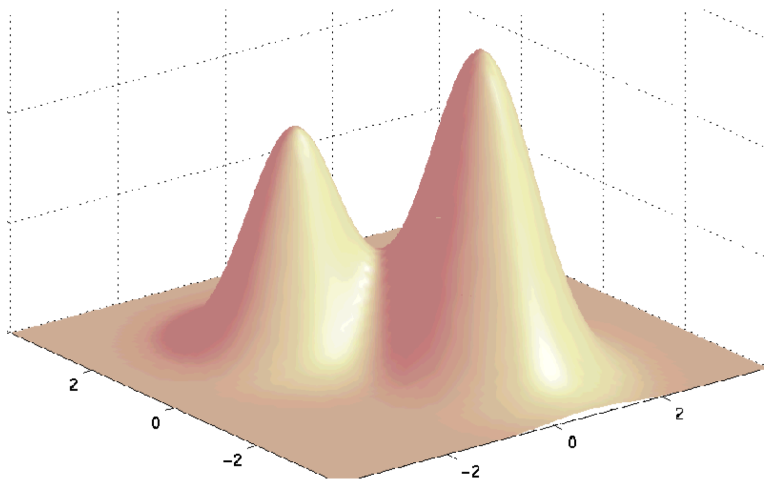
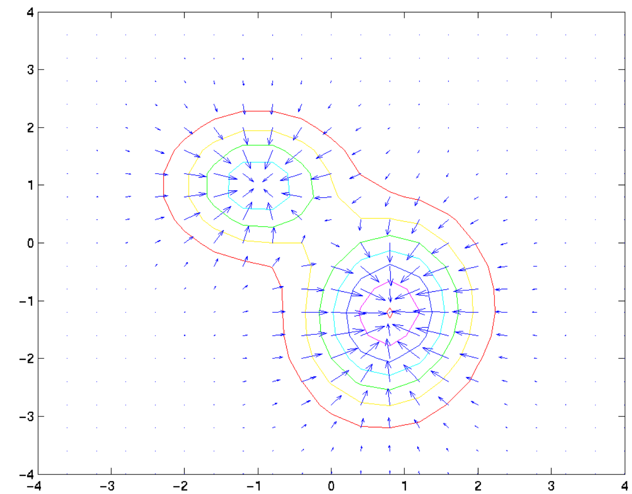
Advanced Machine Learning

Optimisation



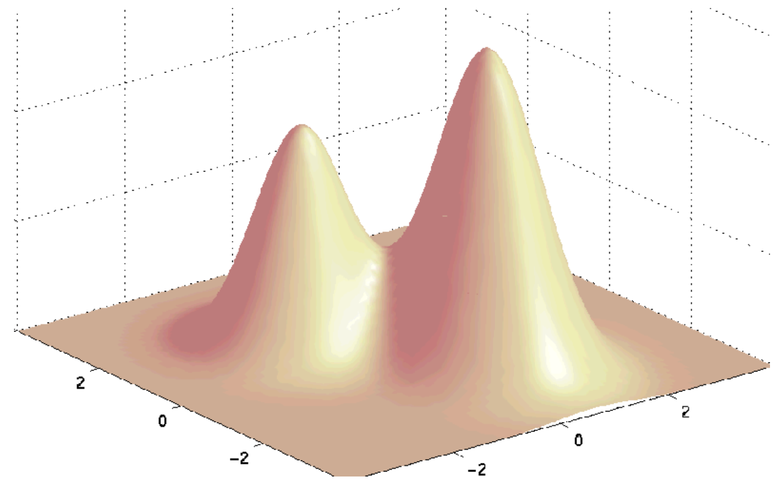


$$z = \mathrm{e}^{-(x+1)^2-(y-1)^2} + 0.6\mathrm{e}^{-(x-1)^2-0.5(y+1)^2+0.1(x-3)(y-3)}$$

Gradient descent, quadratic minima, differing length scales

Outline

1. **Motivation**
2. Gradient Descent
3. Why Gradient Descent is Difficult



ML = Optimisation

- Many learning machines can be thought of as functions of the form
$$\hat{y} = f(\boldsymbol{x}|\boldsymbol{w})$$
(or more generally $\hat{\boldsymbol{y}} = \boldsymbol{f}(\boldsymbol{x}|\boldsymbol{w})$)

- Given an input pattern (set of features) $\boldsymbol{x}$ the learning machine makes a prediction $\hat{y}$

- We try to choose the parameters $\boldsymbol{w}$ so that the predictions are good

- In practice training a learning machine comes down to optimising some loss function

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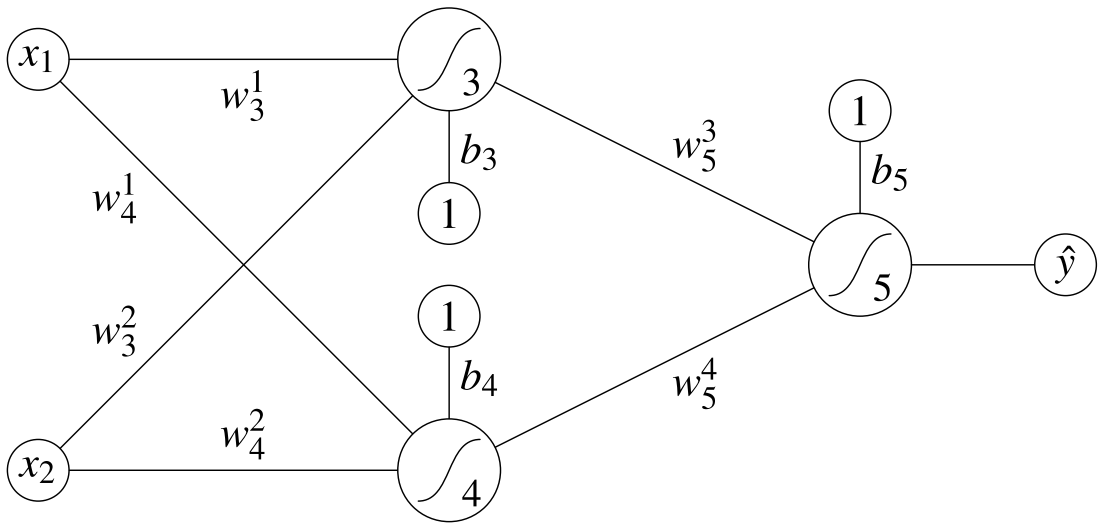
MLP

