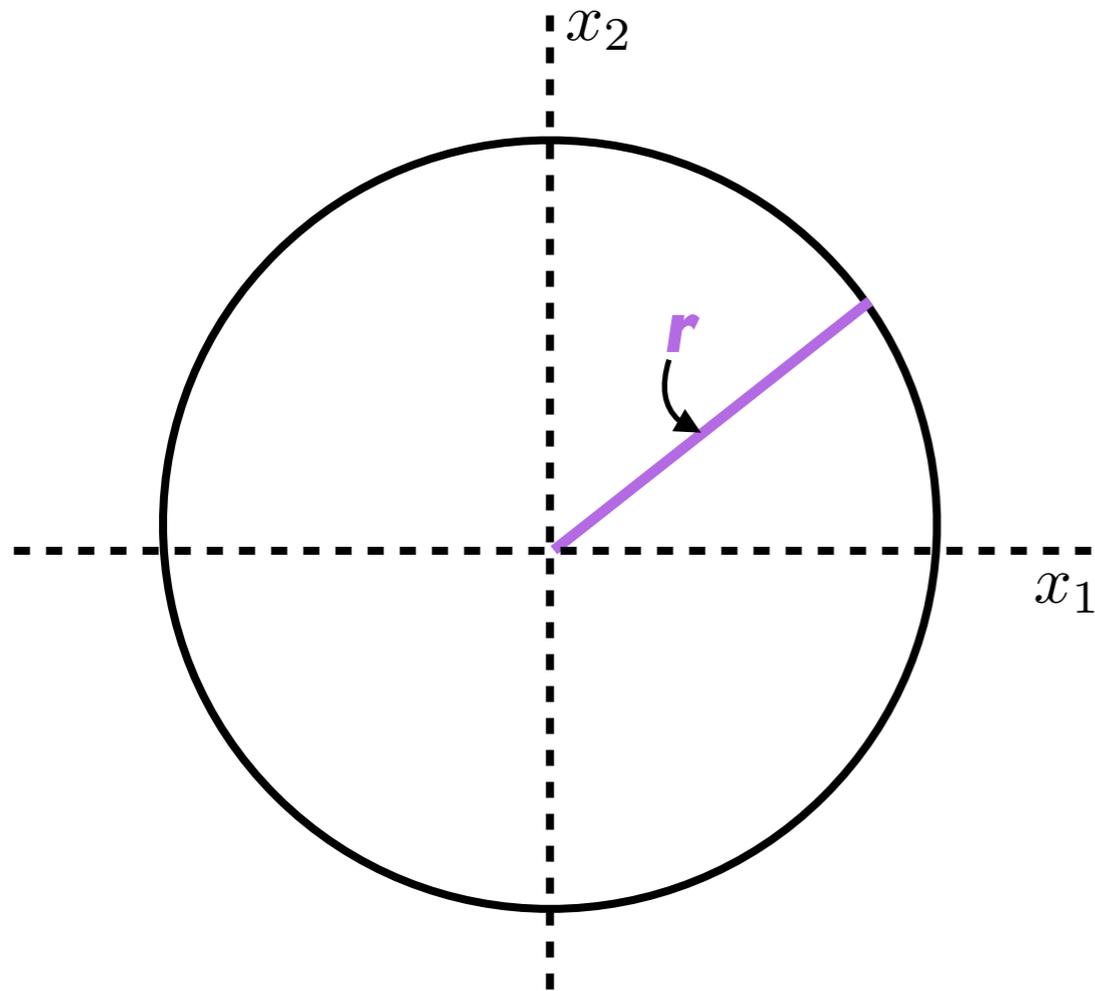
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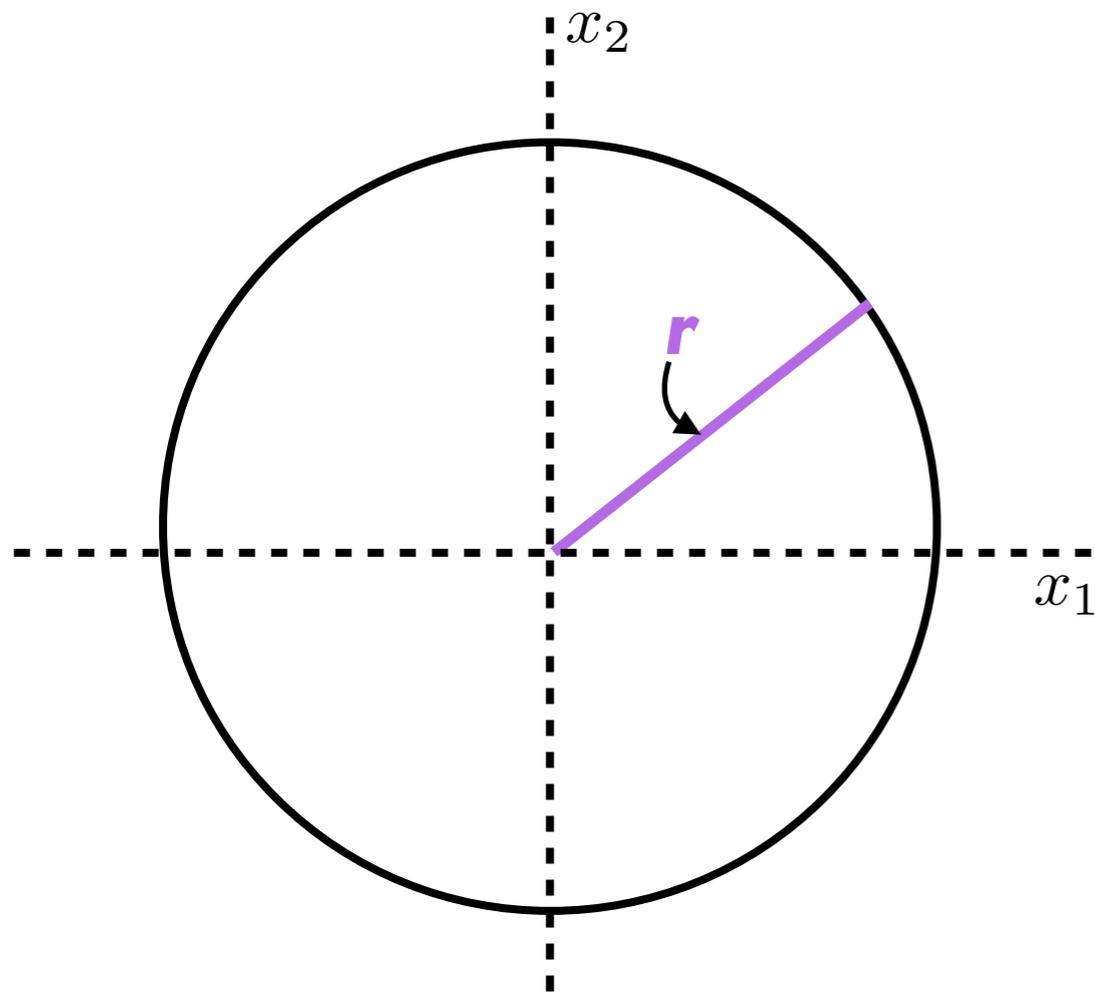
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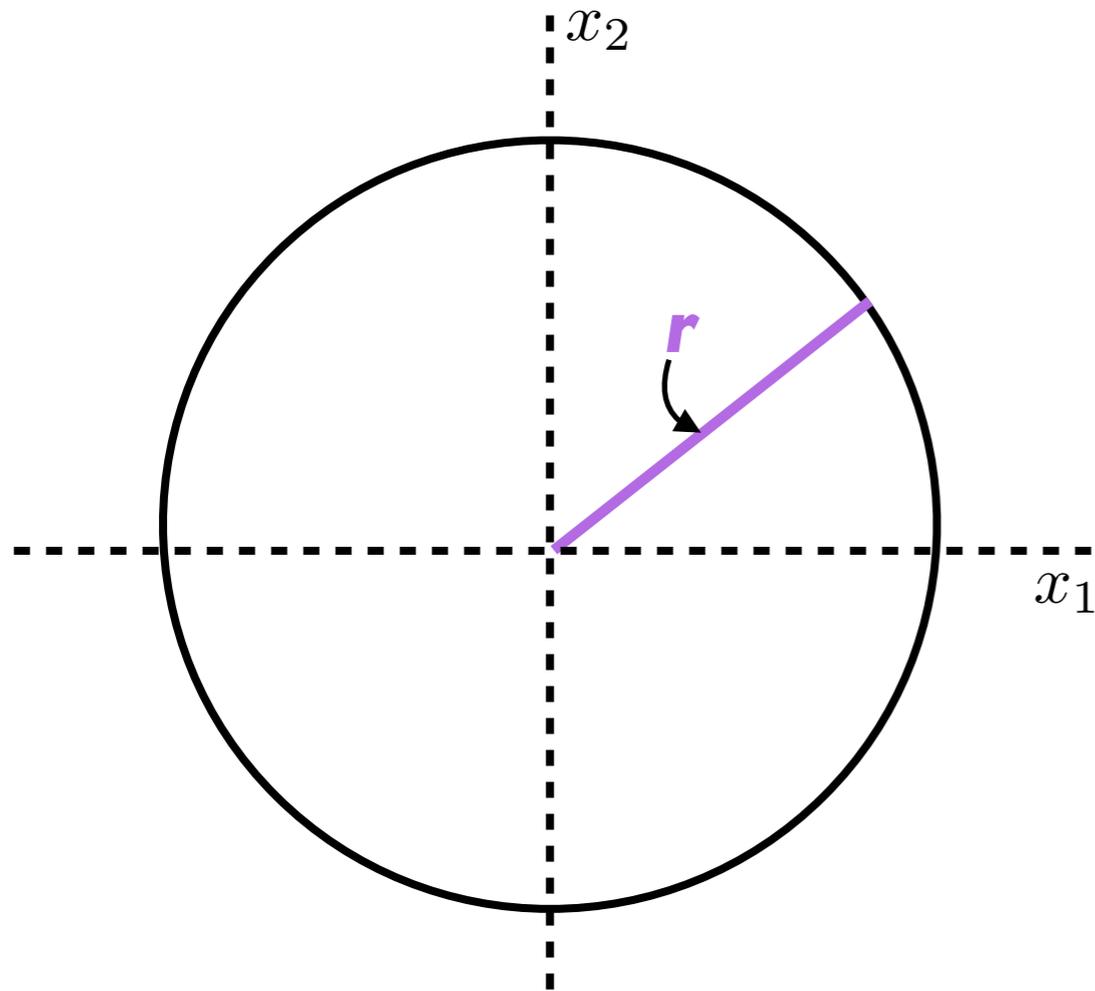
Now consider the path:

$$x(t) = r \cos(t); y(t) = r \sin(t)$$

# Multi-variable Functions

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The circle radius  $r$  is the set of all points where  $F(x_1, x_2) = r^2$



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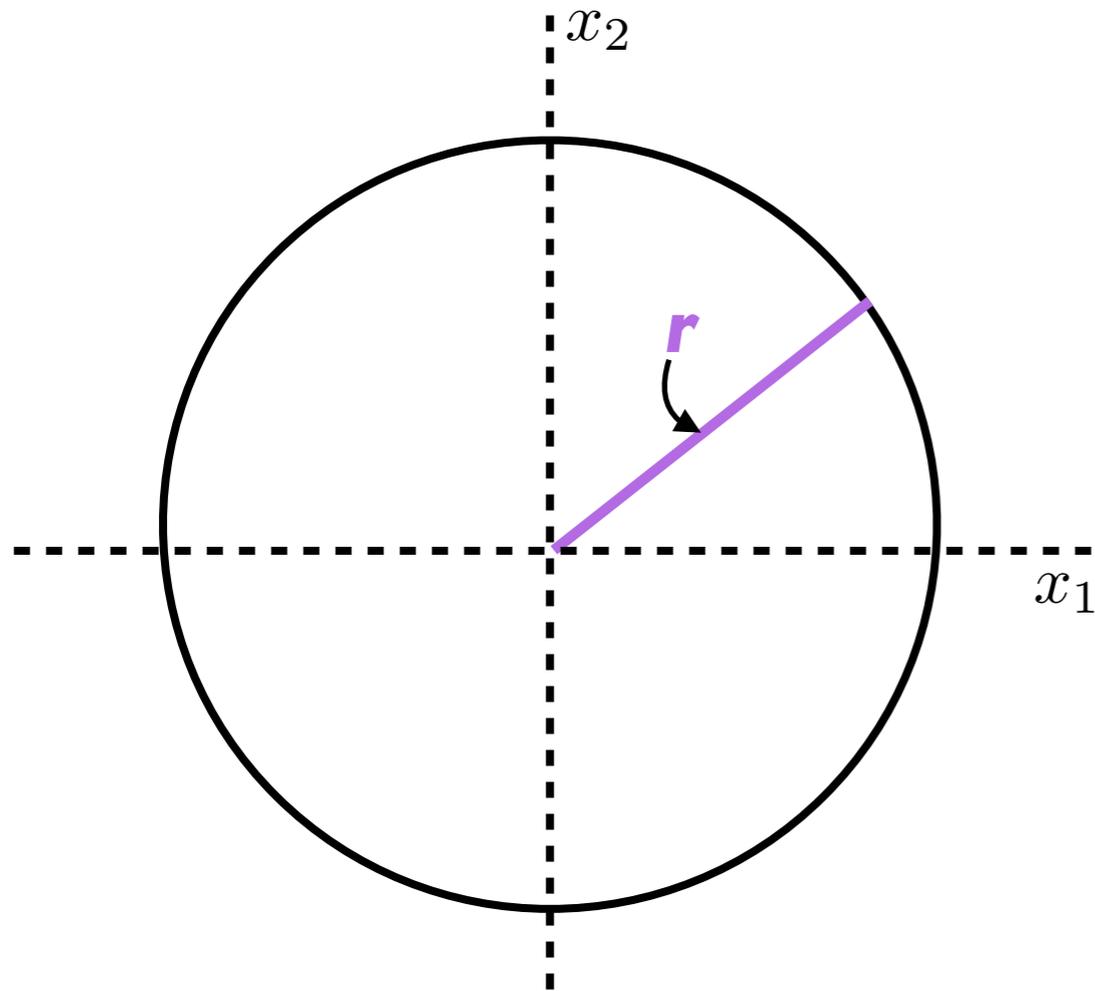
This path is on the circle so  $\mathbf{F}$  is constant:

$$\begin{aligned} F(x(t), y(t)) &= [r \cos(t)]^2 + [r \sin(t)]^2 \\ &= r^2 (\cos^2(t) + \sin^2(t)) = r^2 \end{aligned}$$

# Multi-variable Functions

With these idea in mind, let's consider the function:  $F(x_1, x_2) = x_1^2 + x_2^2$

The circle radius  $r$  is the set of all points where  $F(x_1, x_2) = r^2$



Now consider the path:

$$x(t) = r \cos(t); y(t) = r \sin(t)$$

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Thus:  $\frac{df}{dt} = \frac{d}{dt} [F(x(t))] = 0$

Not a coincidence.

