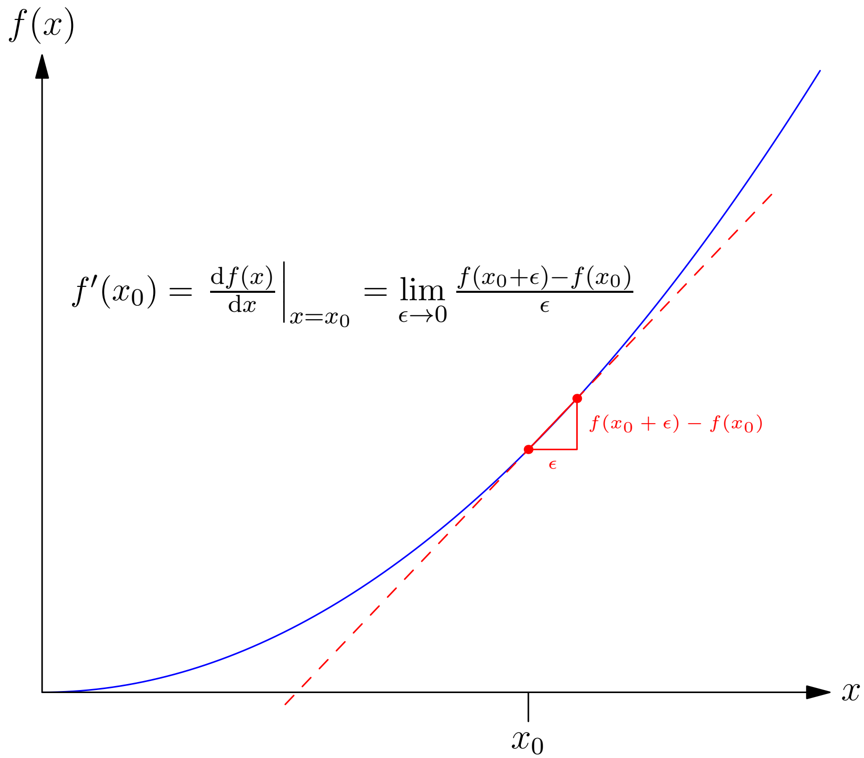
Advanced Machine Learning

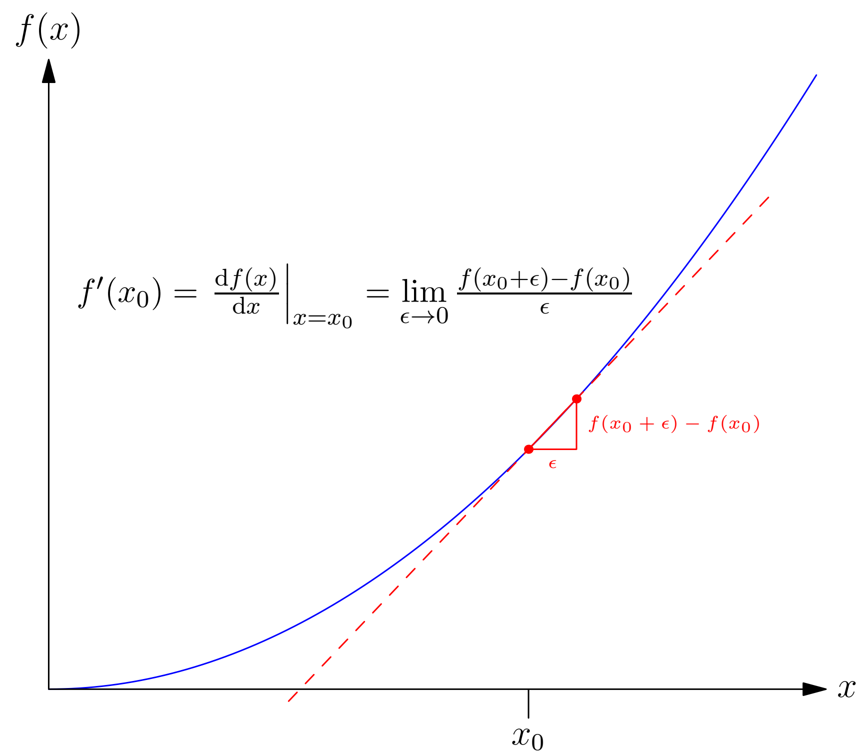
Differential Calculus



Differentiation, product and chain rules, vectors and matrices

Outline

1. **Why Calculus?**
2. Differentiation
3. Vector and Matrix Calculus



Why Calculus?

- Calculus is a fundamental tool of mathematical analysis
- In machine learning differentiation is fundamental tool in optimisation
- Integration is an essential tool in taking expectations over continuous distributions
- Both differentiation and integration crop up elsewhere

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- This material will not be examined explicitly

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- Integration is an essential tool in taking expectations over continuous distributions
- Both differentiation and integration crop up elsewhere
- This material will not be examined explicitly, but I assume elsewhere that you can do calculus

Back to Basics

- You have all done A-level maths so should be familiar with the rules of calculus
- But, it is easy to forget the rules and sometimes we use quite sophisticated tricks
- Although the sophisticated tricks really speed up calculations, it pays to be able to understand where these tricks come from

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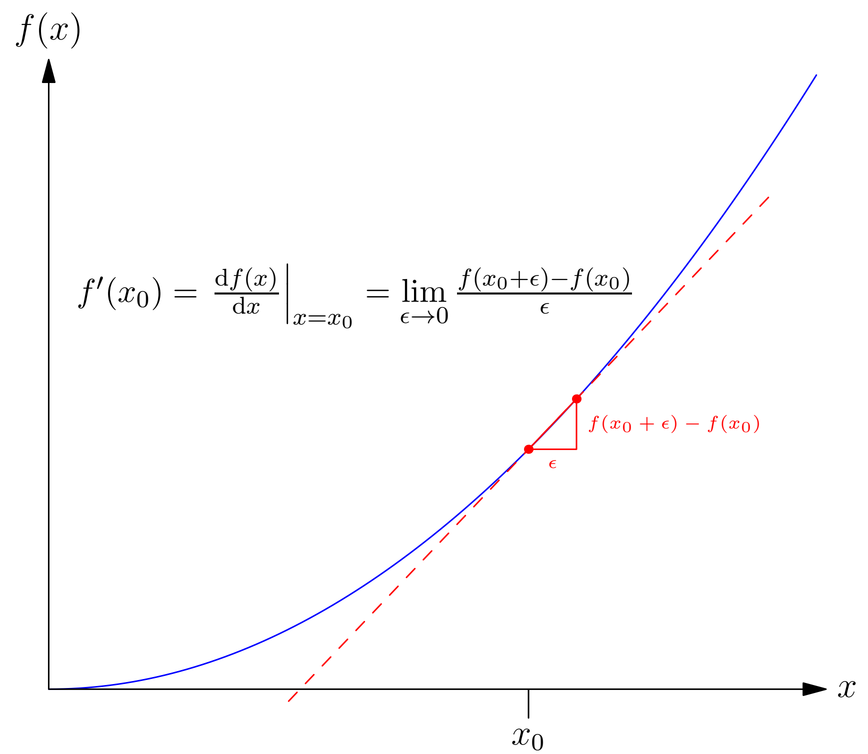
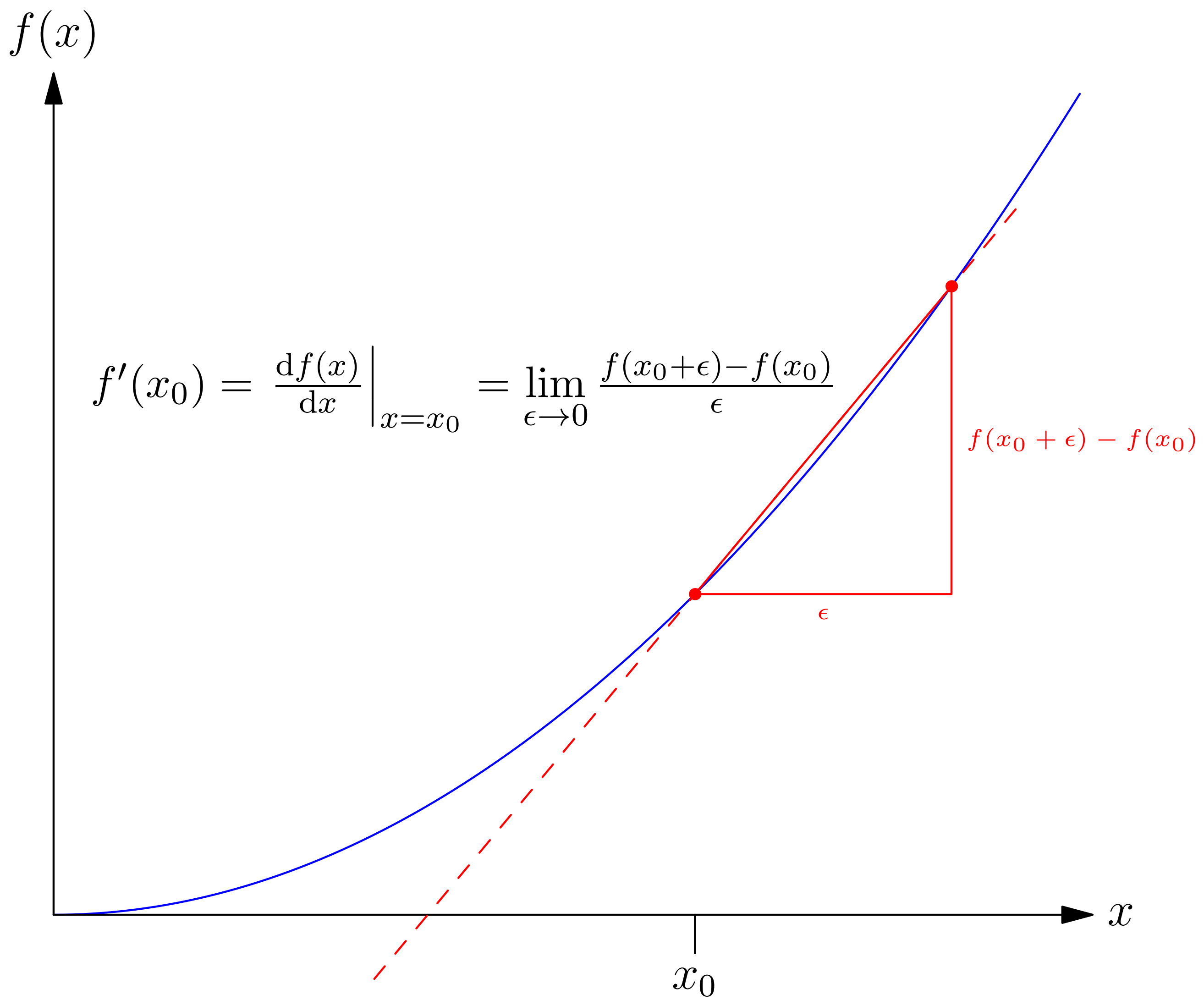