- We can depict a neural network such as an MLP by a diagram



- Stands for the function $(\hat{y} = f(\boldsymbol{x}|\boldsymbol{w}))$

$$\hat{y} = g\big(w_5^3 g(w_3^1 x_1 + w_3^2 x_2 + b_3) + w_5^4 g(w_4^1 x_1 + w_4^2 x_2 + b_4) + b_5\big)$$

where, for example, $g(V) = \frac{1}{1+\mathrm{e}^{-V}}$

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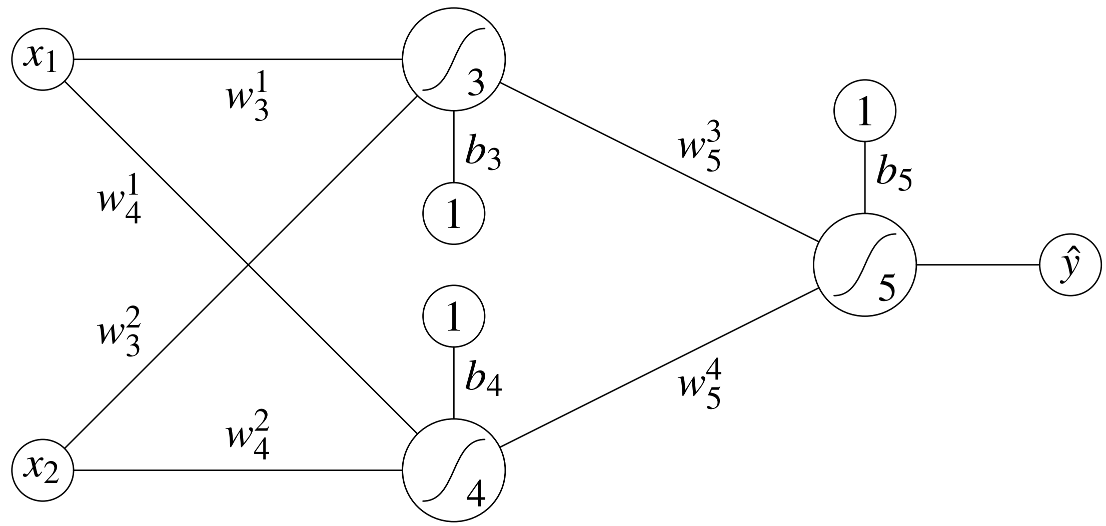

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Training

- Given a (labelled) training dataset

$$\mathcal{D} = \left\{ (\boldsymbol{x}_k, y_k) \middle| k = 1, \ldots, m \right\}$$

- We define an error or loss function that we want to minimise

$$L(\boldsymbol{w}|\boldsymbol{\mathcal{D}}) = \frac{1}{m} \sum_{k=1}^{m} \big(f(\boldsymbol{x}_k|\boldsymbol{w}) - y_k \big)^2$$

- We then use the machine with the weights $\boldsymbol{w}^*$ which minimise $L(\boldsymbol{w}|\mathcal{D})$

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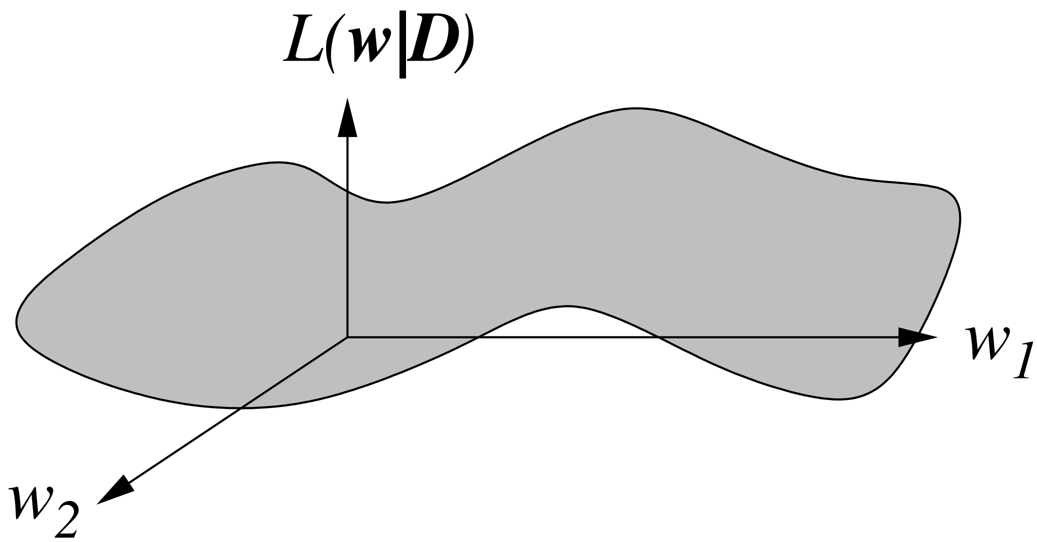
Computing Gradients

- $L(\boldsymbol{w}|\mathcal{D})$ is a complex function of the weights $\boldsymbol{w}$



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- In MLP an efficient algorithm for computing the gradient is known as back-prop

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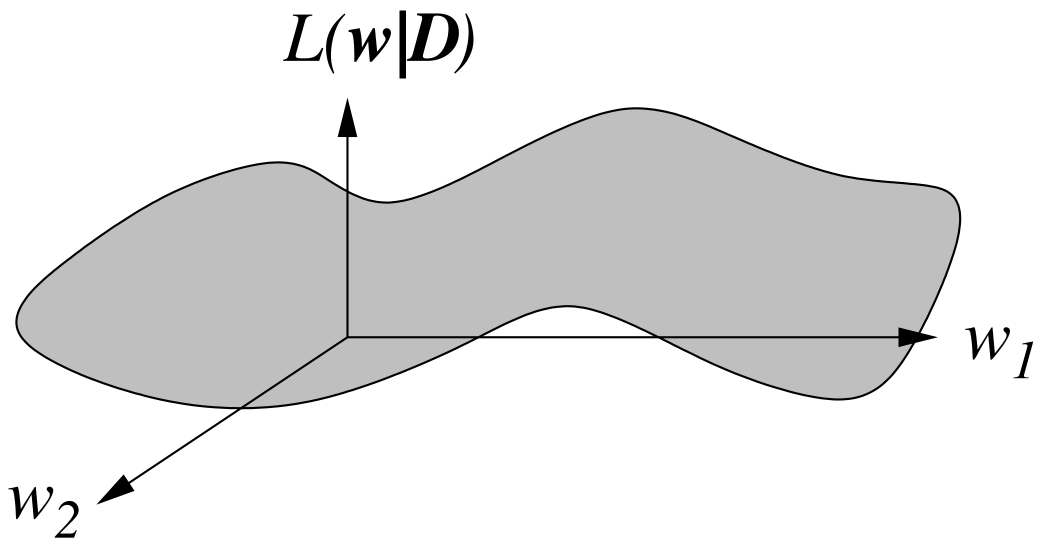

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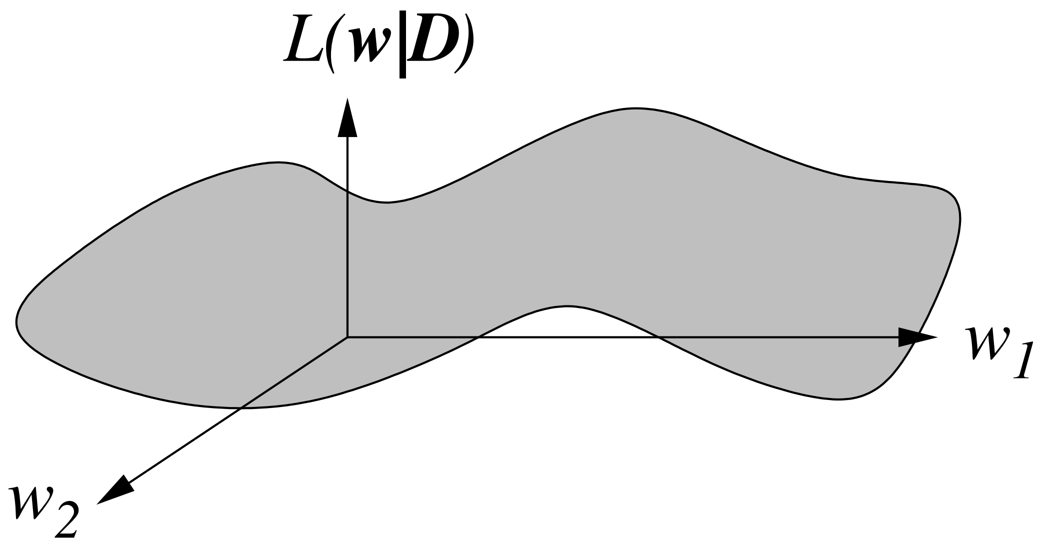