# Multi-variable Functions

In general if a path  $\mathbf{x}(t)$  travels along an isocline of  $\mathbf{F}$ , then:

$$\nabla_x F(x(t)) \cdot \vec{x}'(t) \stackrel{\substack{= \\ \nearrow \text{by the result we proved earlier}}}{=} \frac{d}{dt} [F(x(t))] \stackrel{\substack{= \\ \nwarrow \text{since } \mathbf{F} \text{ is constant along } \mathbf{x}(t)}}}{=} 0$$

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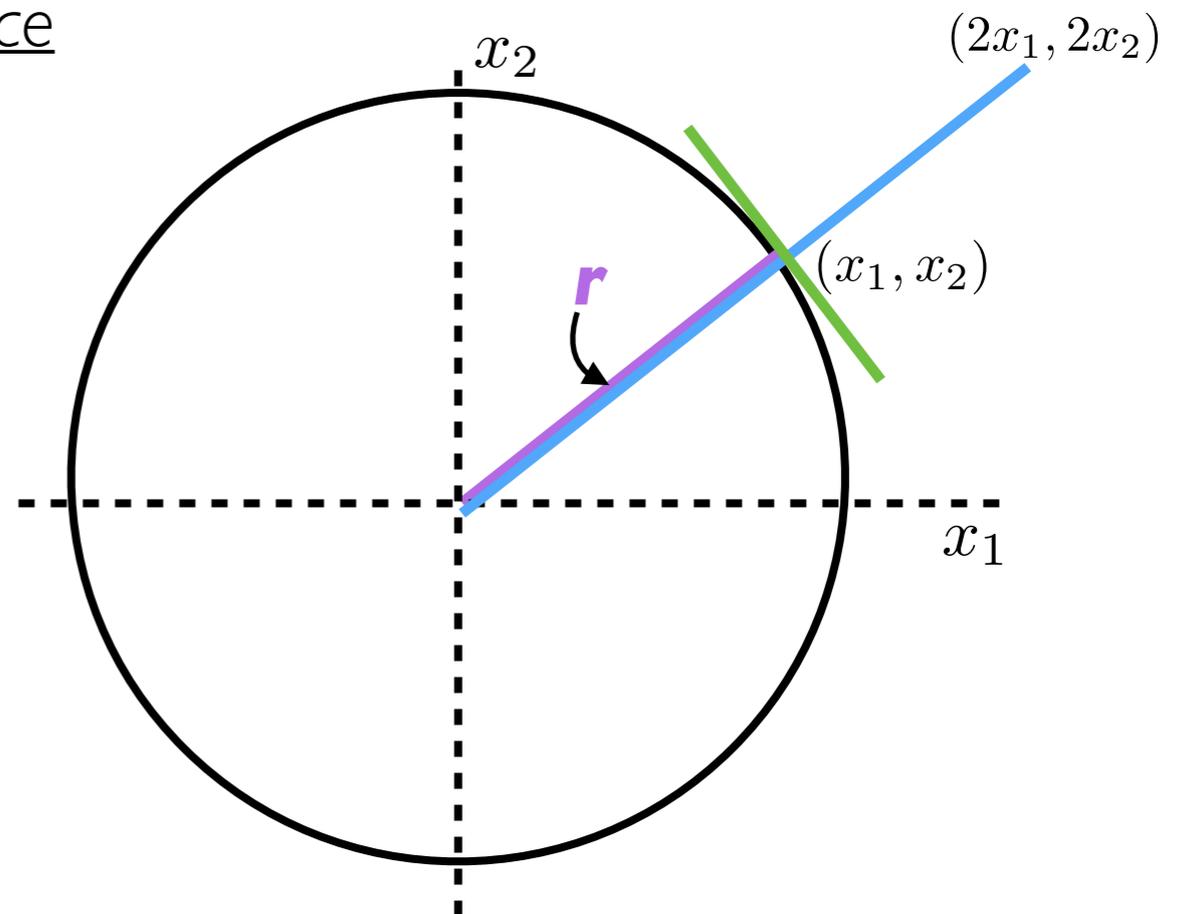
But since  $x(t)$  was any such path, this means the **gradient vector** is always perpendicular to the tangent of the isocline surface

So in our example:

function:  $F(x_1, x_2) = x_1^2 + x_2^2$

isocline:  $F(x_1, x_2) = r^2$   
(circle of radius  $r$ )

gradient:  $\nabla_x F(x_1, x_2) = (2x_1, 2x_2)$



Why do we care about all this? **Constrained Optimization**

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If our goal is to extremize  **$F$**  we seek critical points  $x^*$  s.t.  $\nabla F(x^*) = \vec{0}$

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E.g. suppose we want to maximize

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We can't just seek critical points of  $\mathbf{F}$  because they might not satisfy the constraint.