Differentiation



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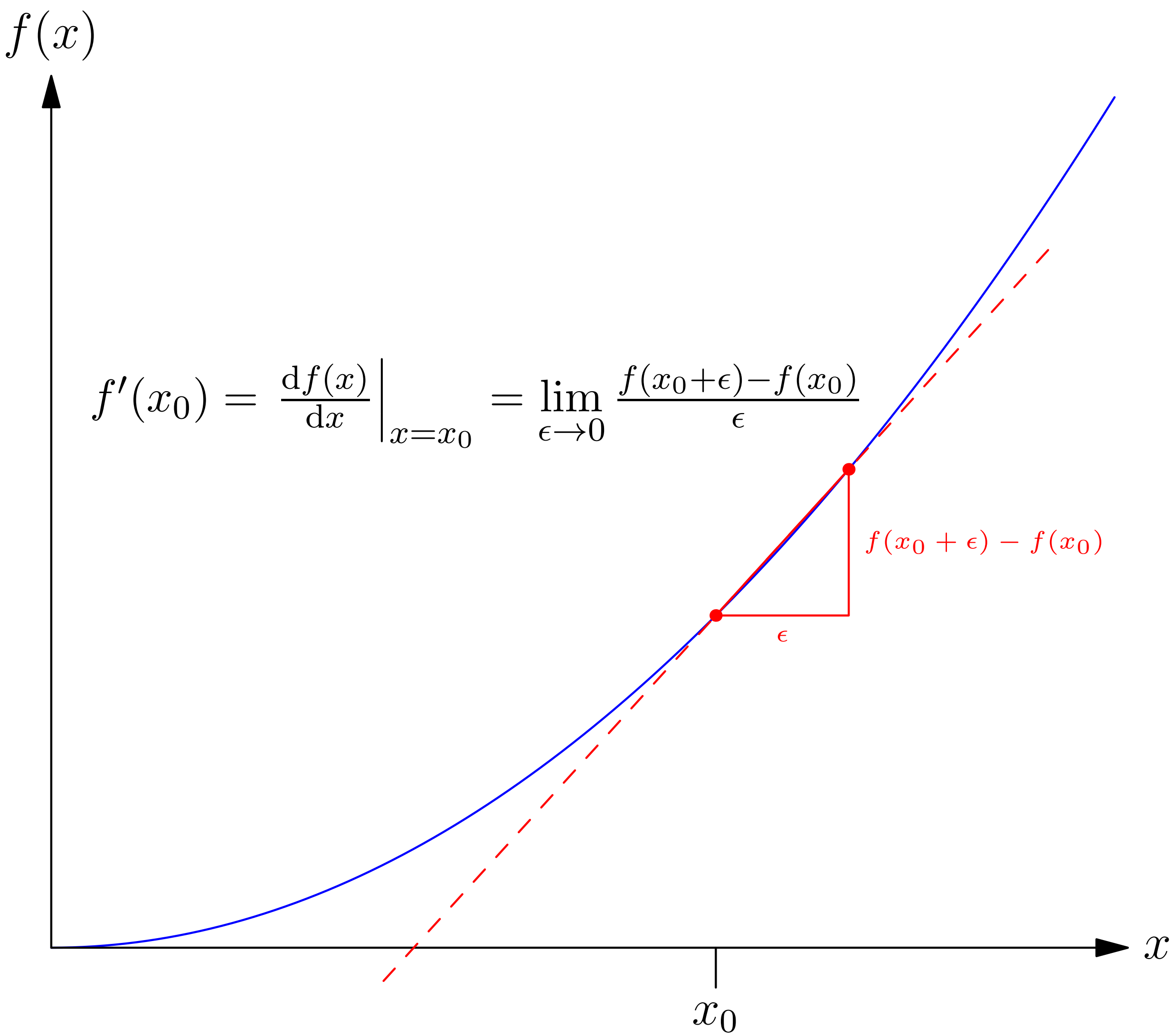
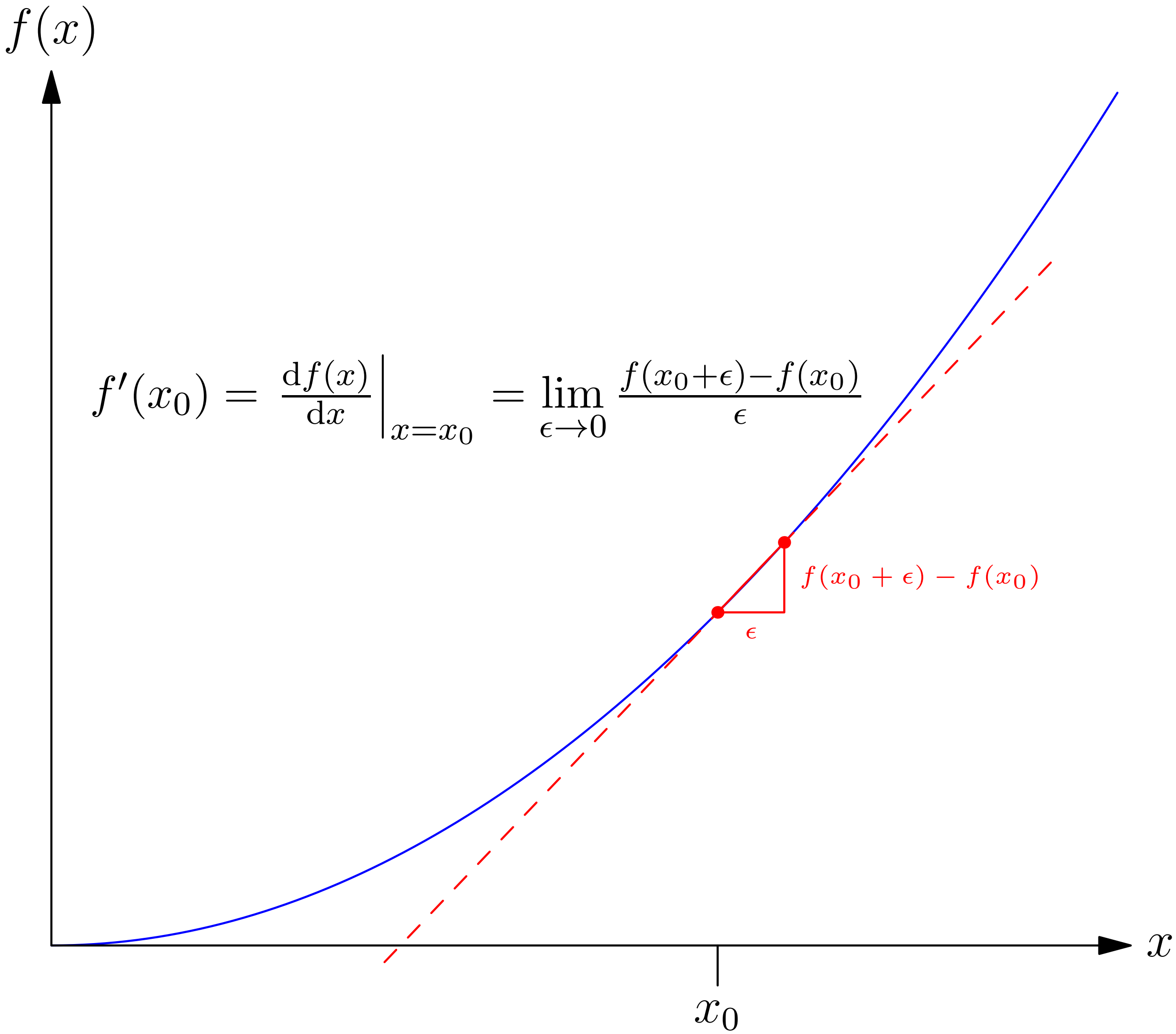


$$f'(x_0) = \left.\frac{\mathrm{d}f(x)}{\mathrm{d}x}\right|_{x=x_0} = \lim_{\epsilon\to 0}\frac{f(x_0+\epsilon)-f(x_0)}{\epsilon}$$

Differentiation



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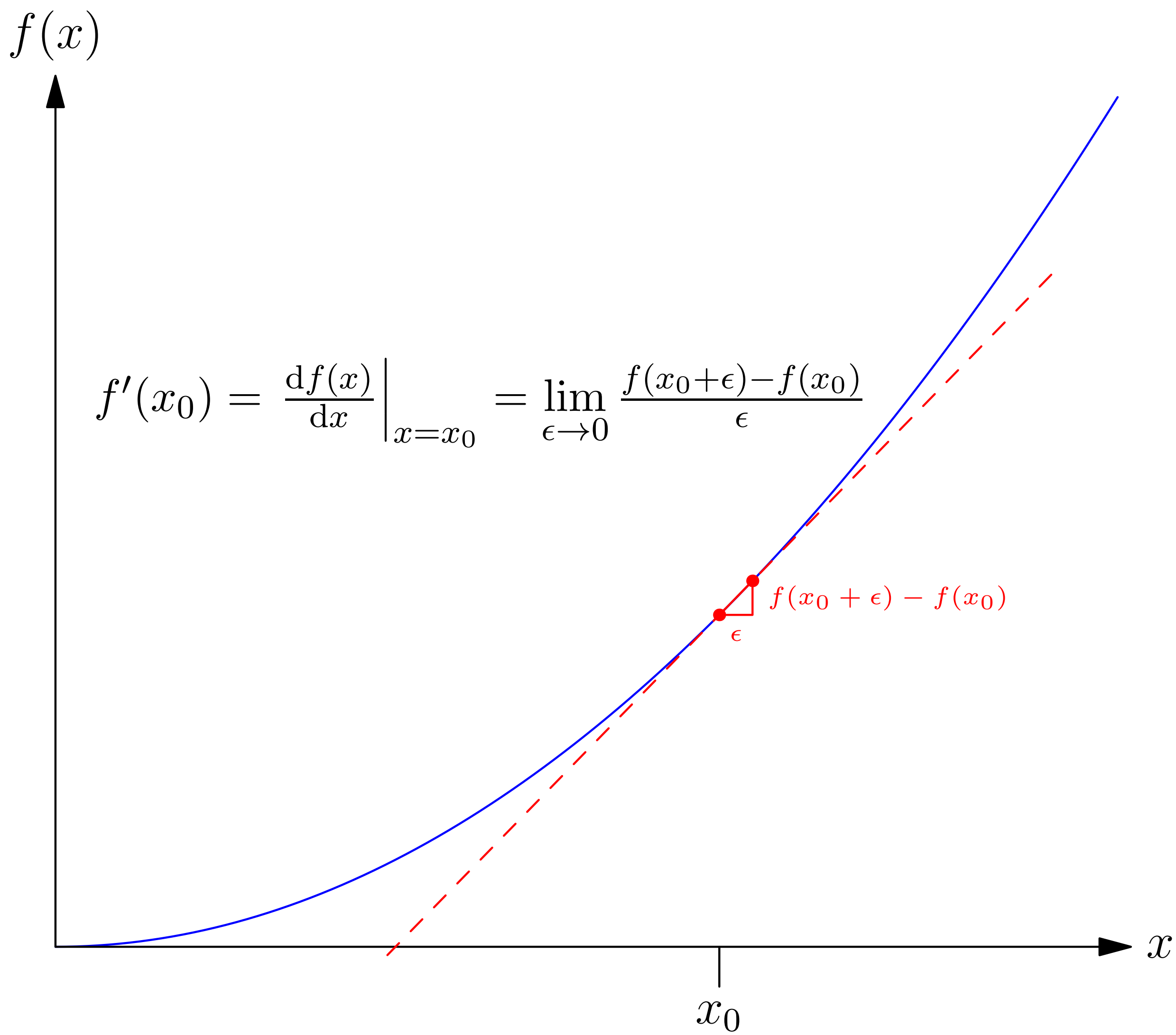

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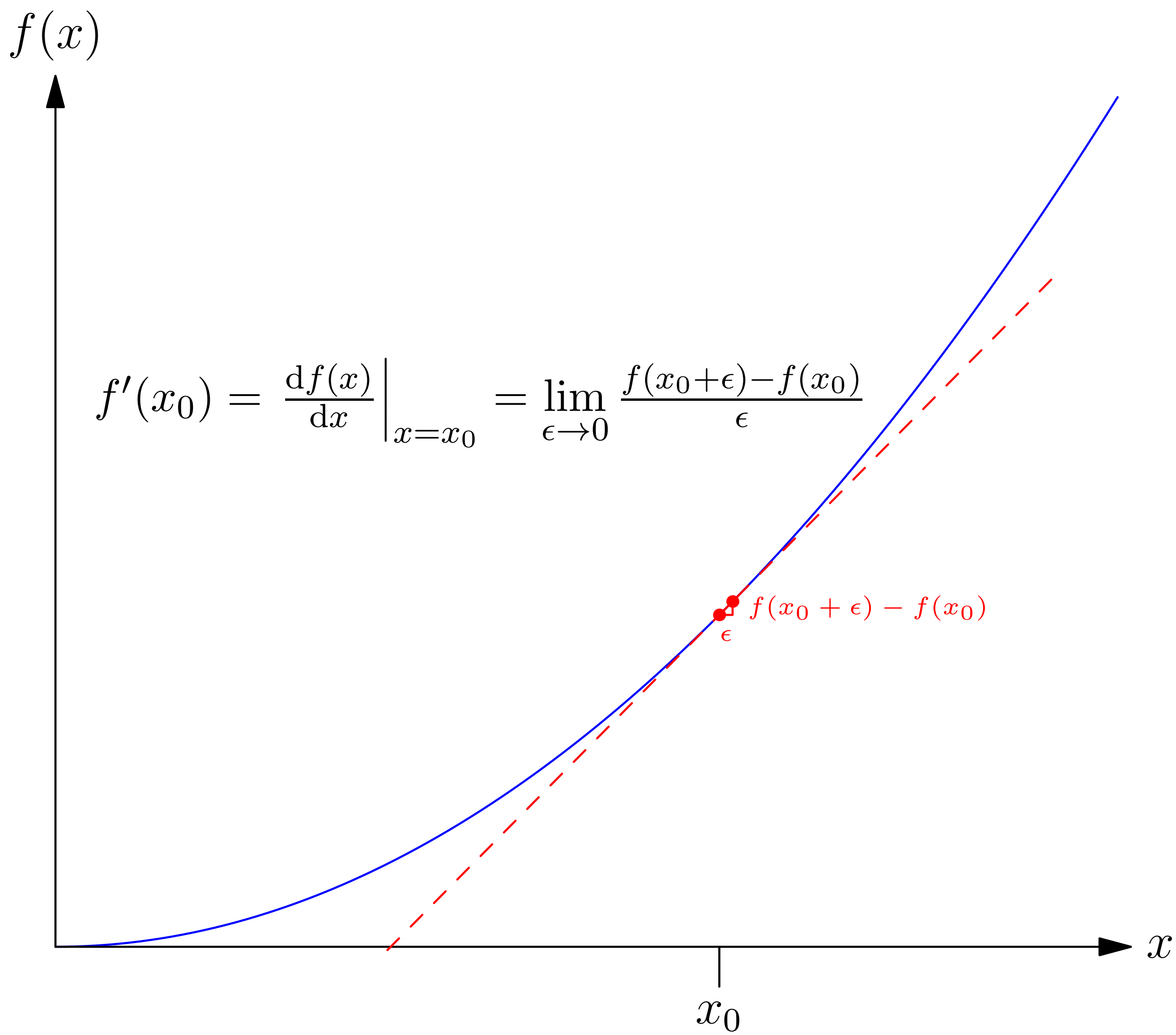

Polynomials

- $f(x) = x^2$

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Linearity of derivatives

- Note that $f(x+\epsilon) = f(x) + \epsilon f'(x) + O(\epsilon^2)$ (from the definition of $f'(x)$)

$$\frac{\mathrm{d}(a f(x) + b g(x))}{\mathrm{d}x} = \lim_{\epsilon \to 0} \frac{(a f(x+\epsilon) + b g(x+\epsilon)) - (a f(x) + b g(x))}{\epsilon}$$