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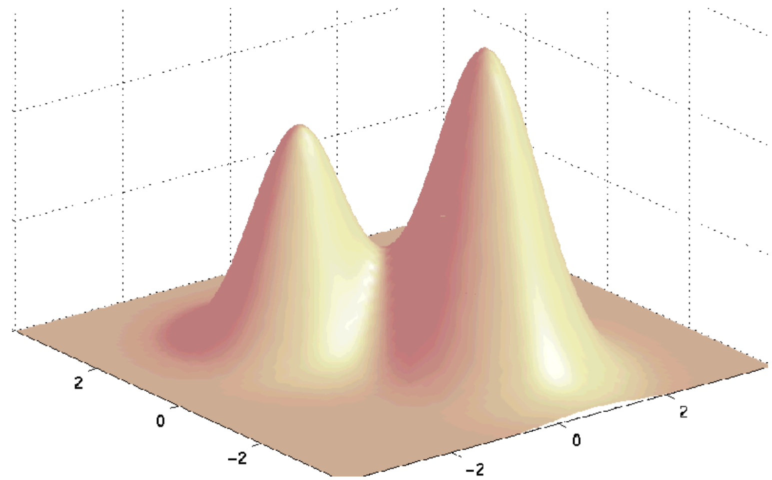

Gradient Optimisation

- A maximum or minimum occurs when $\boldsymbol{\nabla} L(\boldsymbol{w}|\mathcal{D}) = \mathbf{0}$
- E.g.

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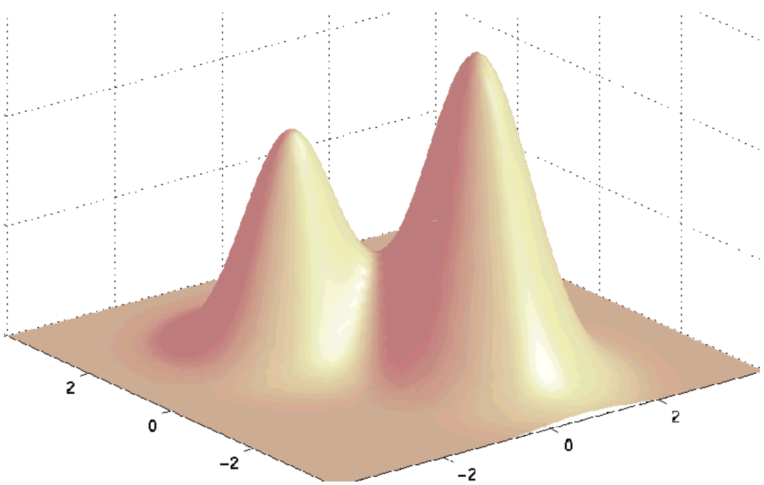

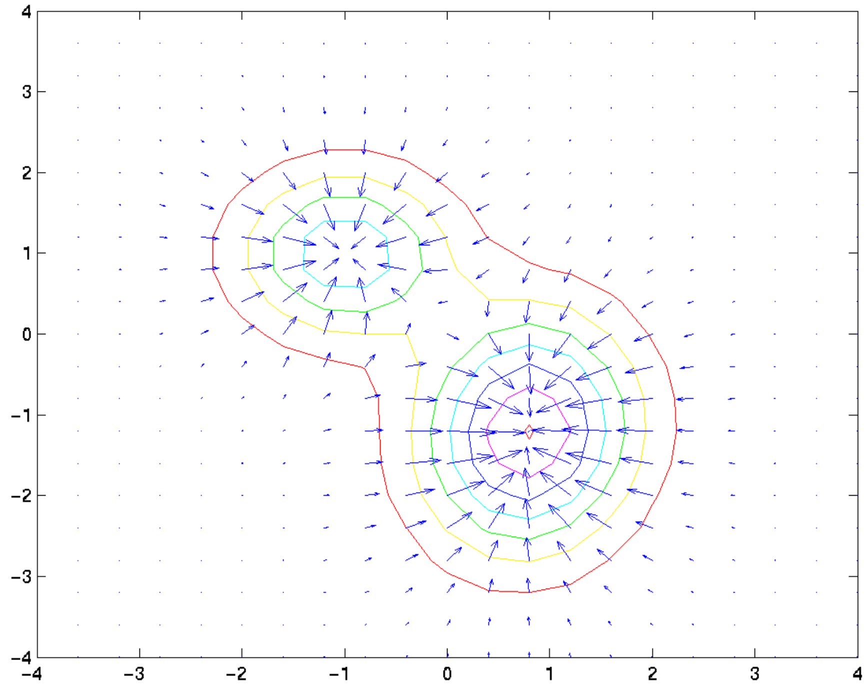

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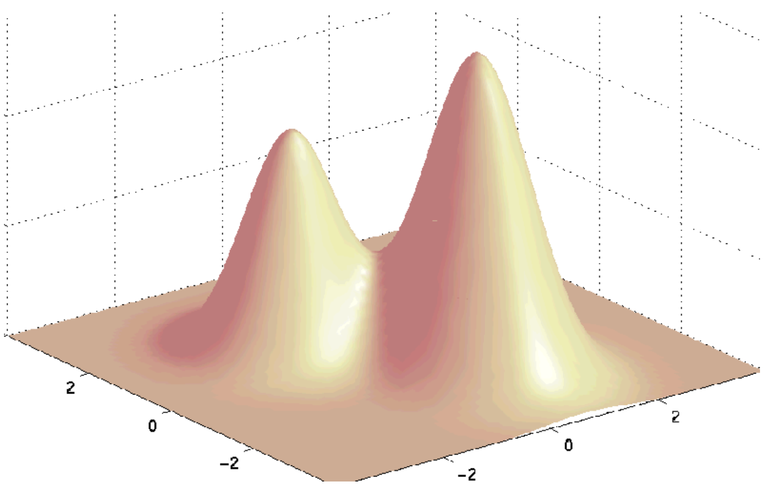