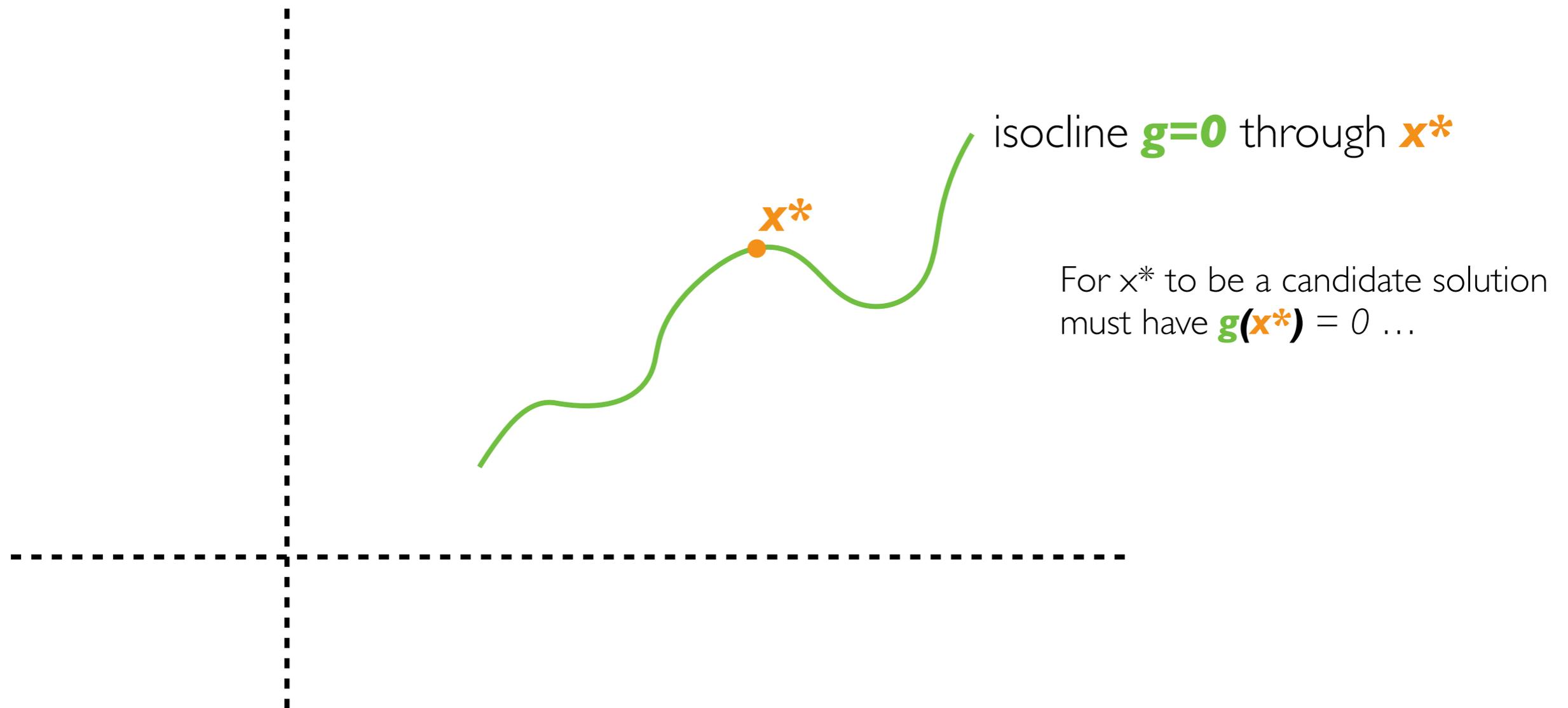
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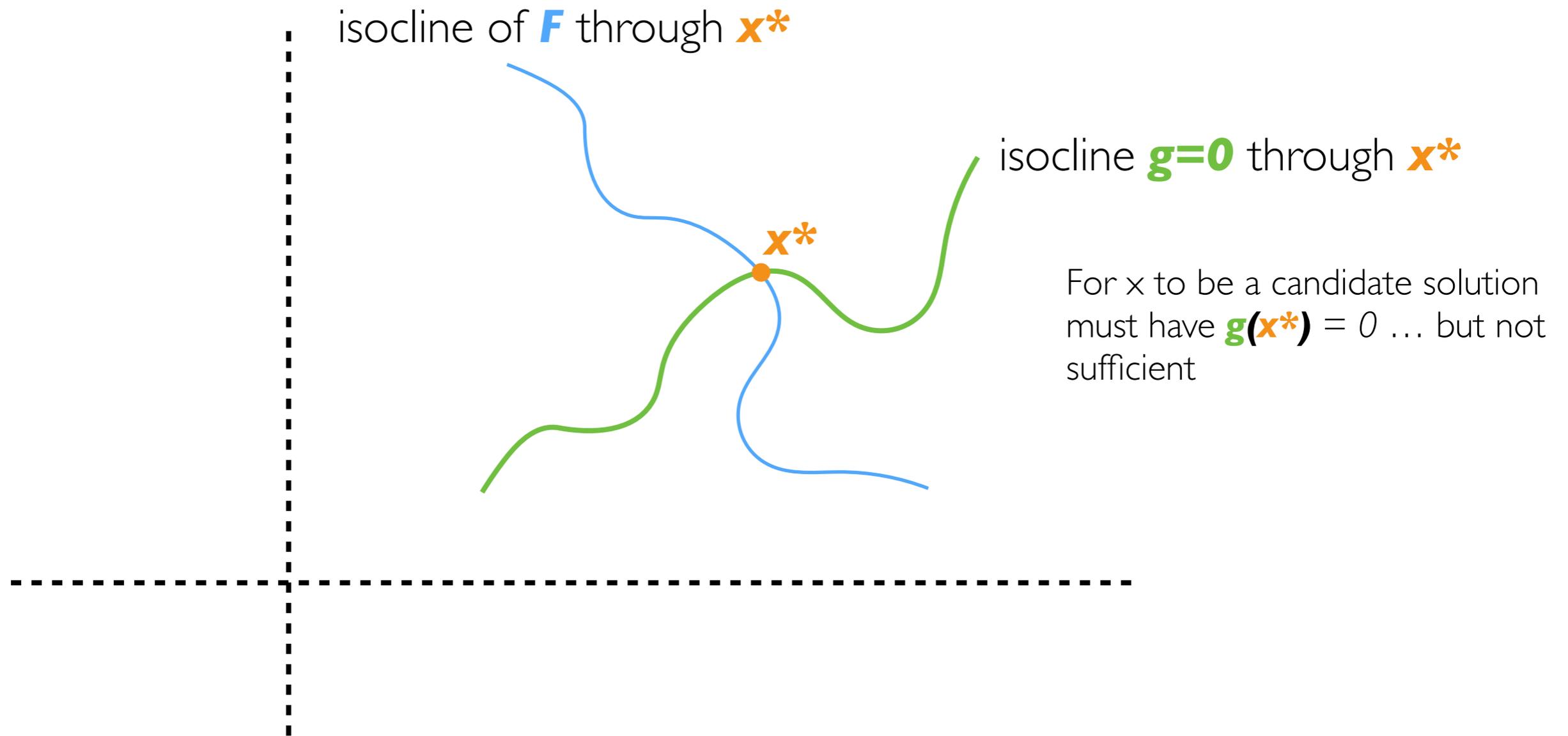
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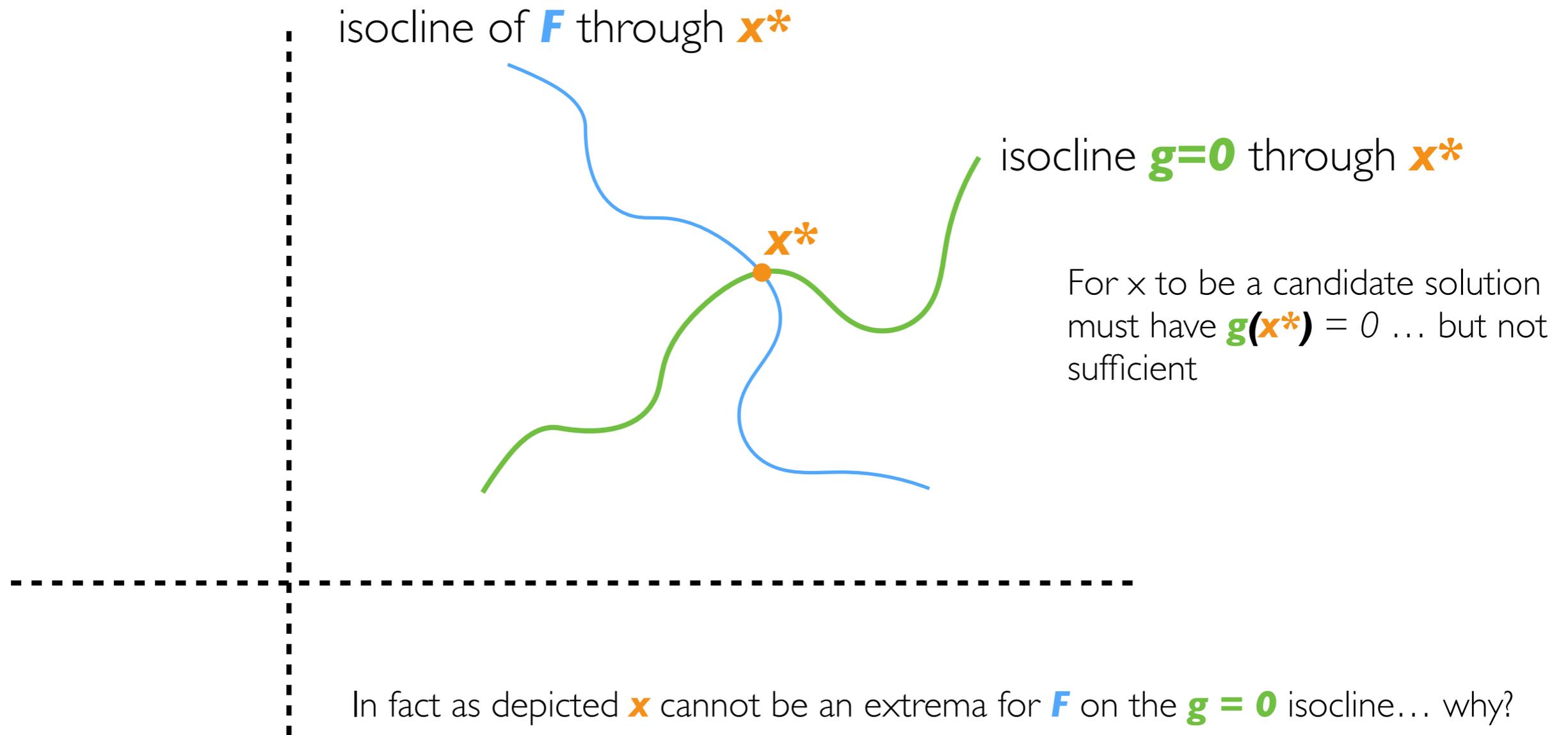