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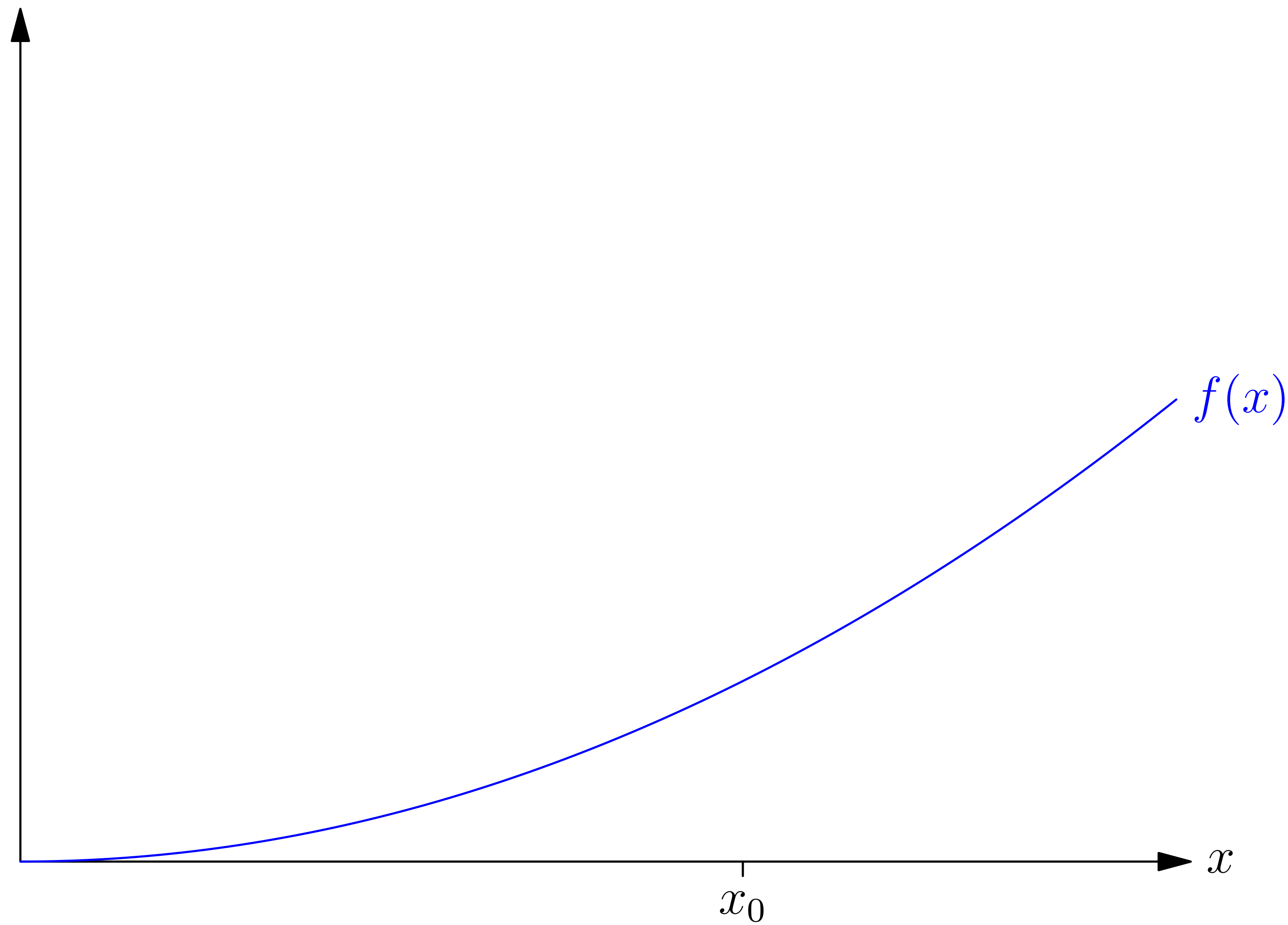
- **Differentiation is a linear operation!**

Linearity in Pictures



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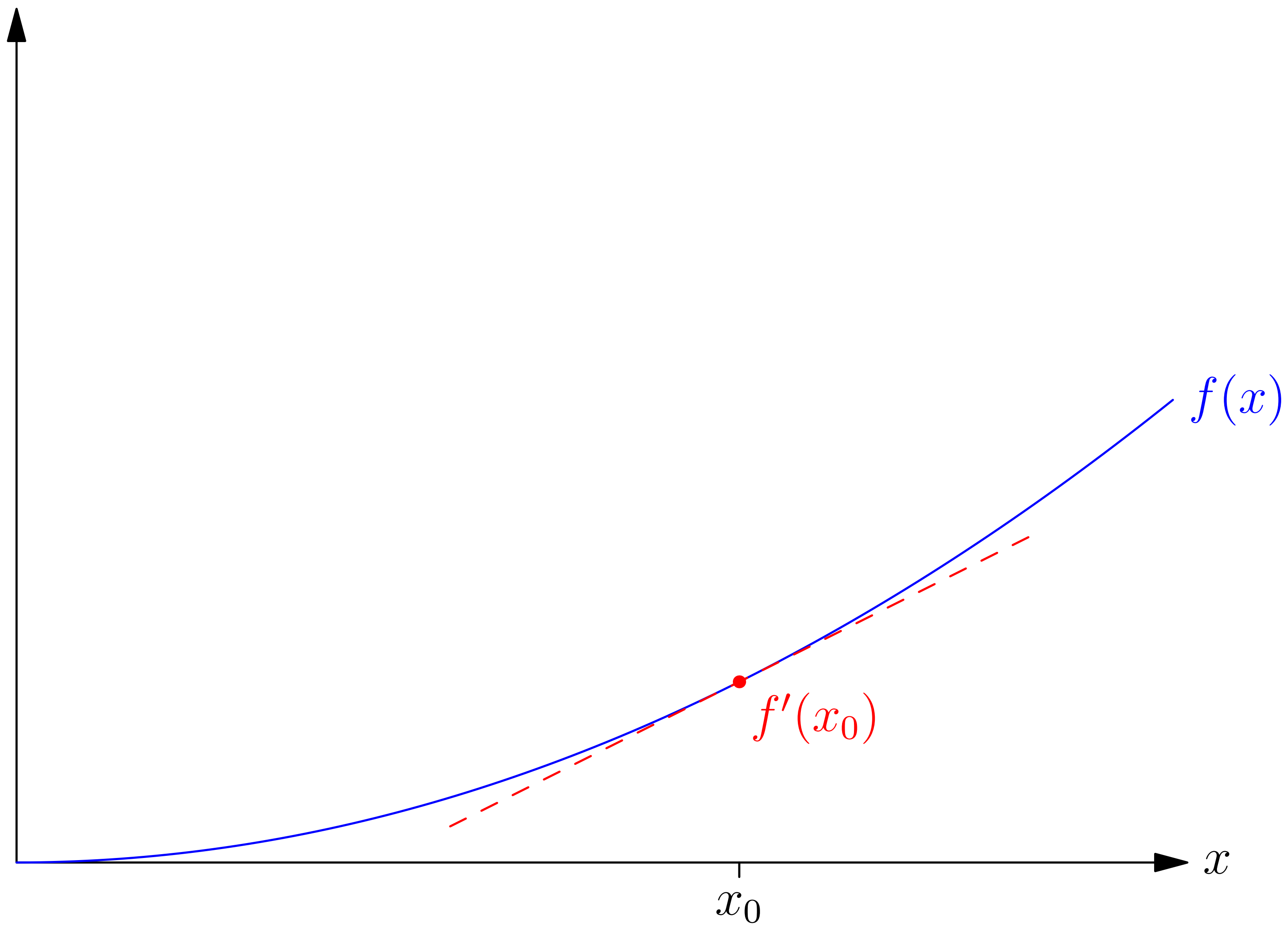

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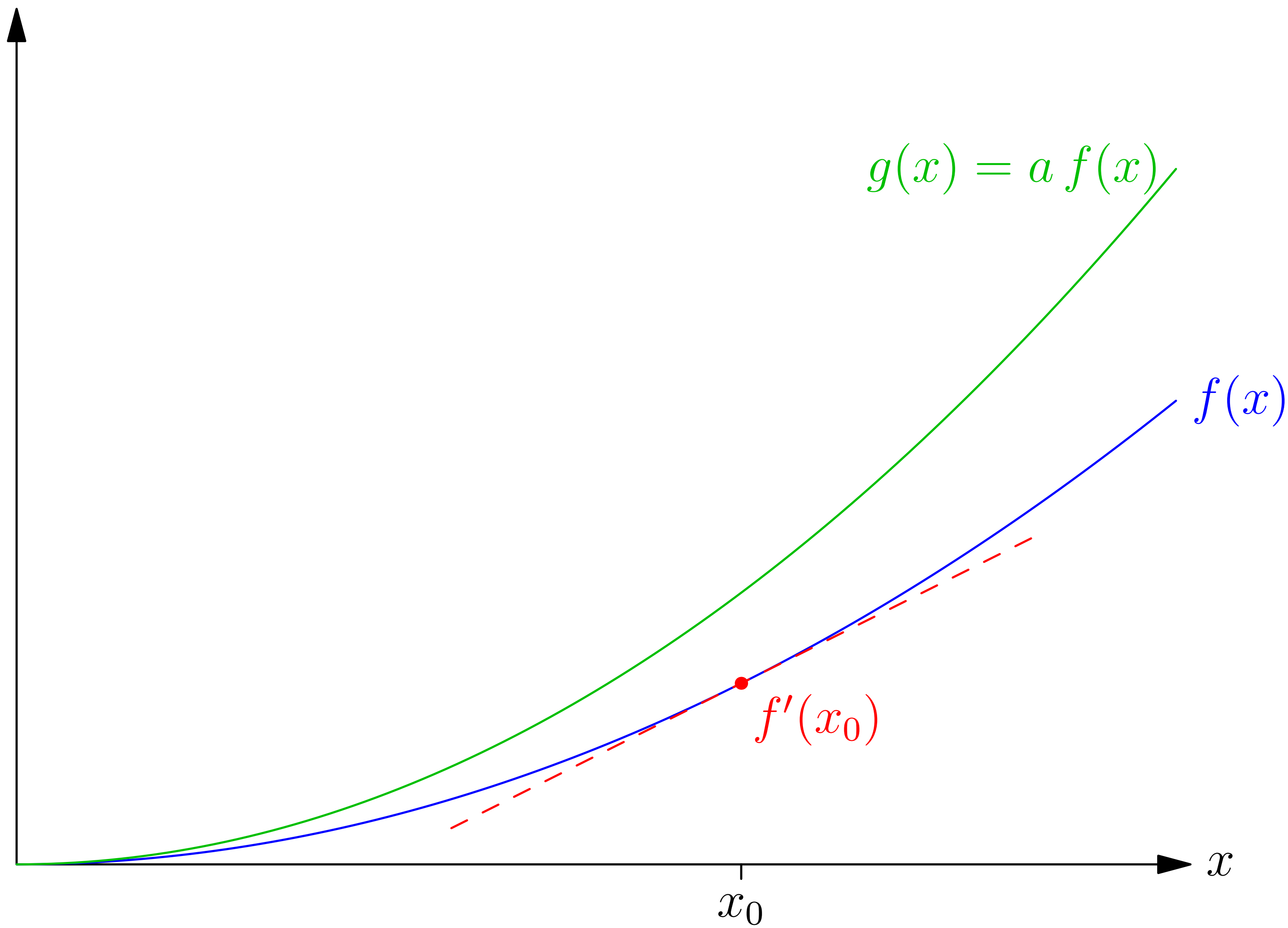

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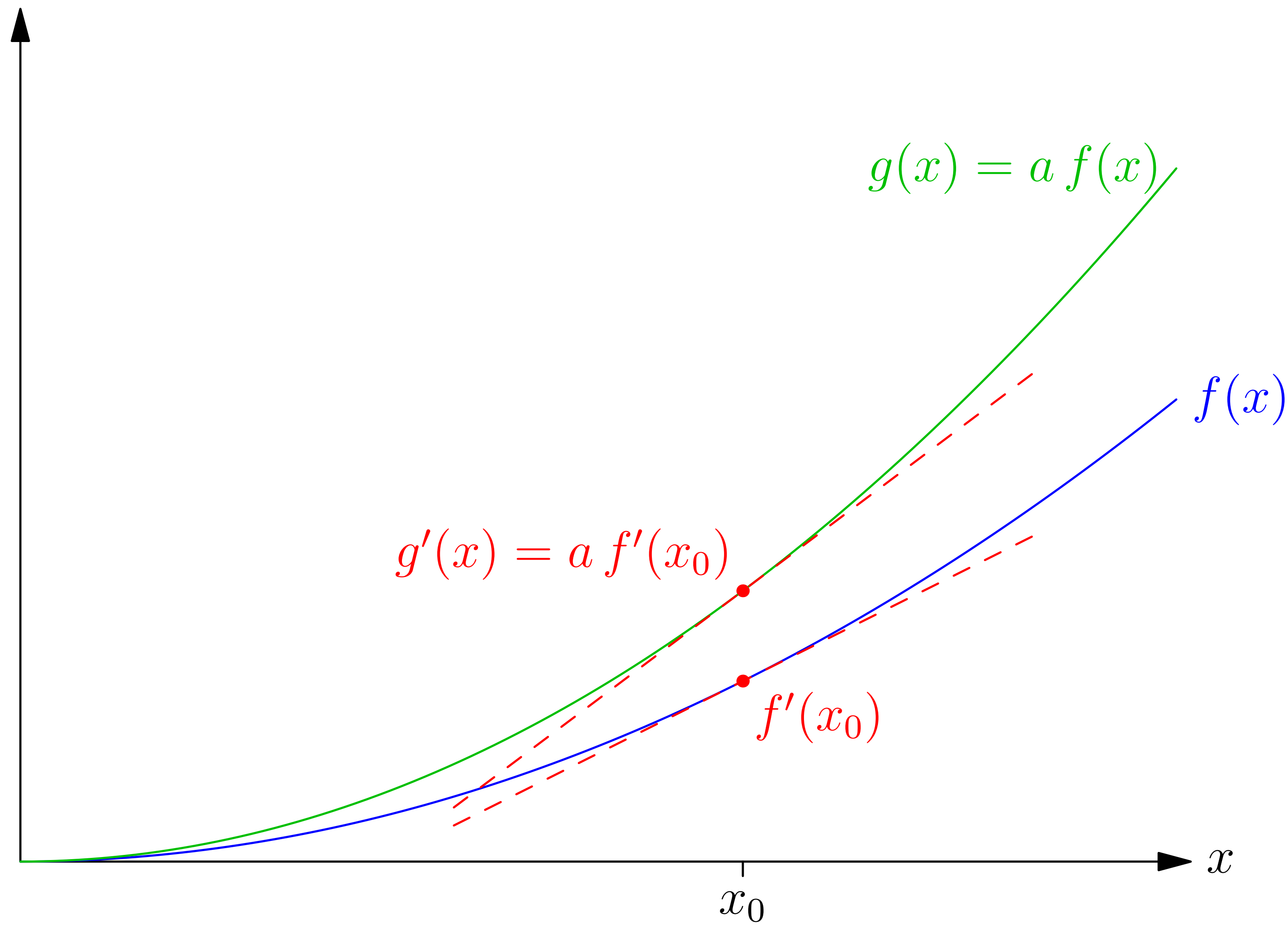