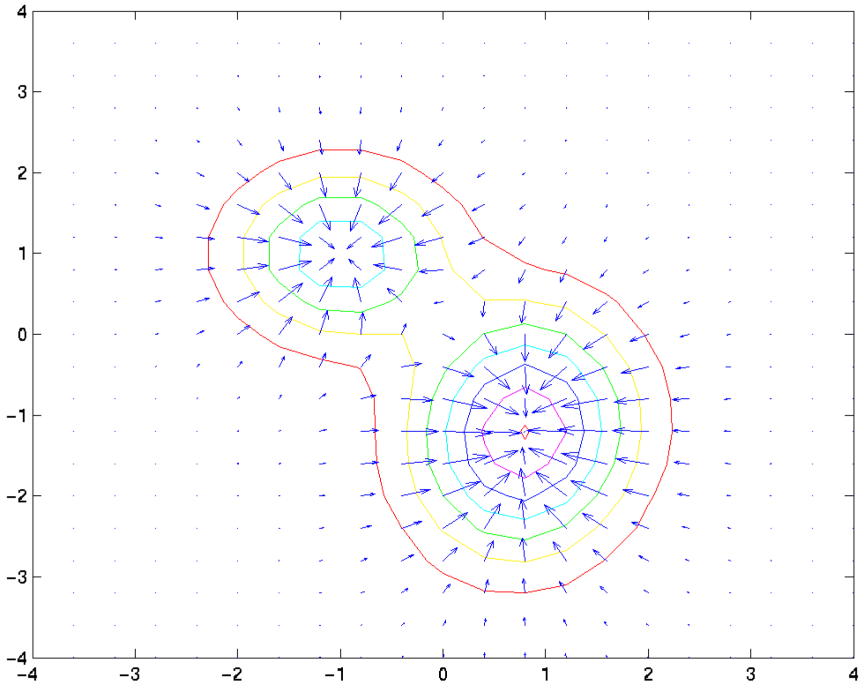

Gradient Descent

- For a simple function $L(\boldsymbol{w}|\mathcal{D})$ we can solve $\boldsymbol{\nabla} L(\boldsymbol{w}|\mathcal{D}) = \boldsymbol{0}$ explicitly. E.g. the linear perceptron

- For a non-linear functions we usually can't solve this set of simultaneous equations

- We can find a maximum or minimum **iteratively**

- If we know the gradient then we can follow the gradient
  - ⋆ Maximisation: $\boldsymbol{w} \to \boldsymbol{w}' = \boldsymbol{w} + r \boldsymbol{\nabla} L(\boldsymbol{w}|\mathcal{D})$
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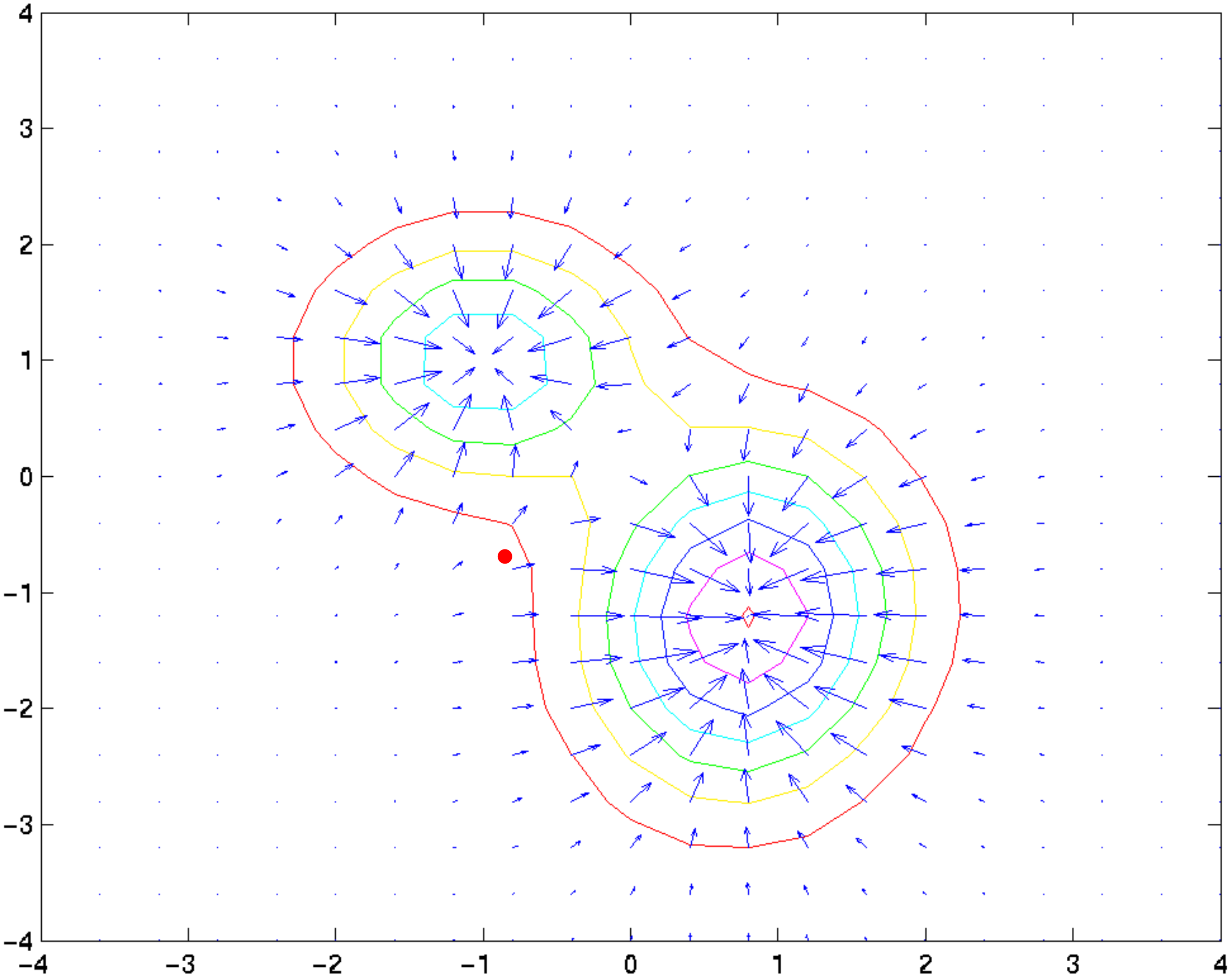
Hill-Climbing



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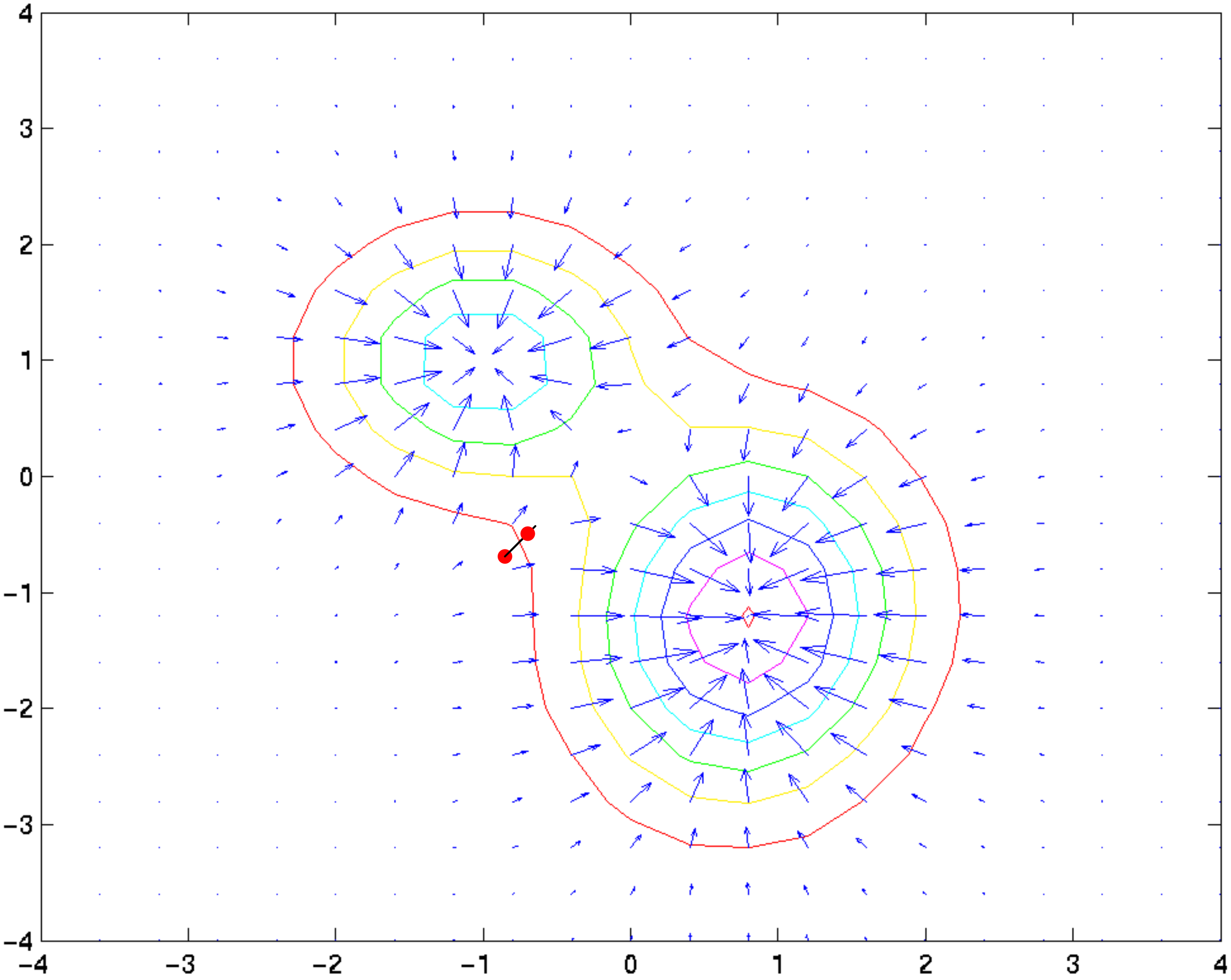