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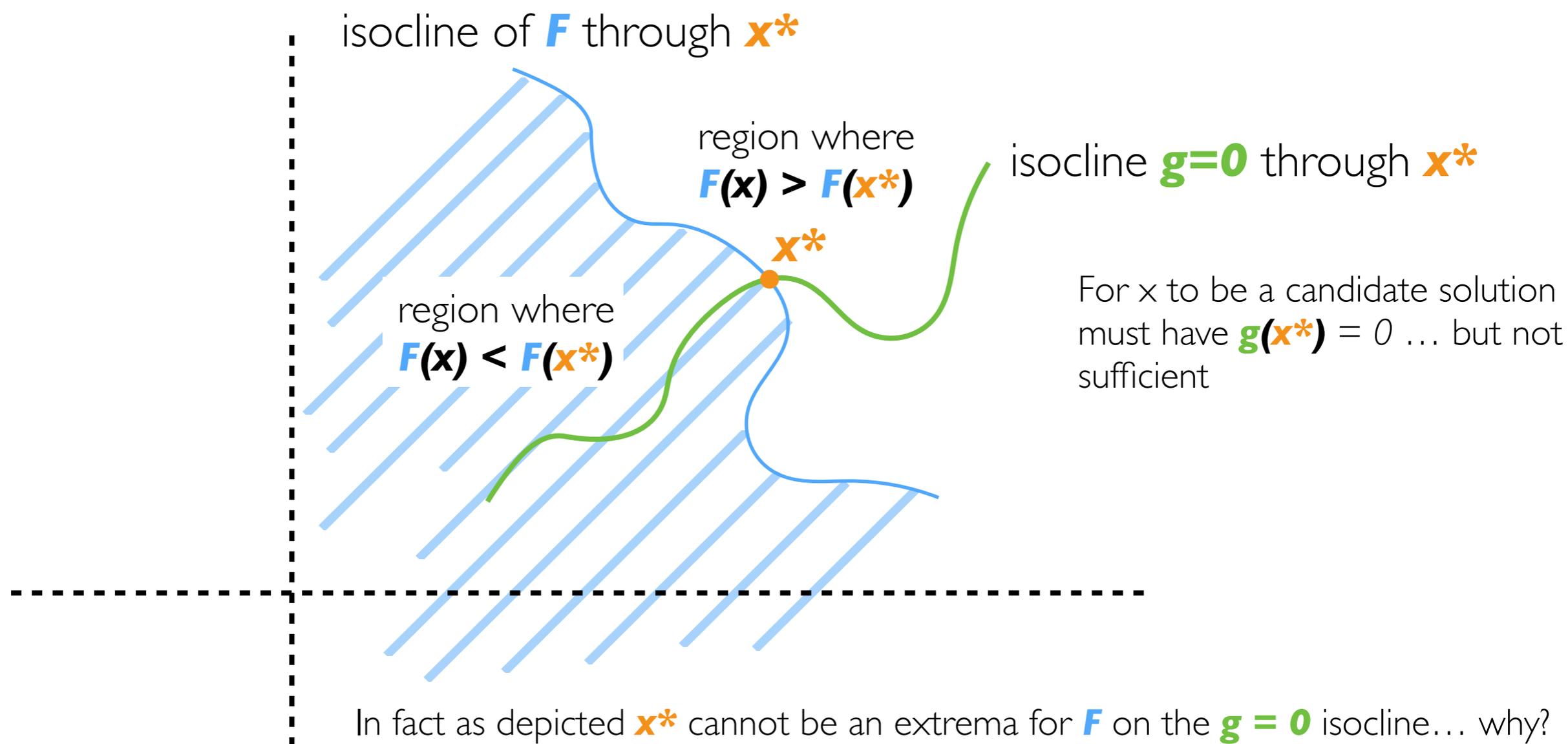
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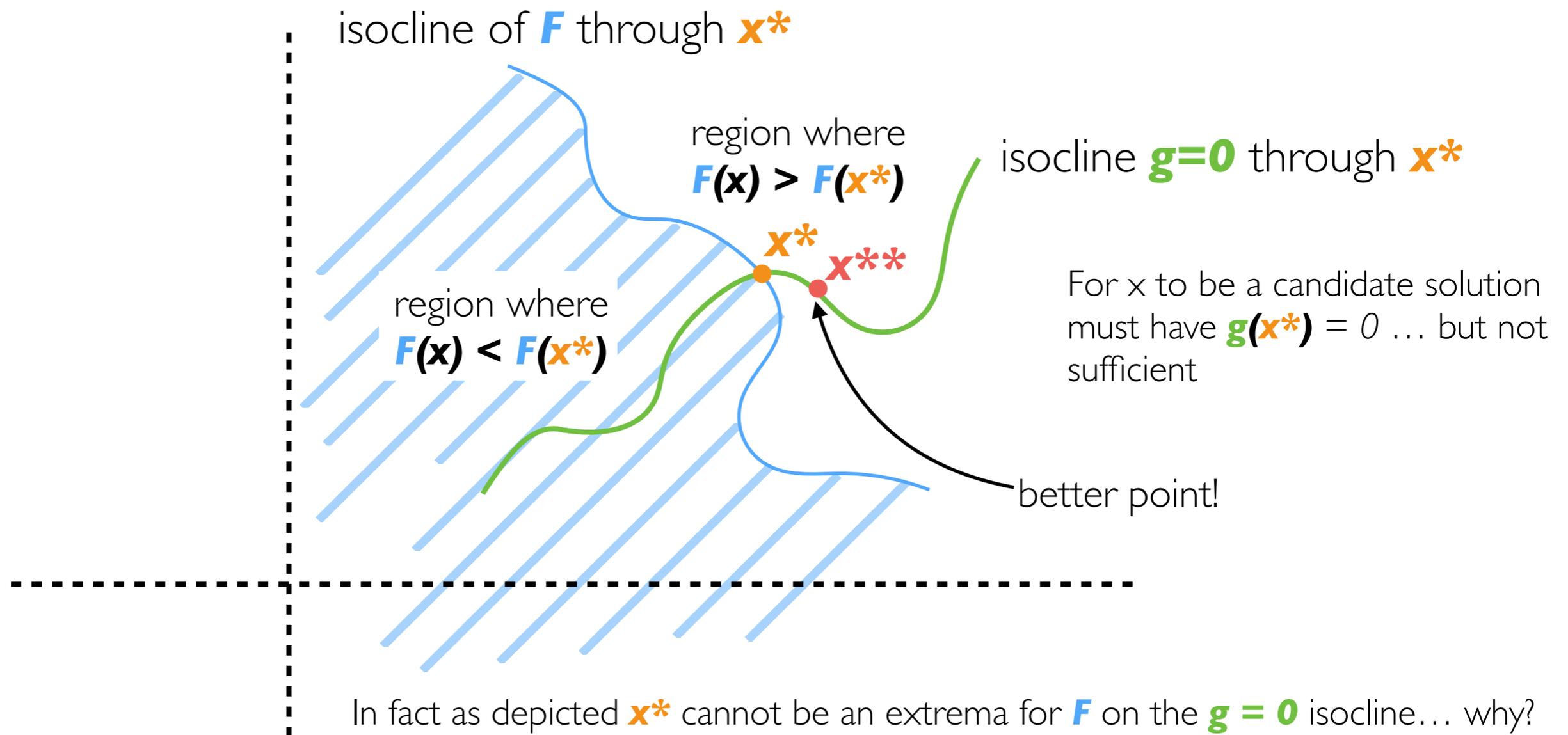
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