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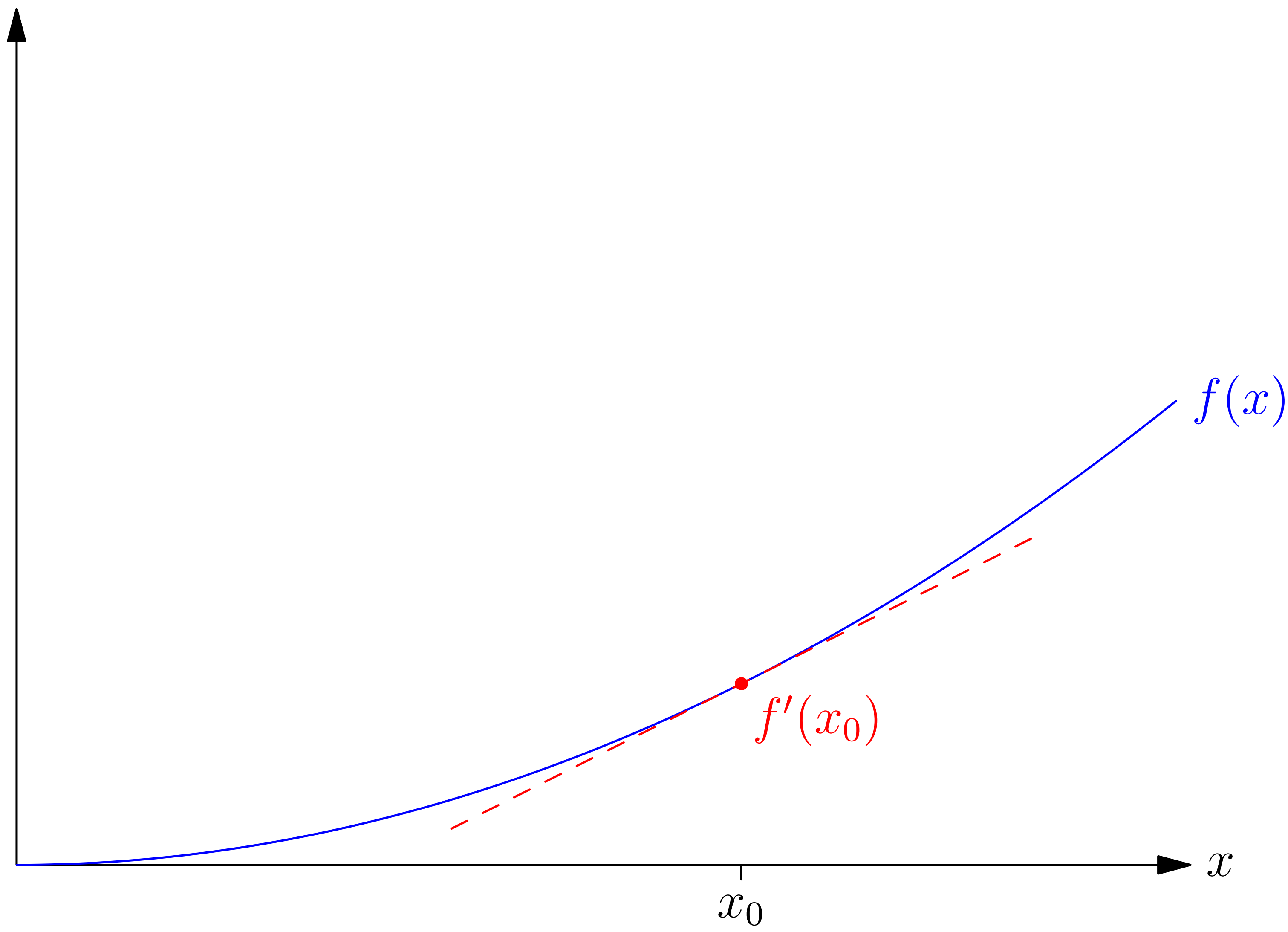

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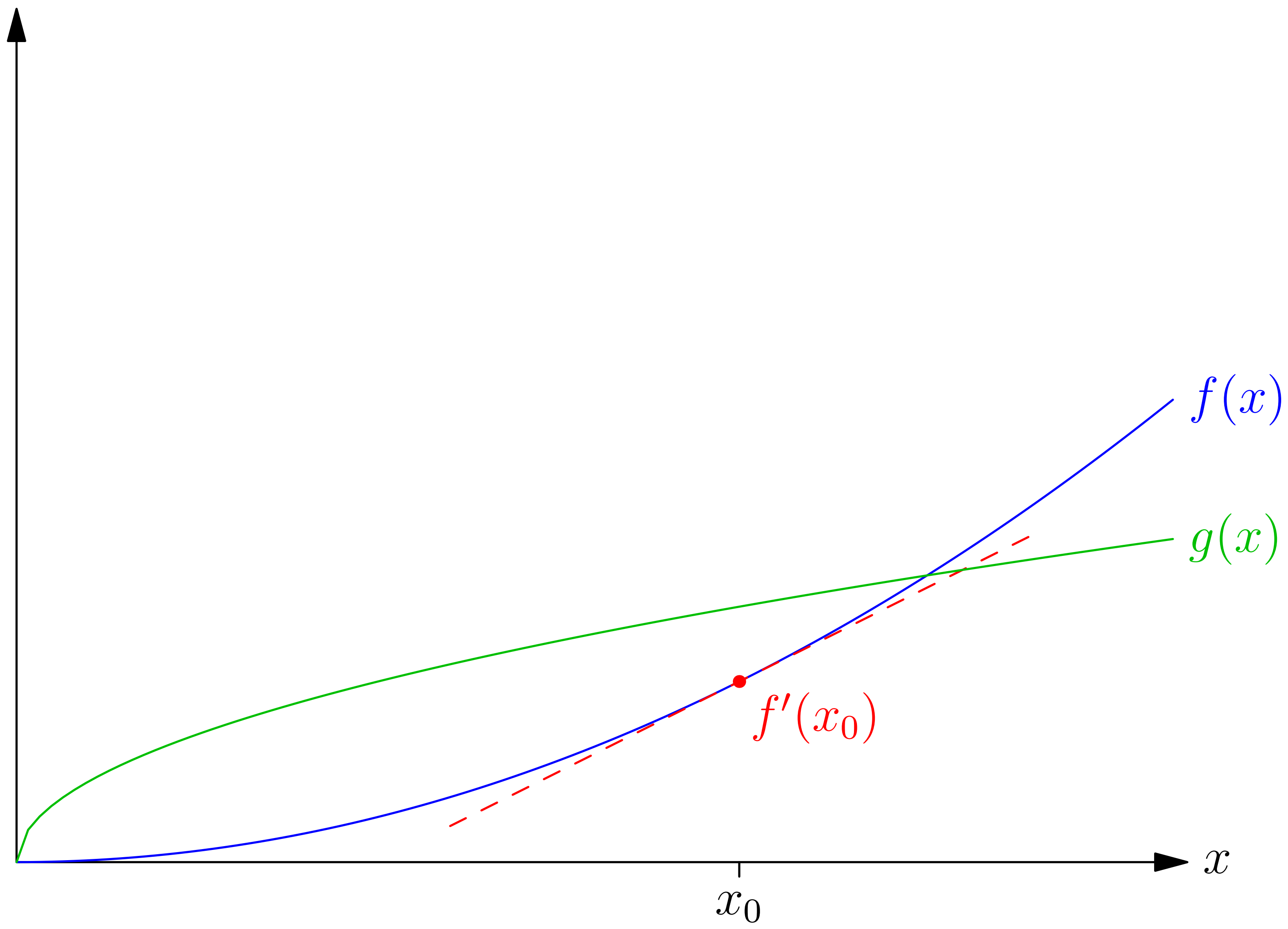

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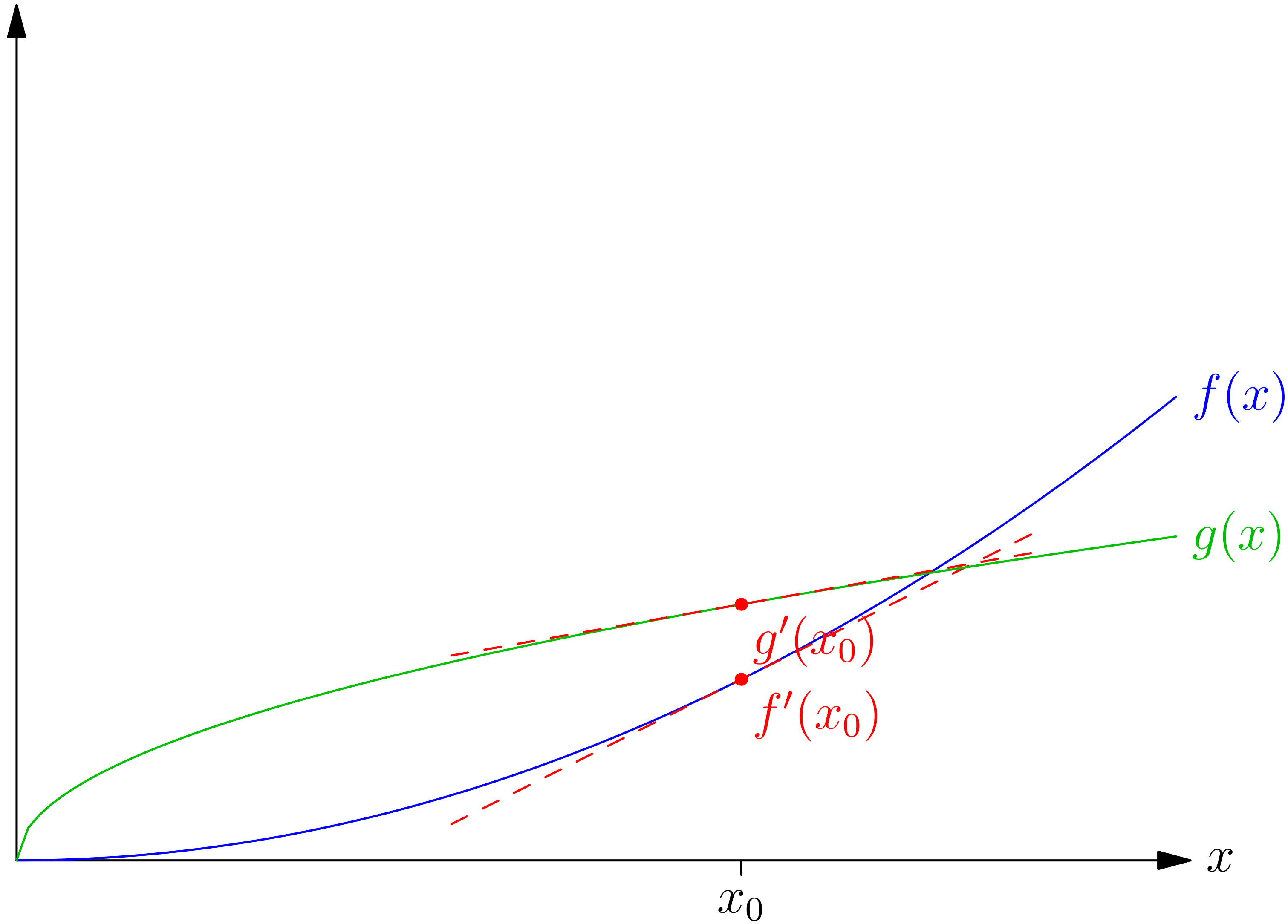