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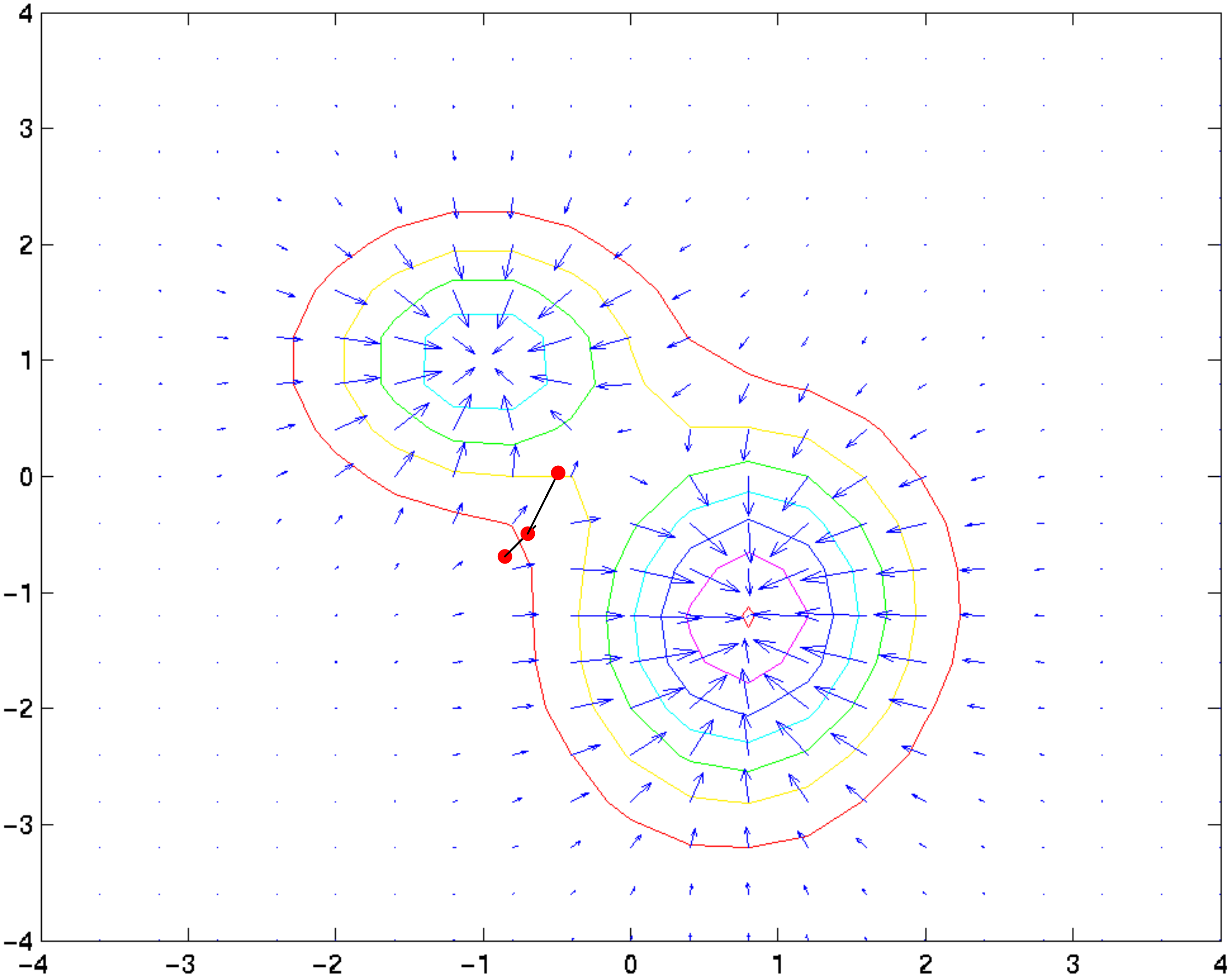