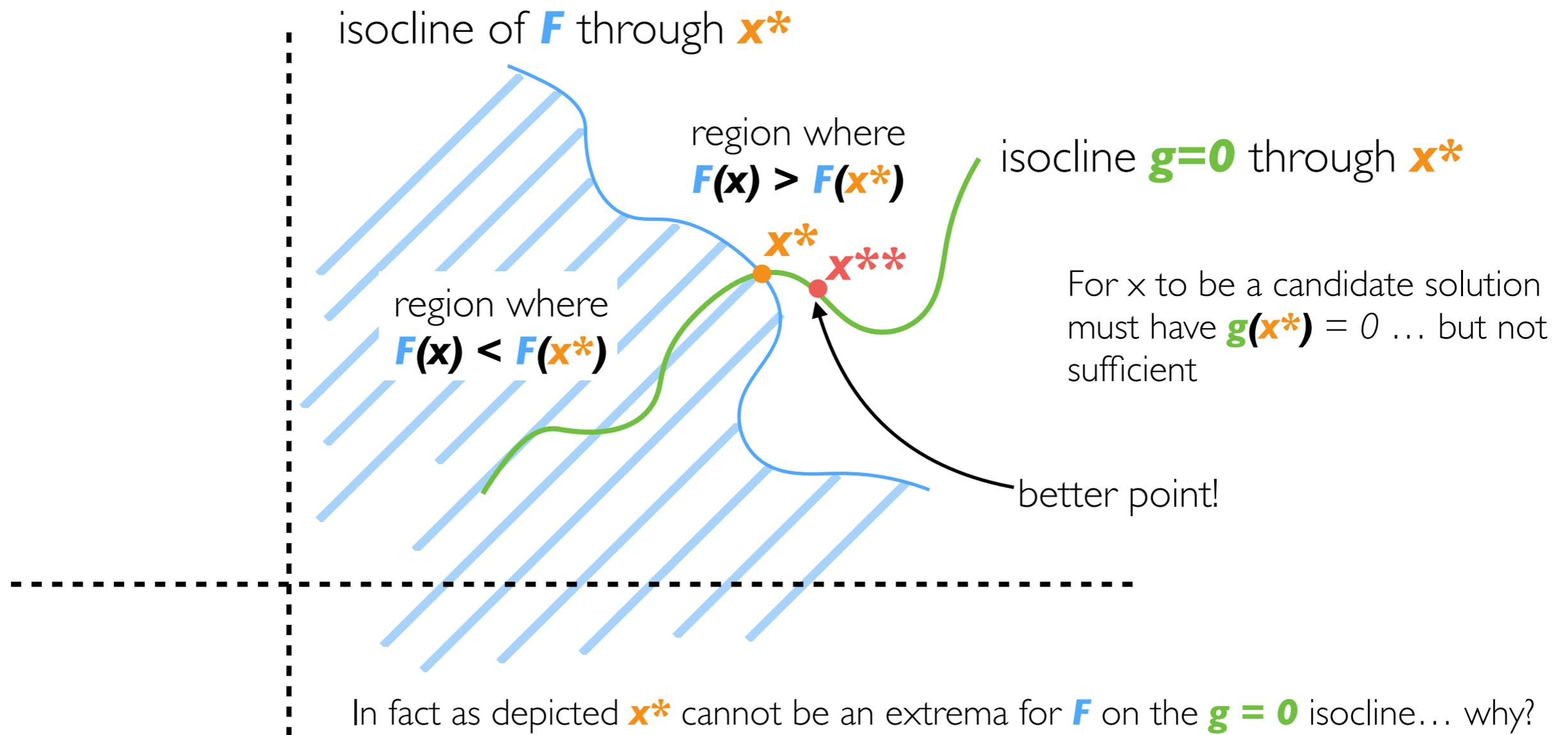
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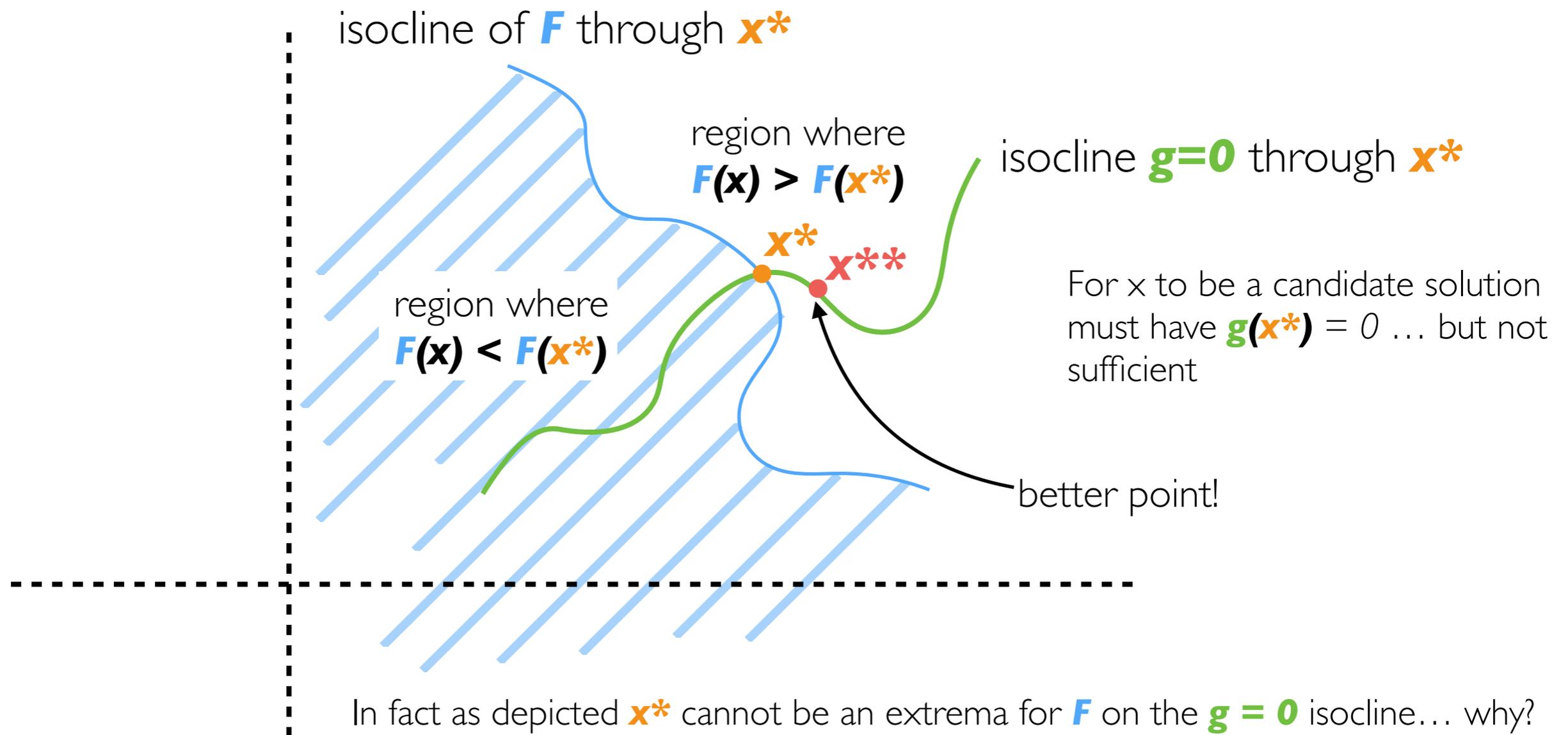
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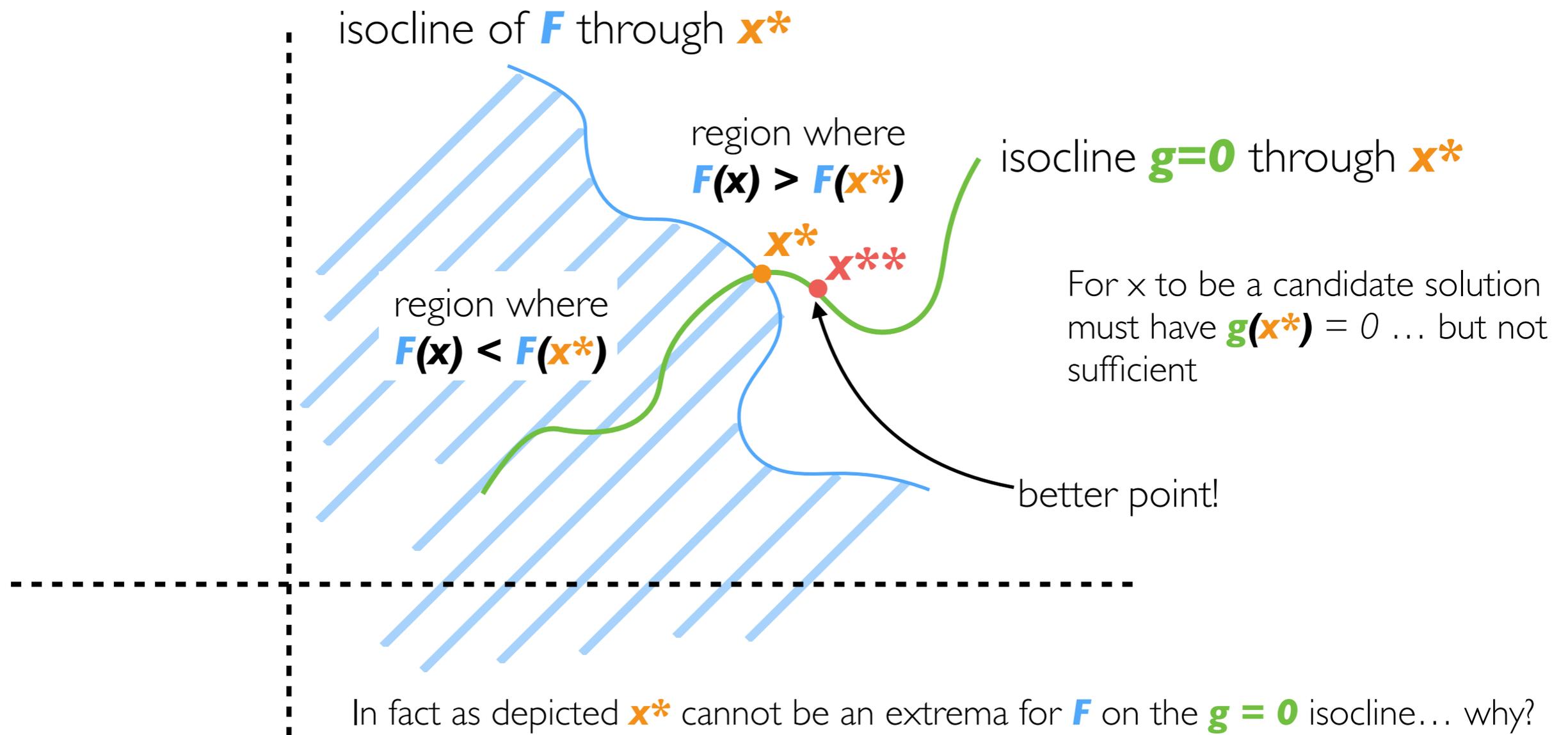