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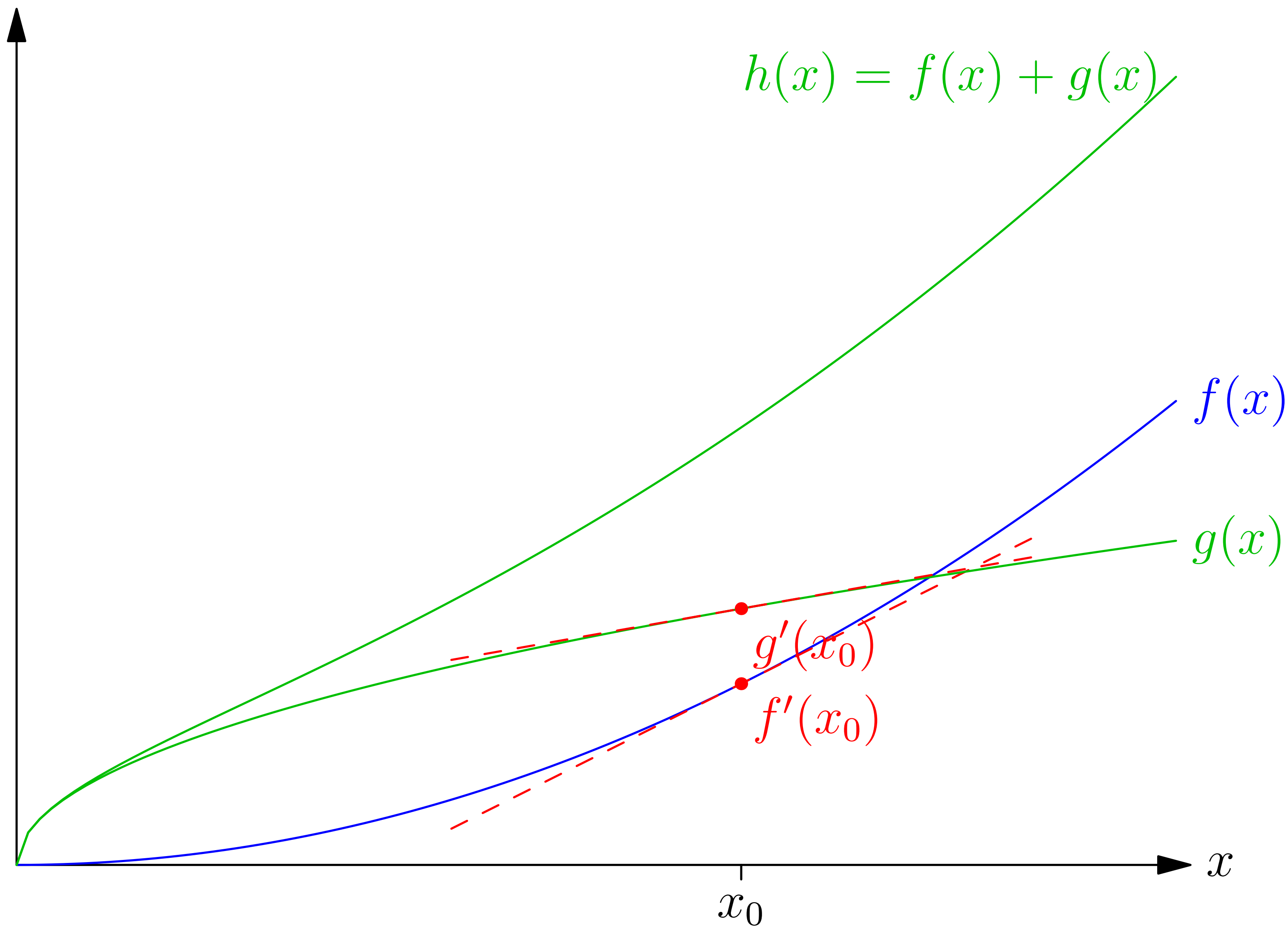

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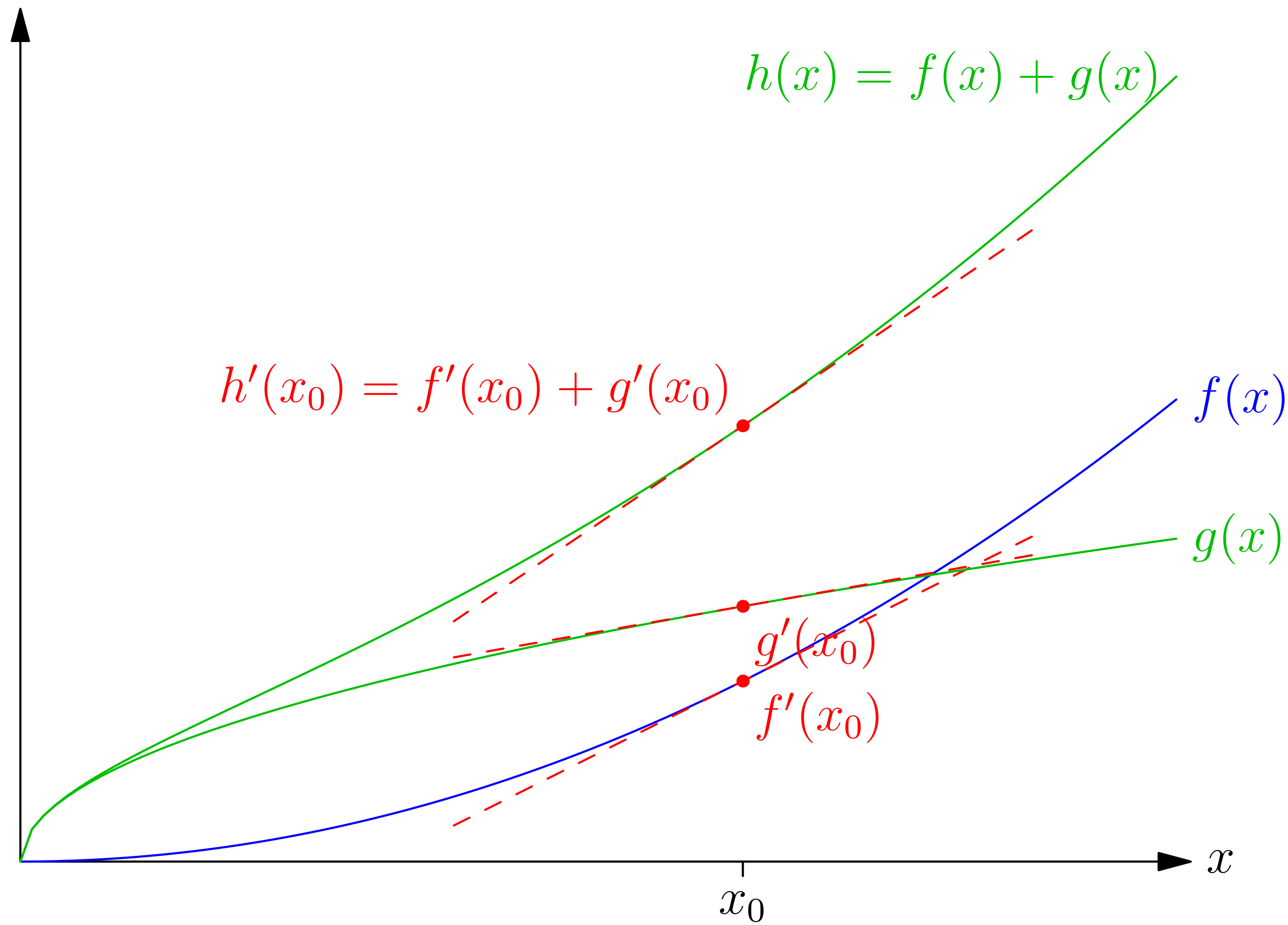

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- This is the **product rule**

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- This is the famous **chain rule**. Together with the product rule it means you can differentiate almost everything

More on chain rules

- We can also write the chain rule as

$$\frac{\mathrm{d}f(g(x))}{\mathrm{d}x} = \frac{\mathrm{d}f(g)}{\mathrm{d}g}\frac{\mathrm{d}g(x)}{\mathrm{d}x}$$

- Sometimes this is neater or easier to remember

$$\frac{\mathrm{d}e^{\cos(x^2)}}{\mathrm{d}x} = \frac{\mathrm{d}e^{\cos(x^2)}}{\mathrm{d}\cos(x^2)}\frac{\mathrm{d}\cos(x^2)}{\mathrm{d}x^2}\frac{\mathrm{d}x^2}{\mathrm{d}x}$$

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$$\begin{aligned} \frac{\mathrm{d} \mathrm{e}^{\cos(x^2)}}{\mathrm{d} x} &= \frac{\mathrm{d} \mathrm{e}^{\cos(x^2)}}{\mathrm{d} \cos(x^2)} \frac{\mathrm{d} \cos(x^2)}{\mathrm{d} x^2} \frac{\mathrm{d} x^2}{\mathrm{d} x} \\ &= \mathrm{e}^{\cos(x^2)} \left(-\sin(x^2)\right) 2x \\ &= -2x \sin(x^2) \mathrm{e}^{\cos(x^2)} \end{aligned}$$

Inverse functions

- Suppose $g(y) = f^{-1}(y)$ is the inverse of $f(x)$ in the sense that $g(f(x)) = f^{-1}(f(x)) = x$

- Using the chain rule

$$\frac{\mathrm{d}g(f(x))}{\mathrm{d}x} = f'(x)g'(f(x))$$

- So $g'(f(x)) = 1/f'(x)$

- Writing $y = f(x)$ so that $x = f^{-1}(y) = g(y)$ we find $g'(y) = 1/f'(g(y))$ that is

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$$\frac{\mathrm{d}g(f(x))}{\mathrm{d}x} = f'(x)g'(f(x)) = 1$$

since $g(f(x)) = x$

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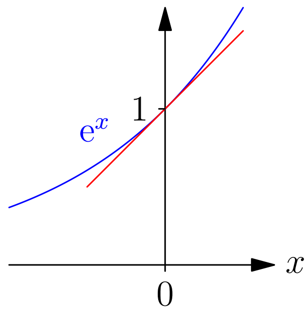

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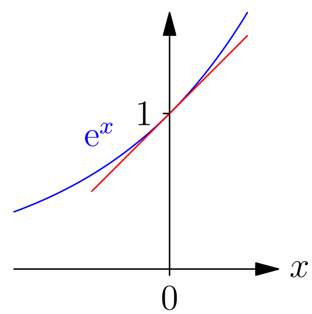

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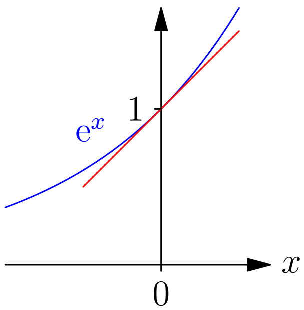

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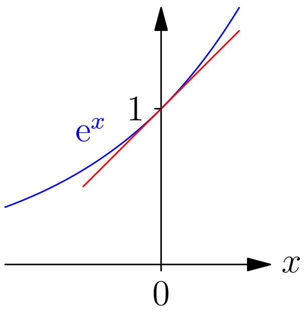

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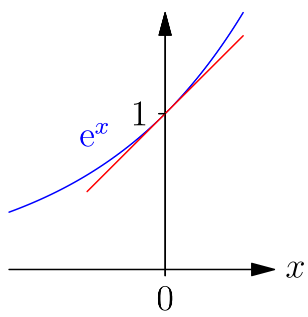

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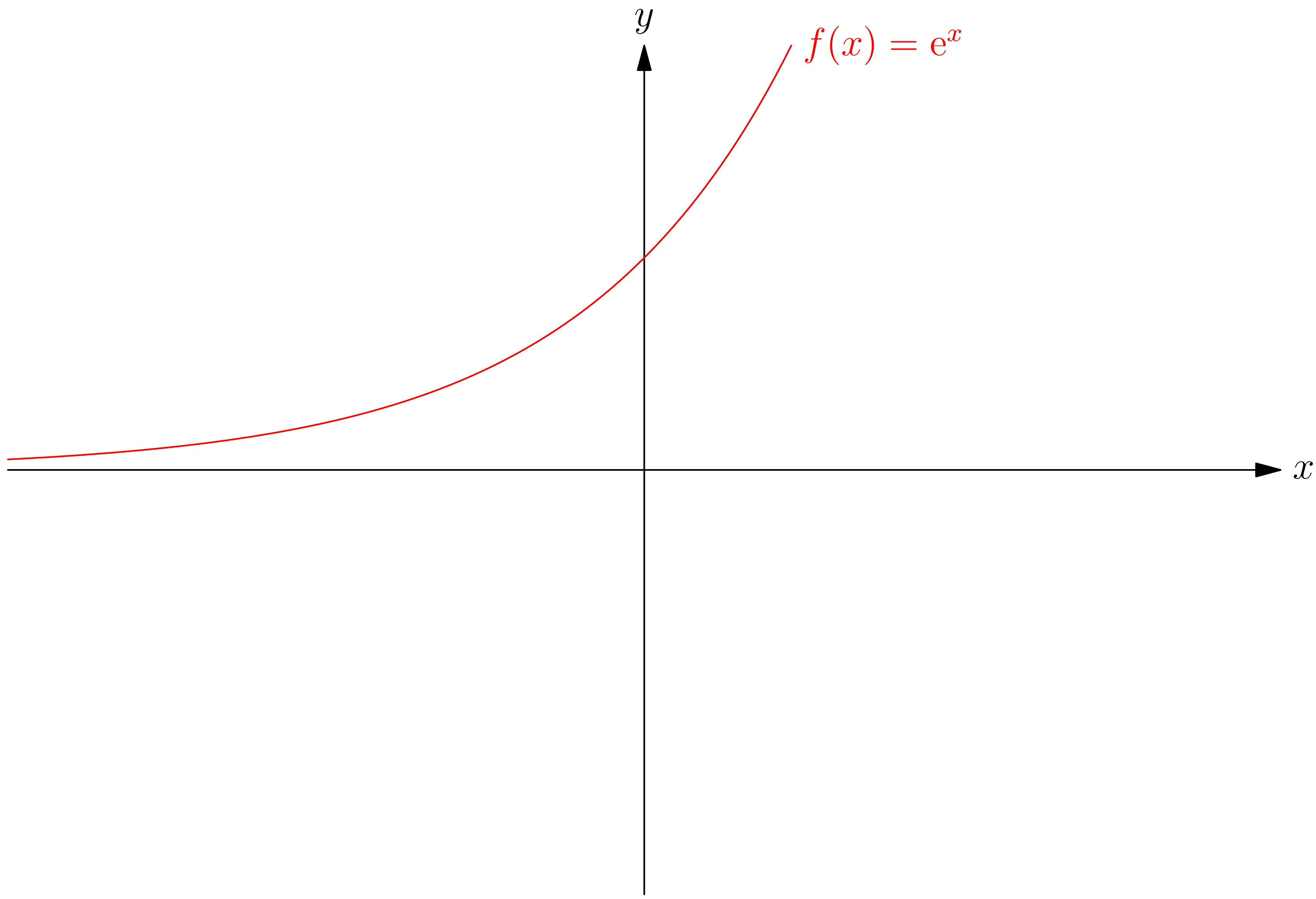
Exponentials and Logarithms