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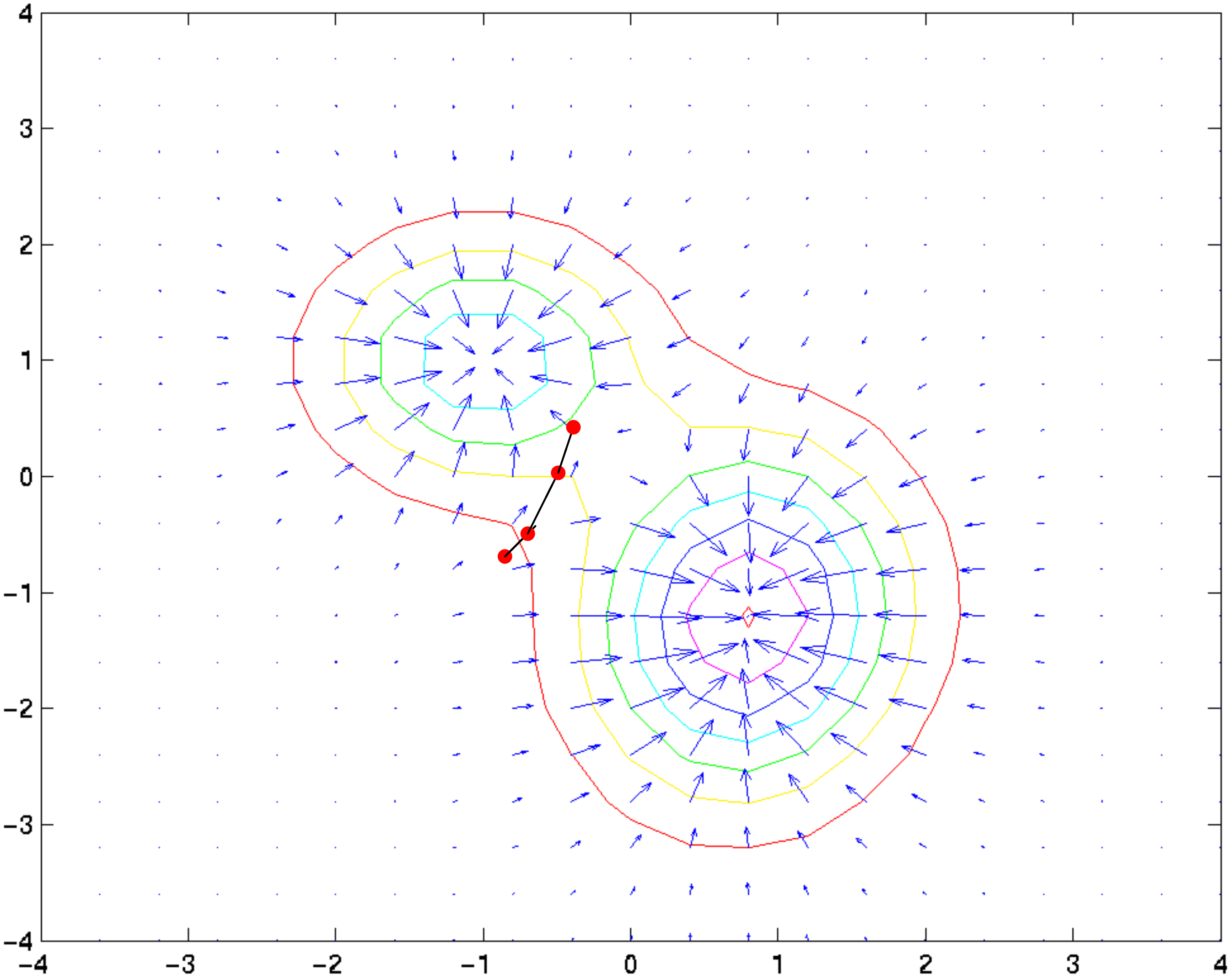

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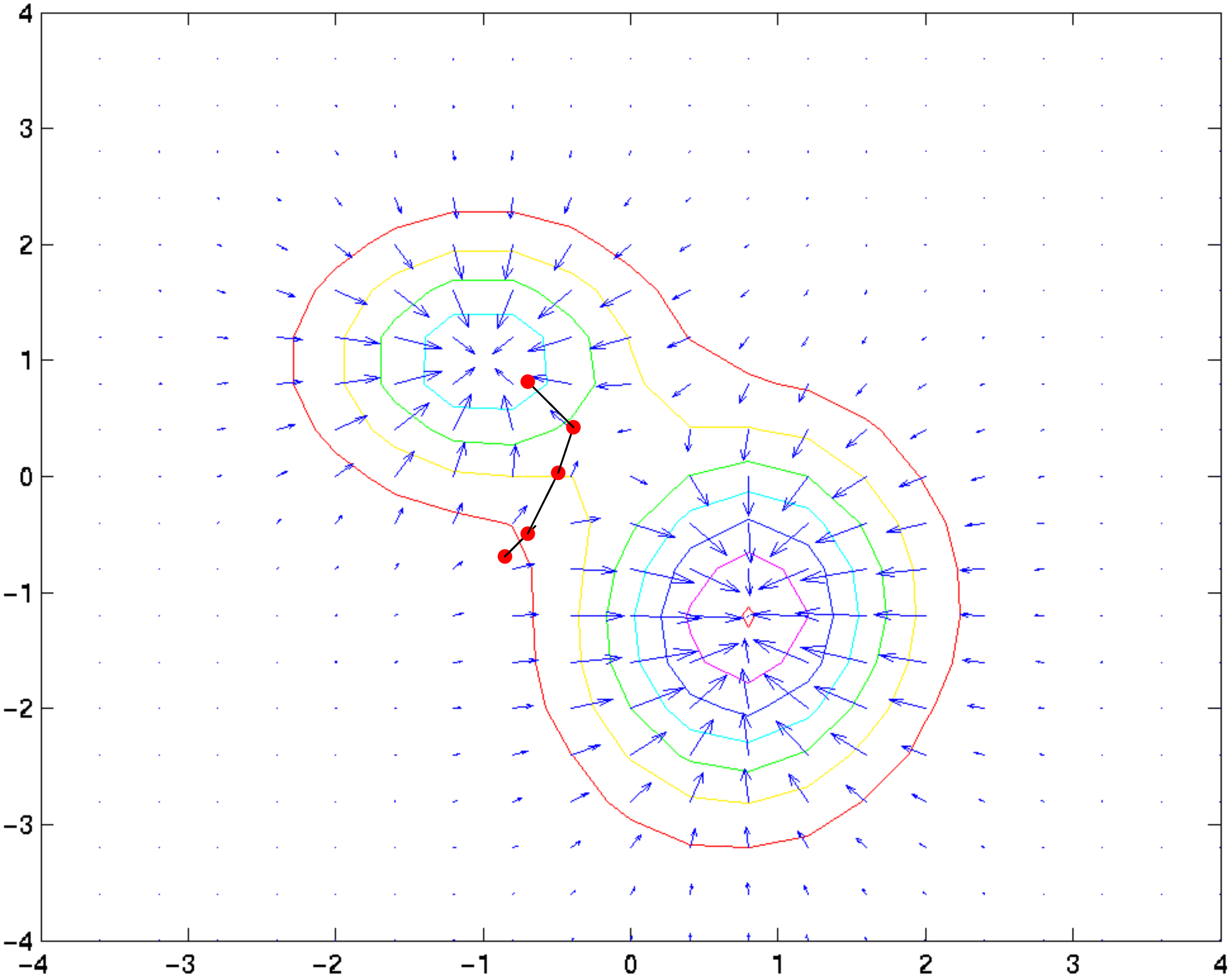