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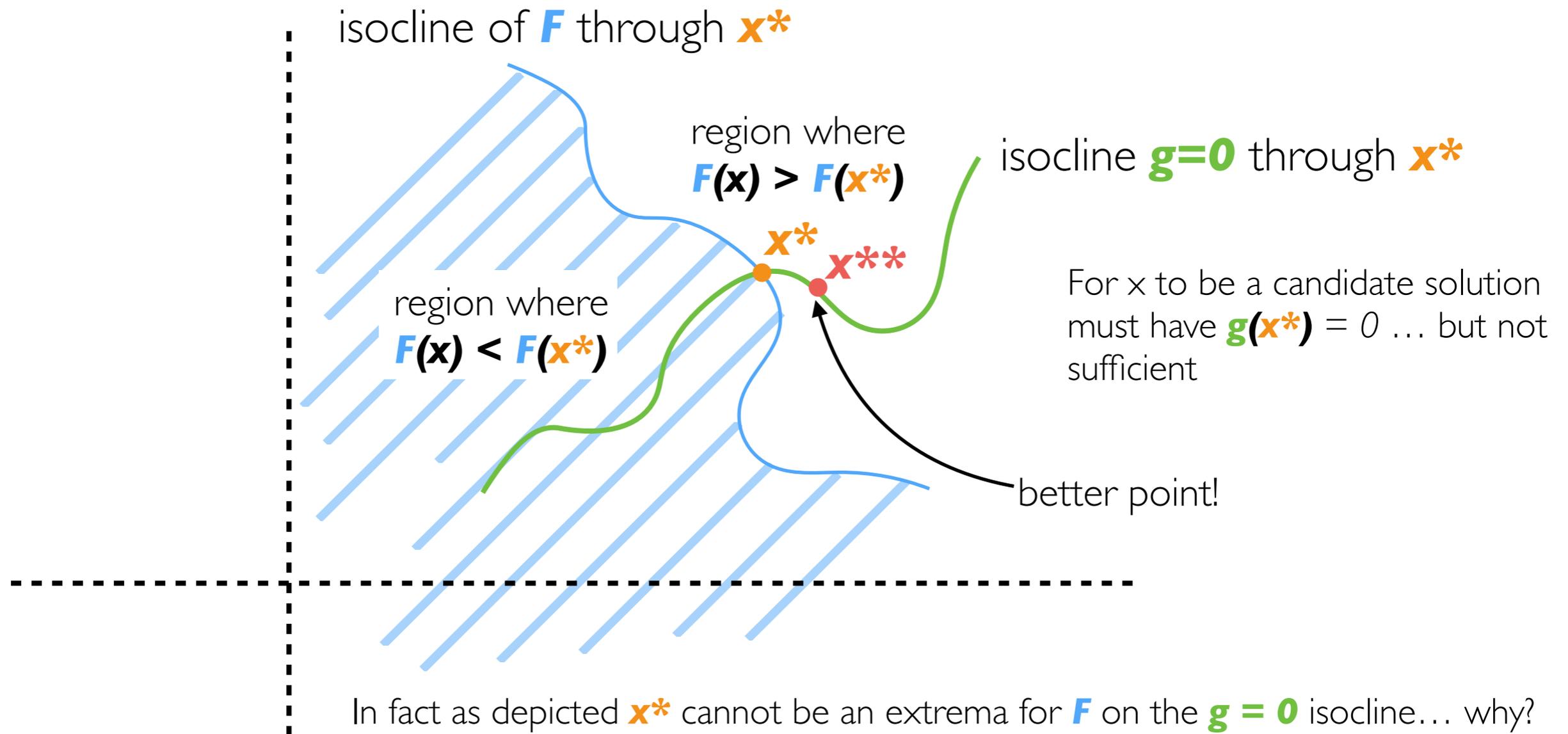
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$$\nabla F(x^*) \quad || \quad \nabla g(x^*)$$