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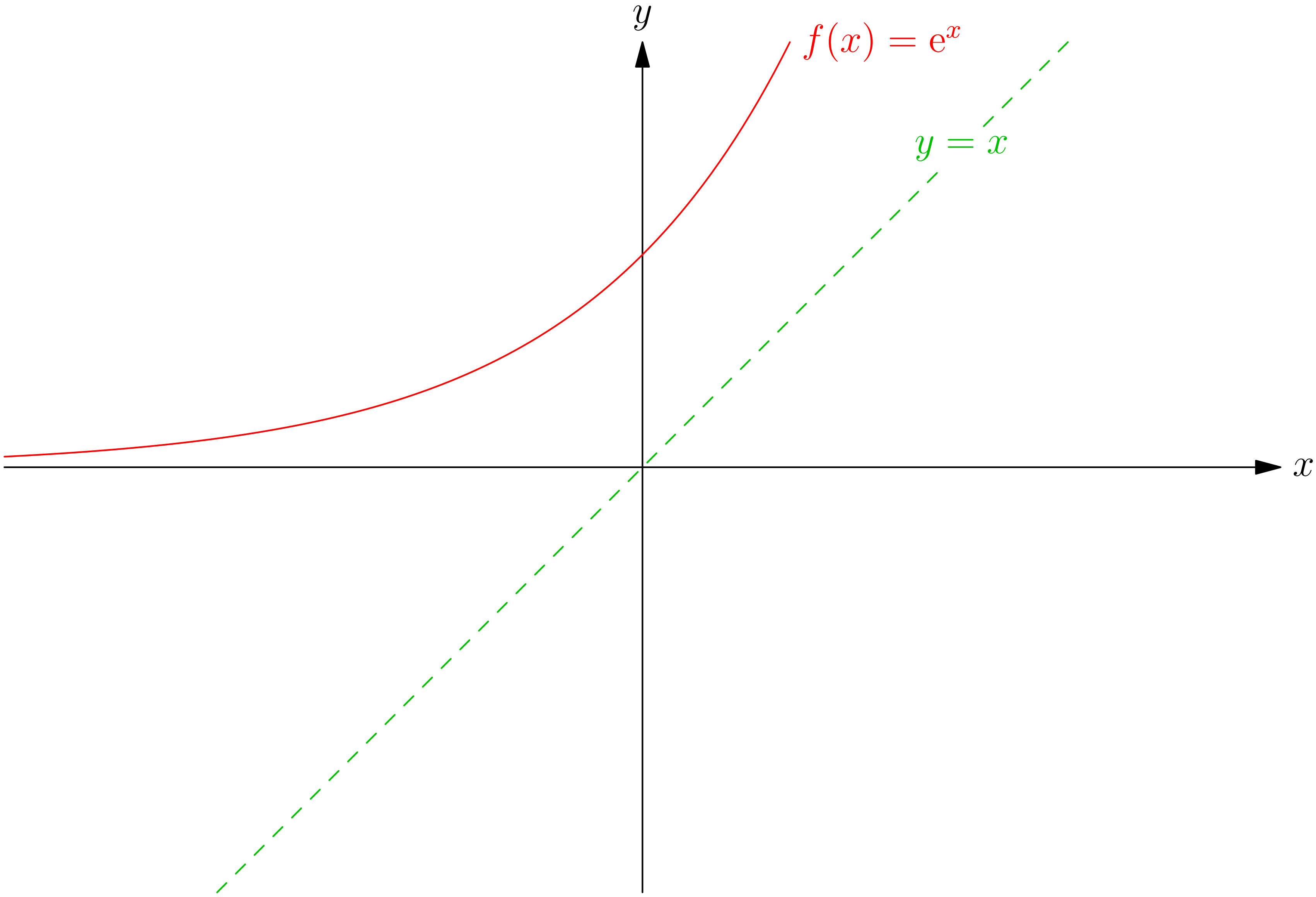

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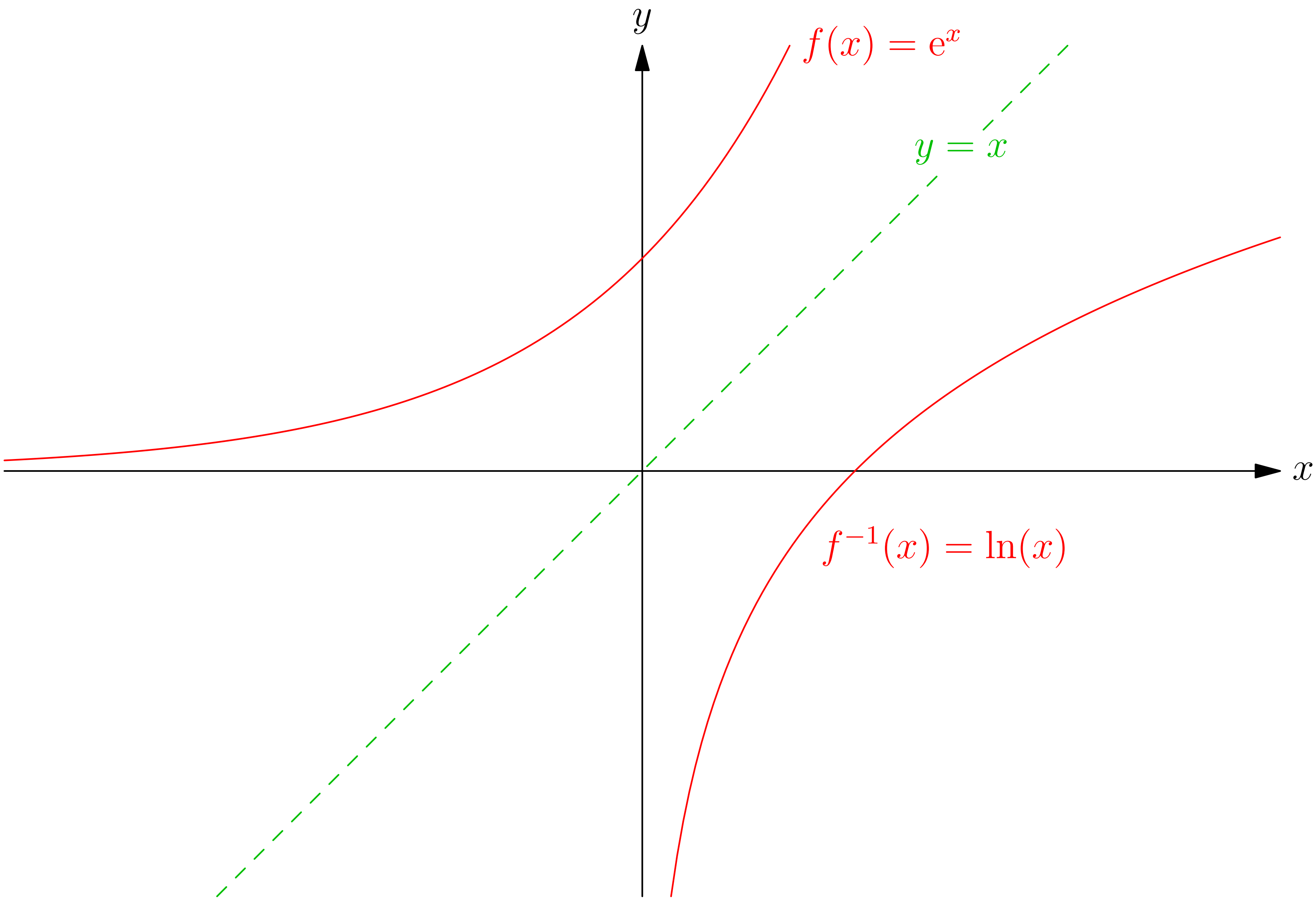

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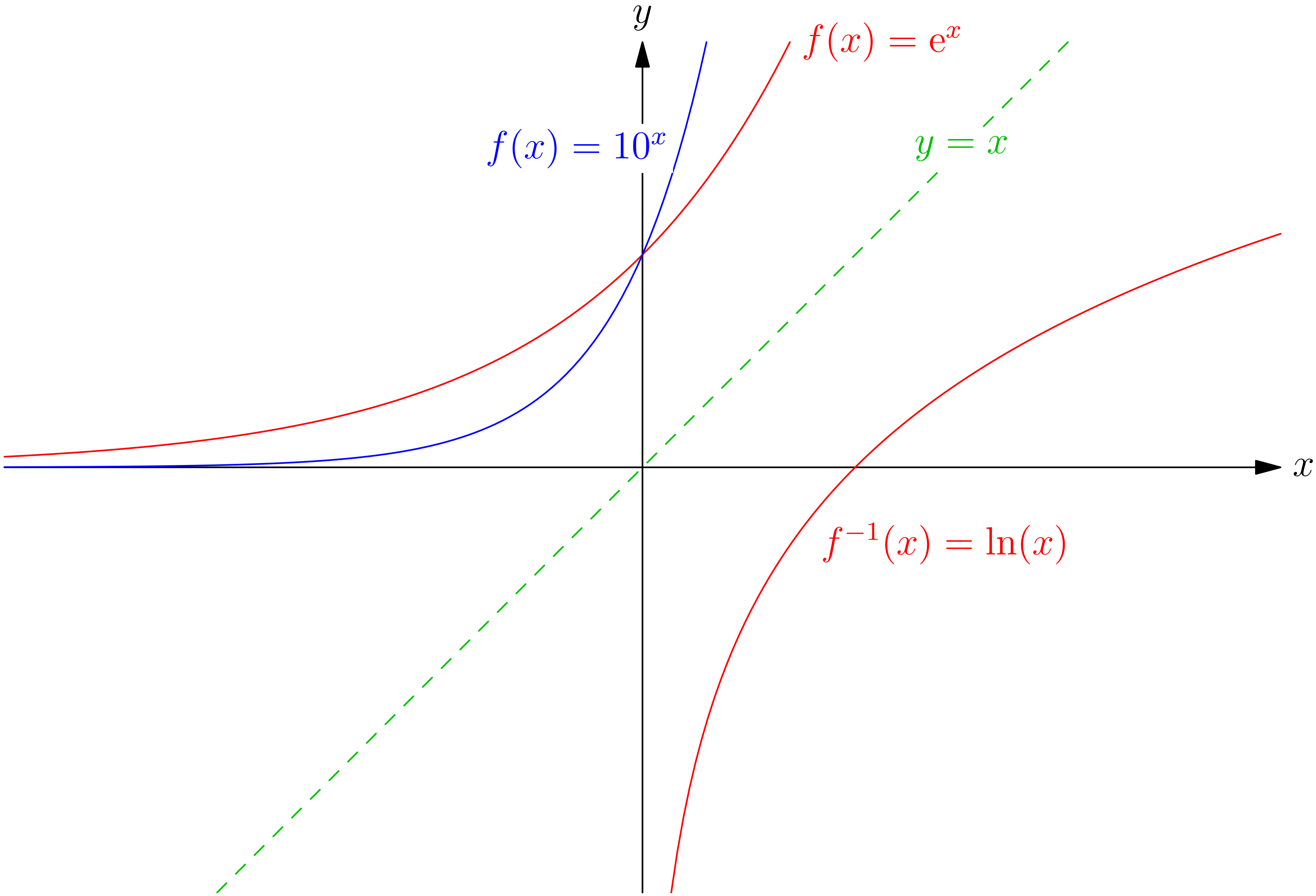