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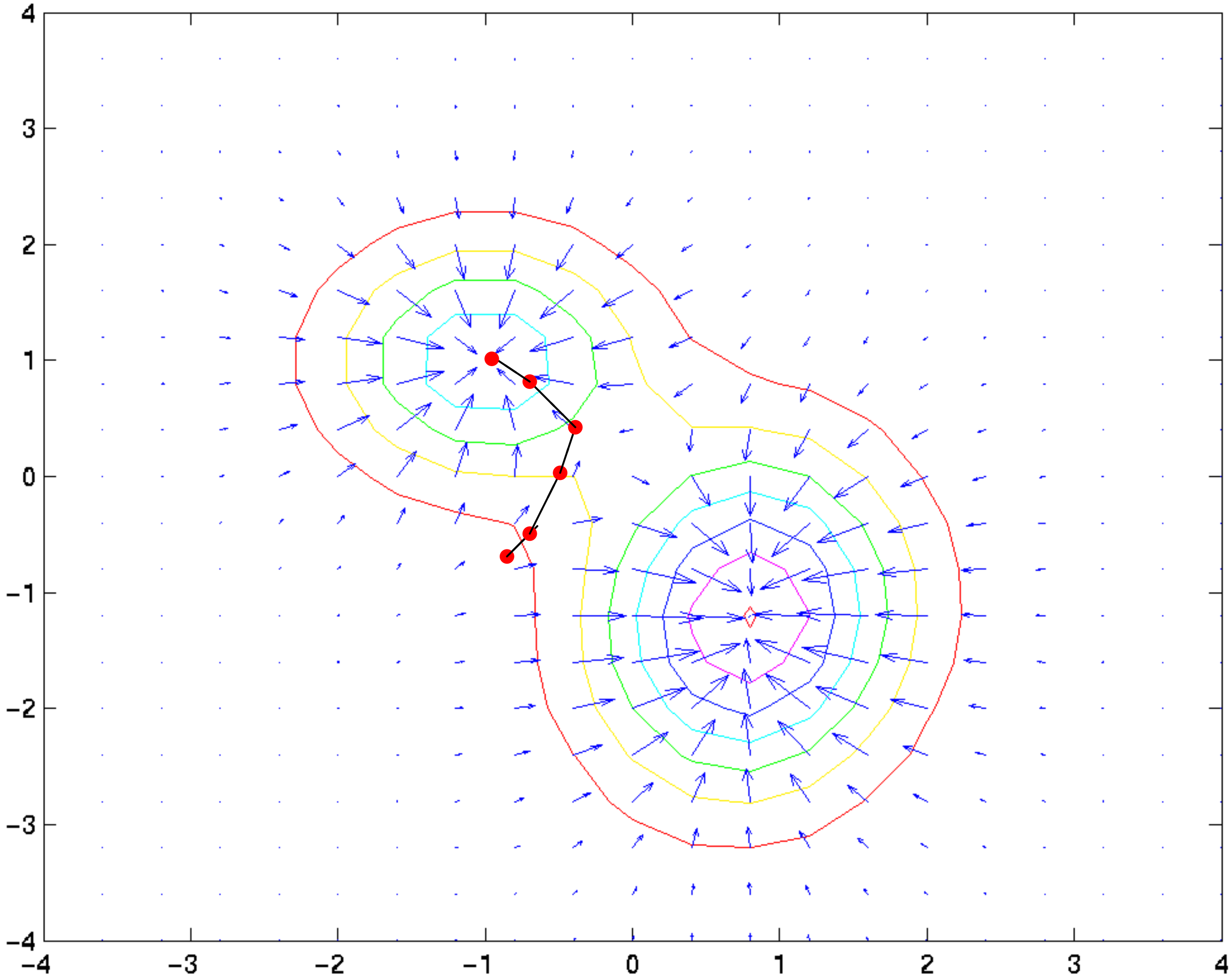
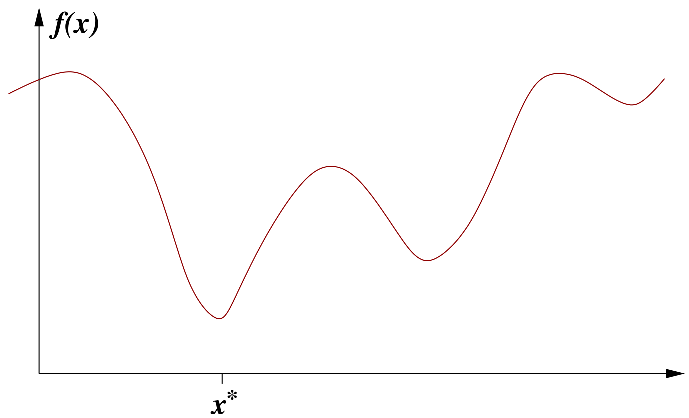


What Goes Right

- Almost all minima are quadratic (Morse's theorem)



- Taylor expanding around a minimum x^*

$$\begin{aligned} f(x) &= f(x^*) + (x - x^*) f'(x^*) + \frac{1}{2}(x - x^*)^2 f''(x^*) + \cdots \\ &= f(x^*) + \frac{1}{2}(x - x^*)^2 f''(x^*) + \frac{1}{3!}(x - x^*)^3 f'''(x^*) + \cdots \end{aligned}$$

- If $x - x^*$ is sufficiently small the higher order terms are negligible

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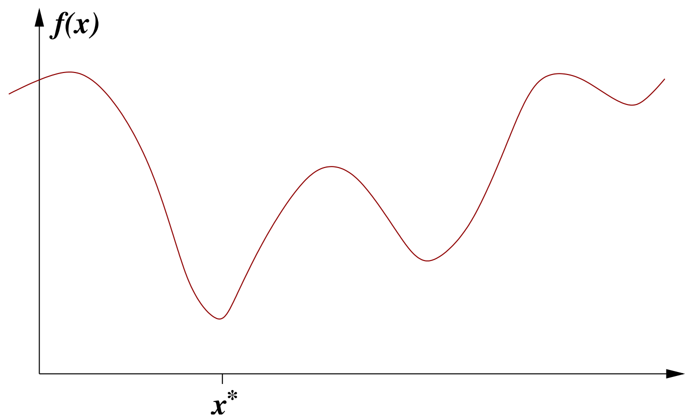

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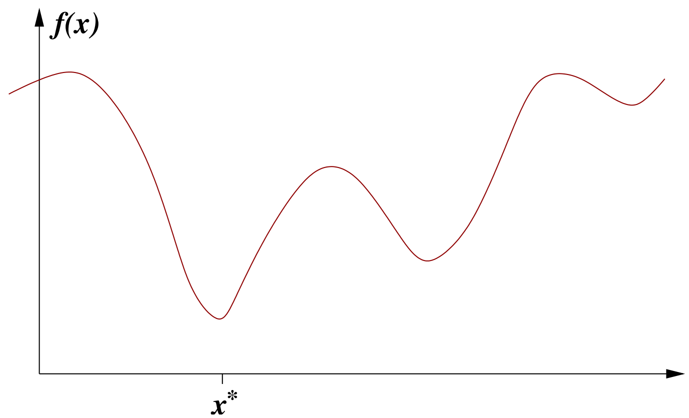

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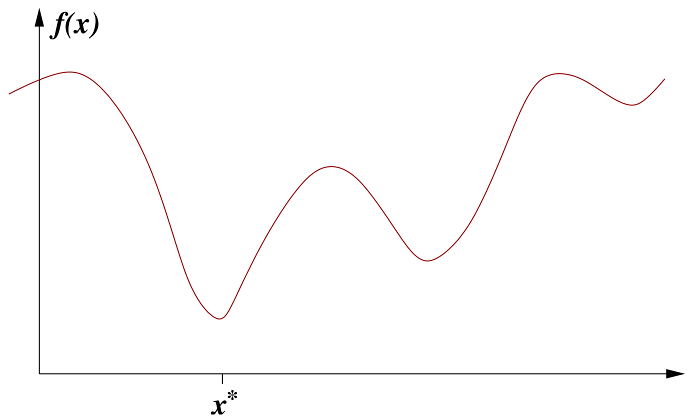

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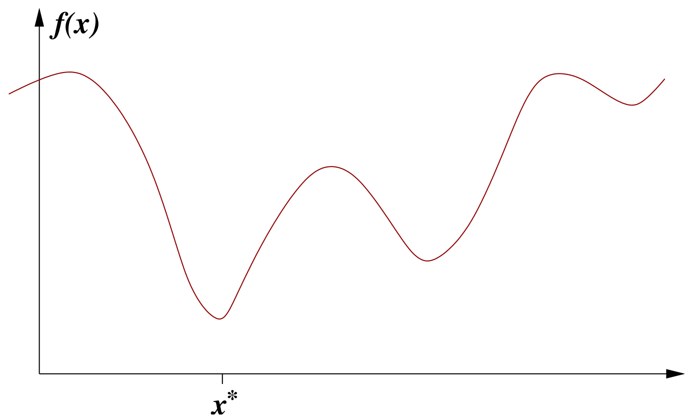