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$$\nabla F(x^*) \parallel \nabla g(x^*) \Rightarrow \nabla F(x^*) = \lambda \nabla g(x^*) \quad \text{scalar}$$

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$$\nabla \mathcal{L}(x_1, x_2, \lambda) = (1 - 2\lambda x_1, 1 - 2\lambda x_2, r^2 - x_1^2 - x_2^2)$$

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$$\begin{array}{c} \parallel \\ 0 \end{array} \Rightarrow x_1 = \frac{1}{2\lambda}, x_2 = \frac{1}{2\lambda}, \lambda = \pm \frac{1}{\sqrt{2}r}$$

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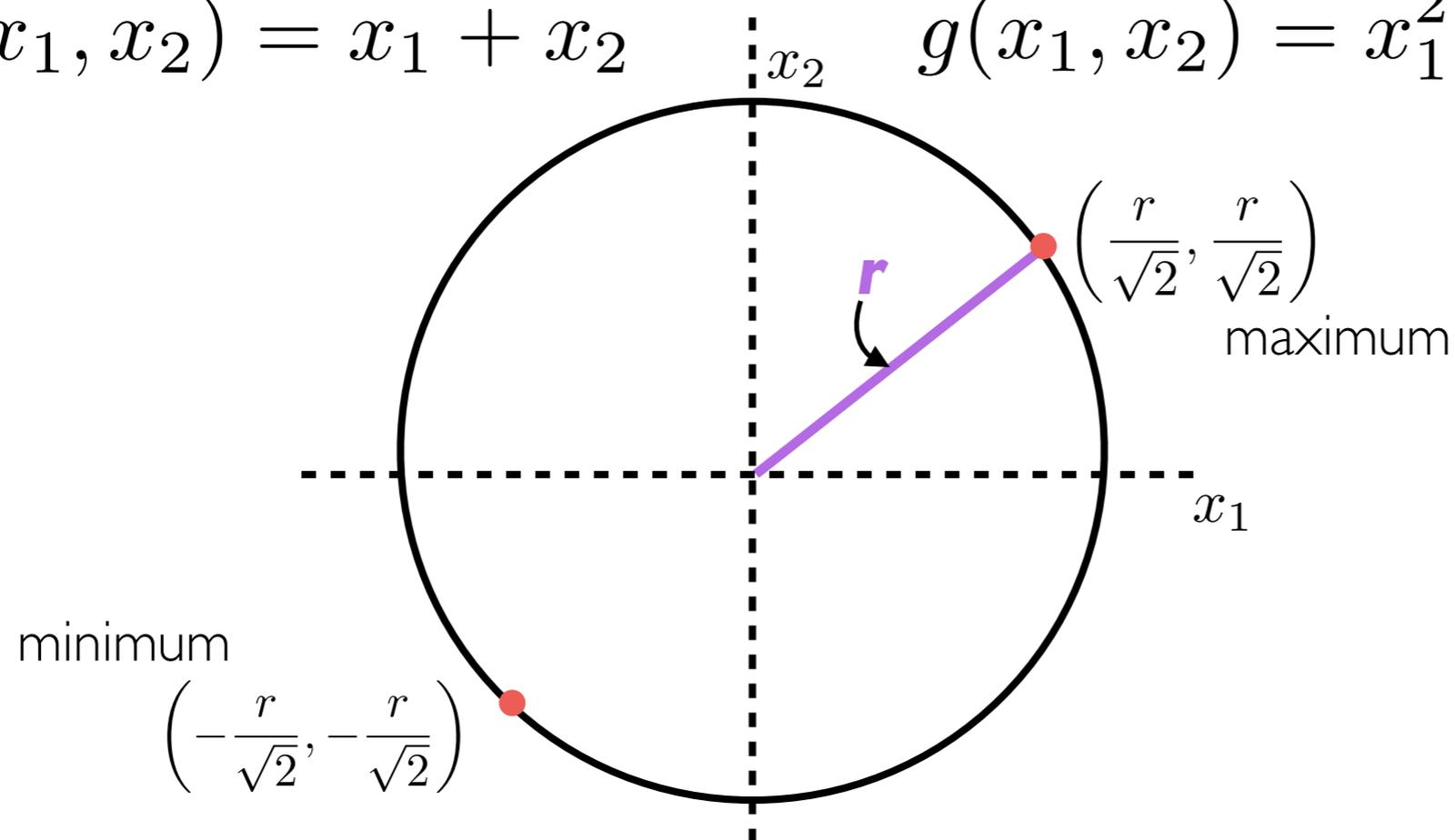
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$$\frac{\partial H(\vec{x})}{\partial x_1} \stackrel{\text{def'n of partial derivative}}{=} \lim_{\Delta x_1 \rightarrow 0} \frac{H(x_1 + \Delta x_1, x_2, \dots) - H(x_1, x_2, \dots)}{\Delta x_1}$$

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applying single-variable chain rule  $\mathbf{m}$   
times

$$= \sum_i \frac{\partial G}{\partial y_i}(\vec{F}(\vec{x})) \frac{\partial F_i}{\partial x_1}(\vec{x})$$

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So in general:

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So in general:

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Or:

$$\nabla H = \nabla \vec{F}(\vec{x}) \cdot \nabla G(\vec{F}(\vec{x}))$$

**n**-vector-  
valued fn

**n****x****m**-matrix  
-valued fn

**m**-vector-  
valued fn

Where  $\nabla \vec{F}$  is the matrix with **ij**-th elt:

$$(\nabla \vec{F})_{ji} = \frac{\partial F_i}{\partial x_j}$$

# Multi-variable Functions

Taylor series for function  $f(\mathbf{x}_1, \dots, \mathbf{x}_n)$  of  $n$  inputs:

$$f(\vec{x}_0, \Delta\vec{x}) = f(\vec{x}_0) + \nabla f(\vec{x}_0) * \Delta\vec{x} + \frac{1}{2} (H[F] \cdot \vec{x}_0) * \Delta x^2 + \dots$$

pointwise mult.

matrix-on-vector multiplication

vector delta

Hessian matrix

$$H[f] = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \frac{\partial^2 f}{\partial x_1 \partial x_3} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2 \partial x_2} & \frac{\partial^2 f}{\partial x_2 \partial x_3} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \frac{\partial^2 f}{\partial x_n \partial x_3} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{bmatrix}$$

shape =  $(\mathbf{n}, \mathbf{n})$