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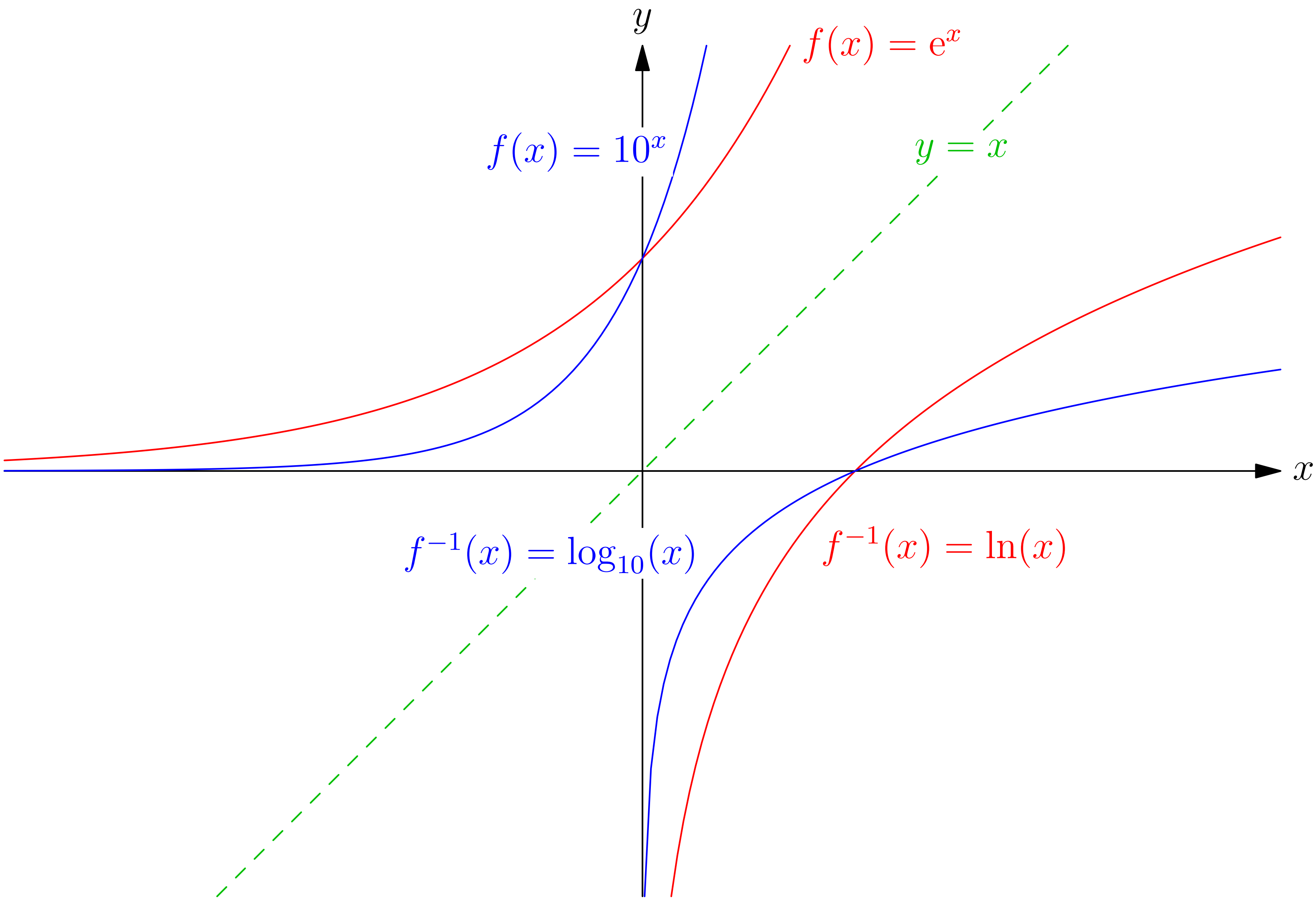

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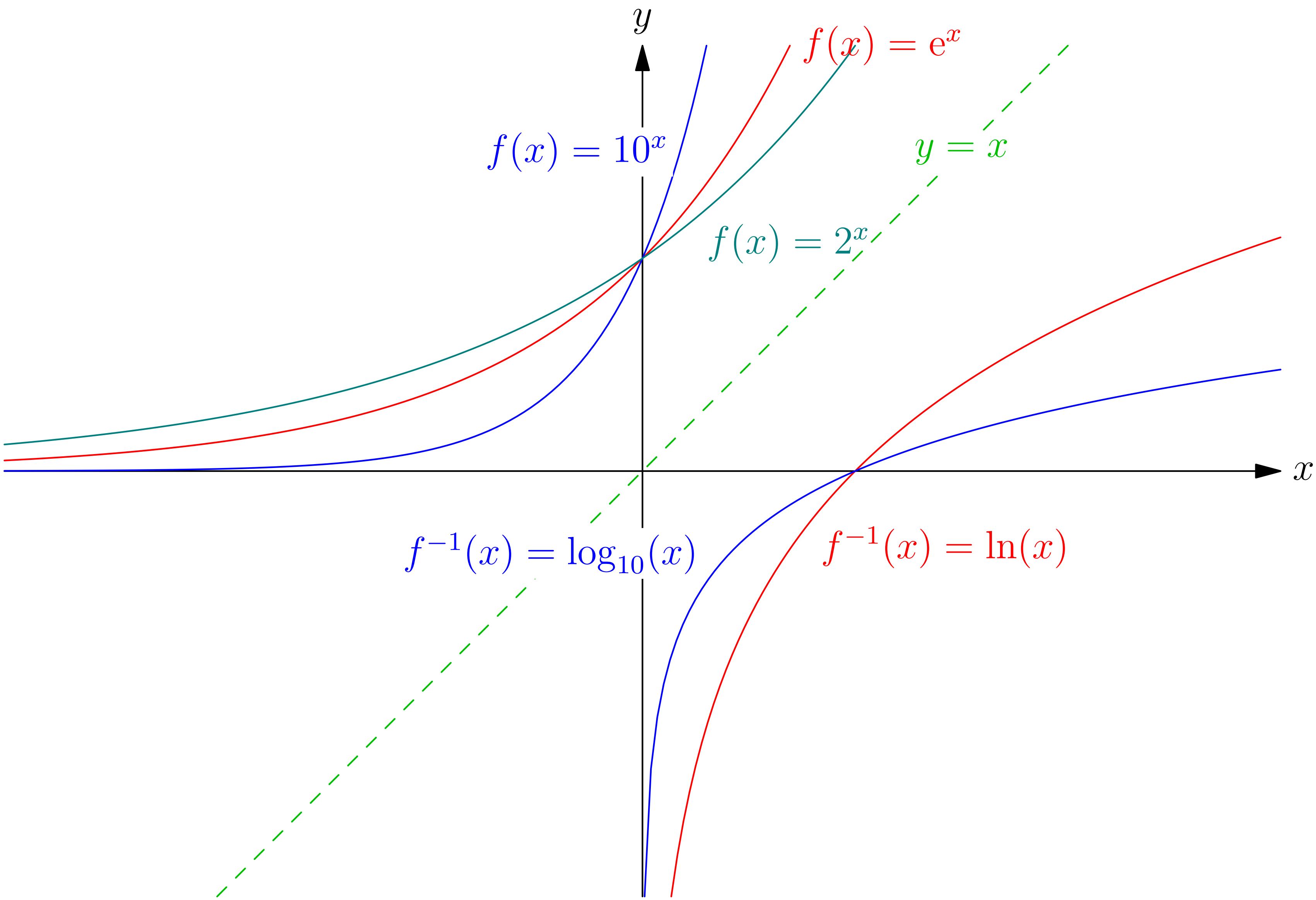

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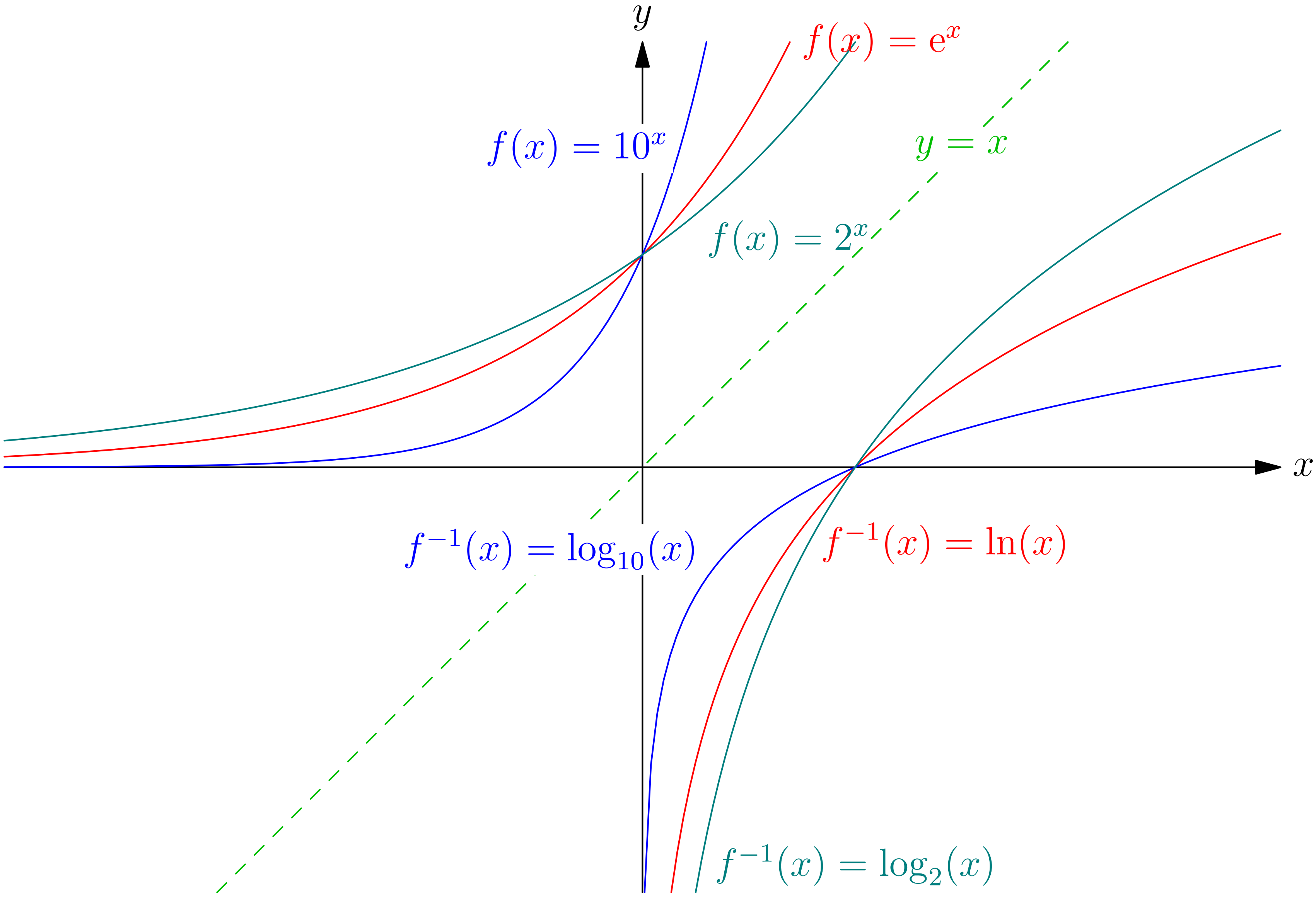
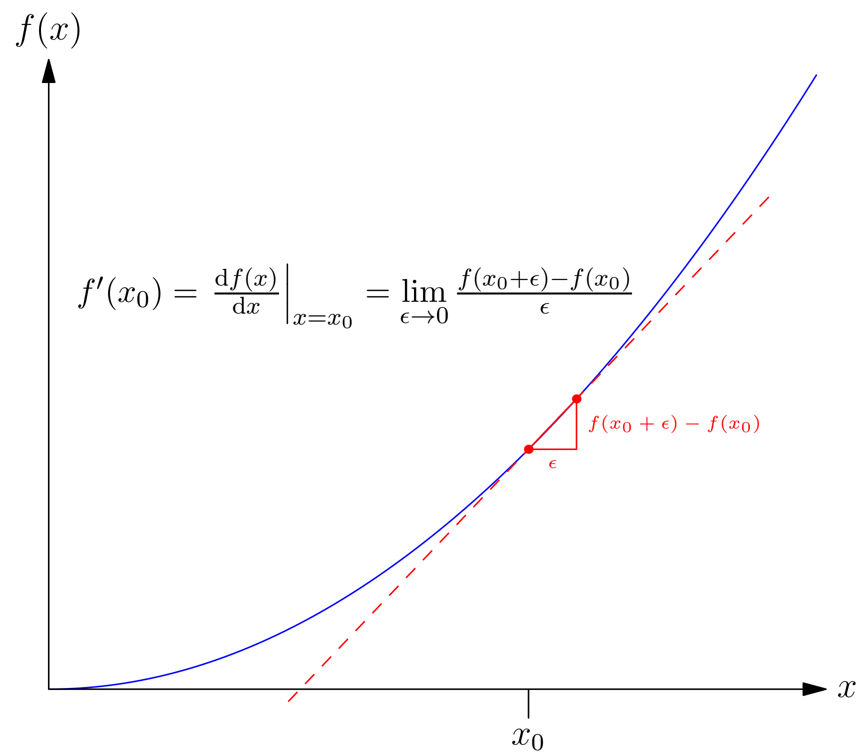


Outline

1. Why Calculus?
2. Differentiation
3. **Vector and Matrix Calculus**



Derivatives in High Dimensions

- When working with functions $f : \mathbb{R}^n \to \mathbb{R}$ in many dimensions then there will typically be different derivative in different directions

- To compute the derivative in a direction $\boldsymbol{u} \in \mathbb{R}^n$ (where $\|\boldsymbol{u}\| = 1$) at a point $\boldsymbol{x} \in \mathbb{R}^n$ we use

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then $g_i(\boldsymbol{x}) = \frac{\partial f(\boldsymbol{x})}{\partial x_i}$

- Recall we defined the vector of first order derivatives of $f(\boldsymbol{x})$ to be the gradient

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This is the start of the high-dimensional Taylor expansion

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- We can compute the gradient by writing out $f(\boldsymbol{x})$ componentwise and performing the partial derivative with respect to x_i

$$\boldsymbol{\nabla} \boldsymbol{w}^{\mathsf{T}} \mathbf{M} \boldsymbol{w}$$

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- It is tedious to compute these things component-wise, but when you need to understand what is going on then go back to the basics

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- Consider $f(\boldsymbol{x}) = \boldsymbol{x}^{\mathsf{T}} \mathbf{M} \boldsymbol{x} + \boldsymbol{a}^{\mathsf{T}} \boldsymbol{x}$

$$\begin{aligned} f(\boldsymbol{x} + \epsilon \boldsymbol{u}) &= (\boldsymbol{x} + \epsilon \boldsymbol{u})^{\mathsf{T}} \mathbf{M} (\boldsymbol{x} + \epsilon \boldsymbol{u}) + \boldsymbol{a}^{\mathsf{T}} (\boldsymbol{x} + \epsilon \boldsymbol{u}) \\ &= f(\boldsymbol{x}) + \epsilon \big(\boldsymbol{u}^{\mathsf{T}} \mathbf{M} \boldsymbol{x} + \boldsymbol{x}^{\mathsf{T}} \mathbf{M} \boldsymbol{u} + \boldsymbol{a}^{\mathsf{T}} \boldsymbol{u} \big) + O(\epsilon^2) \end{aligned}$$

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using $\boldsymbol{x}^\mathsf{T} \mathbf{M} \boldsymbol{u} = \boldsymbol{u}^\mathsf{T} \mathbf{M}^\mathsf{T} \boldsymbol{x}$ and $\boldsymbol{a}^\mathsf{T} \boldsymbol{u} = \boldsymbol{u}^\mathsf{T} \boldsymbol{a}$

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- But $f(\boldsymbol{x} + \epsilon \boldsymbol{u}) = f(\boldsymbol{x}) + \epsilon \boldsymbol{u}^\mathsf{T} \boldsymbol{\nabla} f(\boldsymbol{x}) + O(\epsilon^2)$ so

$$\boldsymbol{\nabla} f(\boldsymbol{x}) = \mathbf{M} \boldsymbol{x} + \mathbf{M}^\mathsf{T} \boldsymbol{x} + \boldsymbol{a}$$

Differentiating Matrices

- Often we have loss functions with respect to a matrix $\boldsymbol{W}$, e.g.

$$L(\boldsymbol{W}) = (\boldsymbol{a}^{\mathsf{T}}\boldsymbol{W}\boldsymbol{b} - c)^2$$

- We might want to find the minimum with respect to $\boldsymbol{W}$

- This occurs at a point $\boldsymbol{W}^*$ where $L(\boldsymbol{W})$ does not increase as we change $\boldsymbol{W}$ in any way

- That is, we seek a $\boldsymbol{W}^*$ such that, for any matrices $\mathbf{U}$

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Generalised Gradient

- We can generalise the idea of gradient to matrices

$$\frac{\partial L(\mathbf{W})}{\partial \mathbf{W}} = \begin{pmatrix} \frac{\partial L(\mathbf{W})}{\partial W_{11}} & \frac{\partial L(\mathbf{W})}{\partial W_{12}} & \cdots & \frac{\partial L(\mathbf{W})}{\partial W_{1m}} \\ \frac{\partial L(\mathbf{W})}{\partial W_{21}} & \frac{\partial L(\mathbf{W})}{\partial W_{22}} & \cdots & \frac{\partial L(\mathbf{W})}{\partial W_{2m}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial L(\mathbf{W})}{\partial W_{n1}} & \frac{\partial L(\mathbf{W})}{\partial W_{n2}} & \cdots & \frac{\partial L(\mathbf{W})}{\partial W_{nm}} \end{pmatrix}$$

- From an identical argument we used for vectors

$$L(\mathbf{W} + \epsilon \mathbf{U}) = L(\mathbf{W}) + \epsilon \operatorname{tr} \mathbf{U}^{\mathsf{T}} \frac{\partial L(\mathbf{W})}{\partial \mathbf{W}} + O(\epsilon^2)$$

where

$$\operatorname{tr} \mathbf{U}^{\mathsf{T}} \mathbf{G} = \sum_i \left[\mathbf{U}^{\mathsf{T}} \mathbf{G} \right]_{ii} = \sum_{ij} U_{ji} G_{ji} = \sum_{ij} U_{ij} G_{ij} = \langle \mathbf{U}, \mathbf{G} \rangle$$

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Example

- Suppose

$$L(\boldsymbol{W}) = \left(\boldsymbol{a}^{\mathsf{T}} \boldsymbol{W} \boldsymbol{b} - c\right)^2$$

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Thus $\frac{\partial L(\mathbf{W})}{\partial \mathbf{W}} = 2\left(\boldsymbol{a}^\mathsf{T}\mathbf{W}\boldsymbol{b} - c\right)\boldsymbol{a}\boldsymbol{b}^\mathsf{T}$

Traces

- The trace of a matrix is the sum of its diagonal elements

$$\mathrm{tr}\boldsymbol{A} = \mathrm{tr}\boldsymbol{A}^{\mathsf{T}} = \sum_i A_{ii}$$

- Clearly $\mathrm{tr}\, c\boldsymbol{A} = c\,\mathrm{tr}\boldsymbol{A}$

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Quick Matrix Differentiation

- Let

$$\partial_{\mathbf{U}} f(\mathbf{X}) = \lim_{\epsilon \to 0} \frac{f(\mathbf{X} + \epsilon \mathbf{U}) - f(\mathbf{X})}{\epsilon}$$

- E.g.

$$\begin{aligned} \partial_{\mathbf{U}} \mathrm{tr} \mathbf{A} \mathbf{X} \mathbf{B} &= \lim_{\epsilon \to 0} \frac{1}{\epsilon} \mathrm{tr} \mathbf{A} \left(\mathbf{X} + \epsilon \mathbf{U} \right) \mathbf{B} - \mathrm{tr} \mathbf{A} \mathbf{X} \mathbf{B} \\ &= \mathrm{tr}\, \mathbf{A} \mathbf{U} \mathbf{B} \end{aligned}$$

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&= \operatorname{tr} \mathbf{A}\mathbf{U}\mathbf{B} = \operatorname{tr} \mathbf{B}^{\mathsf{T}}\mathbf{U}^{\mathsf{T}}\mathbf{A}^{\mathsf{T}} = \operatorname{tr} \mathbf{U}^{\mathsf{T}}\mathbf{A}^{\mathsf{T}}\mathbf{B}^{\mathsf{T}}
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thus

$$\frac{\partial \mathrm{tr} \mathbf{A}\mathbf{X}\mathbf{B}}{\partial \mathbf{X}} = \mathbf{A}^{\top}\mathbf{B}^{\top}$$

Log Determinants

- We often come across logarithms of determinants of matrices, $\log(|\mathbf{M}|)$

- For GP we want to choose $\mathbf{K}$ to maximise the marginal likelihood, $\log\big(|\mathbf{K} + \sigma^2\mathbf{I}|\big)$

- To find the derivative of $\log(|\mathbf{X}|)$ we consider

$$\log(|\mathbf{X} + \epsilon\mathbf{U}|) = \log\big(|\mathbf{X}(\mathbf{I} + \epsilon\mathbf{X}^{-1}\mathbf{U})|\big)$$

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⋆ Using $|\mathbf{AB}| = |\mathbf{A}||\mathbf{B}|$

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$\star$ Using $|\mathbf{AB}| = |\mathbf{A}||\mathbf{B}|$
$\star$ Using $\log(ab) = \log(a) + \log(b)$

Determinants

$$|\mathbf{I} + \epsilon \mathbf{M}| = \begin{vmatrix} 1 + \epsilon M_{11} & \epsilon M_{12} \\ \epsilon M_{21} & 1 + \epsilon M_{22} \end{vmatrix}$$

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Determinants

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$$|\mathbf{I}+\epsilon\,\mathbf{M}| = \begin{vmatrix} 1+\epsilon\,M_{11} & \text{[redacted]} & & & \\ \text{[redacted]} & 1+\epsilon\,M_{22} & \epsilon\,M_{32} & \epsilon\,M_{42} & \epsilon\,M_{52} \\ & \epsilon\,M_{23} & 1+\epsilon\,M_{33} & \epsilon\,M_{43} & \epsilon\,M_{53} \\ & \epsilon\,M_{24} & \epsilon\,M_{34} & 1+\epsilon\,M_{44} & \epsilon\,M_{54} \\ & \epsilon\,M_{25} & \epsilon\,M_{35} & \epsilon\,M_{45} & 1+\epsilon\,M_{55} \end{vmatrix}$$

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Determinants

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Determinants

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Determinants

$$|\mathbf{I}+\epsilon\mathbf{M}| = \begin{vmatrix} 1+\epsilon M_{11} & \epsilon M_{12} \\ \epsilon M_{21} & 1+\epsilon M_{22} \end{vmatrix} = (1+\epsilon M_{11})(1+\epsilon M_{22}) - \epsilon^2 M_{21} M_{12}$$

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$$= (1+\epsilon\,M_{11})\,C_{11}\; -\epsilon\,M_{21}\,C_{21} + \epsilon\,M_{31}\,C_{31} - \epsilon\,M_{41}\,C_{41}$$

Determinants

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$$= (1+\epsilon\, M_{11})\, C_{11} \;-\epsilon\, M_{21}\, C_{21} +\epsilon\, M_{31}\, C_{31} -\epsilon\, M_{41}\, C_{41} +\epsilon\, M_{51}\, C_{51}$$

Determinants

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$$= (1 + \epsilon\, M_{11})\,(1 + \epsilon\, M_{22})\, C'_{22} + O(\epsilon^2)$$

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$$= \prod_i (1 + \epsilon\,M_{ii}) + O(\epsilon^2)$$

Determinants

$$|\mathbf{I} + \epsilon \mathbf{M}| = \begin{vmatrix} 1 + \epsilon M_{11} & \epsilon M_{12} \\ \epsilon M_{21} & 1 + \epsilon M_{22} \end{vmatrix} = (1 + \epsilon M_{11})(1 + \epsilon M_{22}) - \epsilon^2 M_{21} M_{12}$$

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$$= (1 + \epsilon \sum_i M_{ii}) + O(\epsilon^2)$$

Determinants

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$$=(1+\epsilon\ \mathrm{tr}\ \mathbf{M}) + O(\epsilon^2)$$

Putting it Together

- Recall

$$\log(|\mathbf{X} + \epsilon \mathbf{U}|) - \log(|\mathbf{X}|) = \log\big(|\mathbf{I} + \epsilon \mathbf{X}^{-1}\mathbf{U}|\big)$$

Putting it Together

- Recall

$$
\begin{aligned}
\log(|\mathbf{X} + \epsilon\mathbf{U}|) - \log(|\mathbf{X}|) &= \log\big(|\mathbf{I} + \epsilon\mathbf{X}^{-1}\mathbf{U}|\big) \\
&= \log\big(1 + \epsilon \operatorname{tr} \mathbf{X}^{-1}\mathbf{U} + O(\epsilon)^2\big)
\end{aligned}
$$

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\end{aligned}
$$

using $\log(1+x) = x + \frac{x^2}{2} + \cdots$

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&= \epsilon \operatorname{tr} \mathbf{X}^{-1}\mathbf{U} + O(\epsilon)^2 \\
&= \epsilon \operatorname{tr} \mathbf{U}^{\mathsf{T}} \big(\mathbf{X}^{-1}\big)^{\mathsf{T}} + O(\epsilon)
\end{aligned}
$$

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Putting it Together

- Recall

$$\begin{aligned}\log(|\mathbf{X}+\epsilon\mathbf{U}|)-\log(|\mathbf{X}|) &= \log\big(|\mathbf{I}+\epsilon\mathbf{X}^{-1}\mathbf{U}|\big)\\ &= \log\big(1+\epsilon\,\mathrm{tr}\,\mathbf{X}^{-1}\mathbf{U}+O(\epsilon)^2\big)\\ &= \epsilon\,\mathrm{tr}\,\mathbf{X}^{-1}\mathbf{U}+O(\epsilon)^2\\ &= \epsilon\,\mathrm{tr}\,\mathbf{U}^{\mathsf{T}}\big(\mathbf{X}^{-1}\big)^{\mathsf{T}}+O(\epsilon)\end{aligned}$$

using $\log(1+x) = x + \frac{x^2}{2} + \cdots$

- Thus $\partial_{\mathbf{U}}\log(|\mathbf{X}|) = \mathrm{tr}\,\mathbf{U}^{\mathsf{T}}\big(\mathbf{X}^{-1}\big)^{\mathsf{T}}$

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$$
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&= \epsilon \operatorname{tr} \mathbf{X}^{-1}\mathbf{U} + O(\epsilon)^2 \\
&= \epsilon \operatorname{tr} \mathbf{U}^{\mathsf{T}} \big(\mathbf{X}^{-1}\big)^{\mathsf{T}} + O(\epsilon)
\end{aligned}
$$

using $\log(1+x) = x + \frac{x^2}{2} + \cdots$

- Thus $\partial_{\mathbf{U}} \log(|\mathbf{X}|) = \operatorname{tr} \mathbf{U}^{\mathsf{T}} \big(\mathbf{X}^{-1}\big)^{\mathsf{T}}$

- Or

$$
\frac{\partial \log(|\mathbf{X}|)}{\partial \mathbf{X}} = \big(\mathbf{X}^{-1}\big)^{\mathsf{T}}
$$

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- With care you can differentiate most expressions
- The chain and product rule are incredibly powerful tools
- We can generalise differentiation to vectors and matrices
- There are a number of surprisingly useful results

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- Next stop: integration