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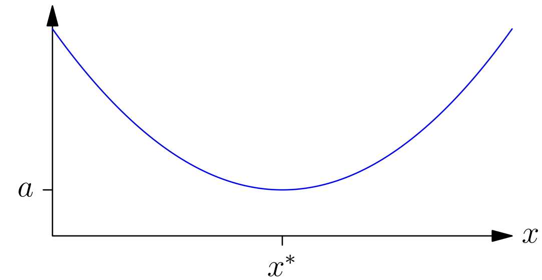
Newton's Method

- If we were in a quadratic minimum

$$f(x) = a + \frac{b}{2}(x - x^*)^2$$



- then

$$f'(x) = b(x - x^*), \qquad f''(x) = b$$

- so

$$x - x^* = \frac{f'(x)}{b} = \frac{f'(x)}{f''(x)}$$

- or

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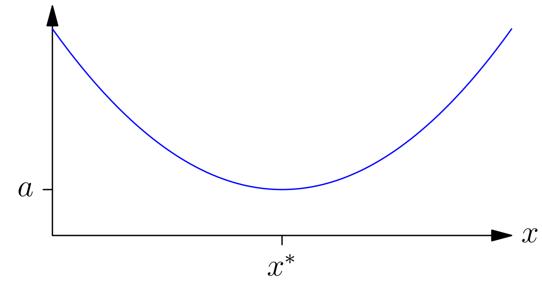

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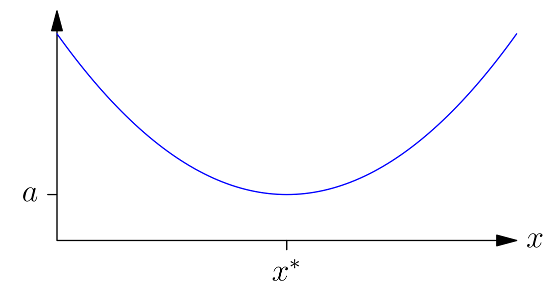

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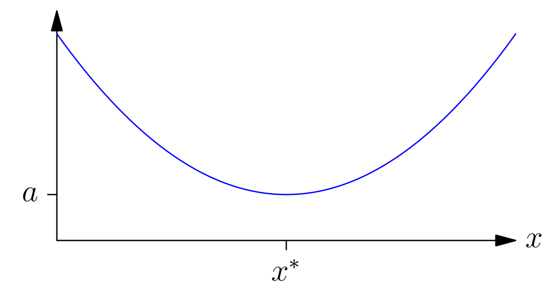

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Newton's Method

- This is Newton's methods
- For non-quadratic functions Newtons method converges **quadratically** provided we are sufficiently close to a minimum
- If we are at a distance $x - x^* = \epsilon$ from the minima then after one cycle we will be a distance ϵ^2 after two cycles we will be at a distance ϵ^4, etc.
- If we are too far from a minimum we might go anywhere!
- We should follow the gradient until we are near the minimum

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- If we are at a distance $x - x^* = \epsilon$ from the minima then after one cycle we will be a distance ϵ^2 after two cycles we will be at a distance ϵ^4, etc.
- If we are too far from a minimum we might go anywhere!
- We should follow the gradient until we are near the minimum

Taylor's Expansion in High Dimensions

- We can generalise these results to many dimensions
- The Taylor expansion of a function $f(\boldsymbol{x})$ about $\boldsymbol{x}_0$

$$f(\boldsymbol{x}) = f(\boldsymbol{x}_0) + (\boldsymbol{x} - \boldsymbol{x}_0)^{\mathsf{T}} \boldsymbol{\nabla} f(\boldsymbol{x}_0) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}_0)^{\mathsf{T}} \mathbf{H}(\boldsymbol{x} - \boldsymbol{x}_0) + \cdots$$

where $\mathbf{H}$ is the **Hessian** matrix with elements

$$H_{ij} = \frac{\partial^2 f(\boldsymbol{x}_0)}{\partial x_i \partial x_j}$$

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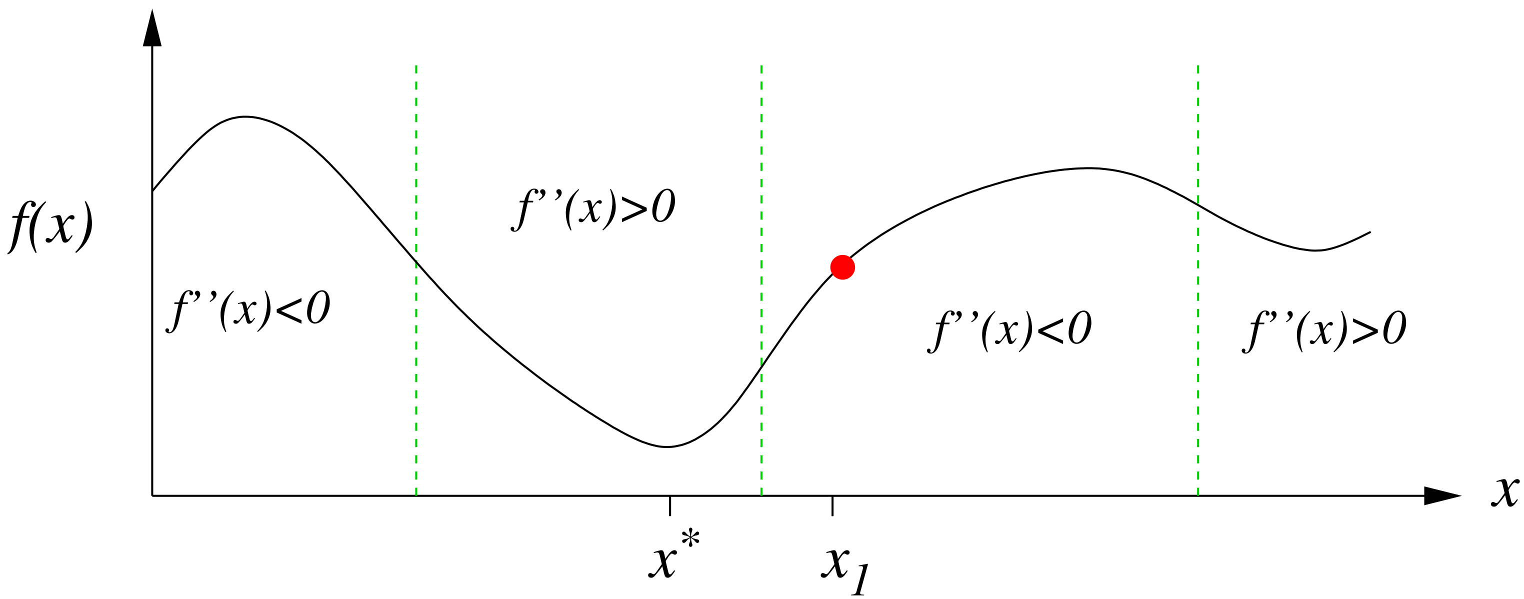
- If we are optimising N parameters the Hessian is an $N \times N$ matrix
- It is time-consuming to compute (and prone to errors when coding)

- Away from minima they can be misleading



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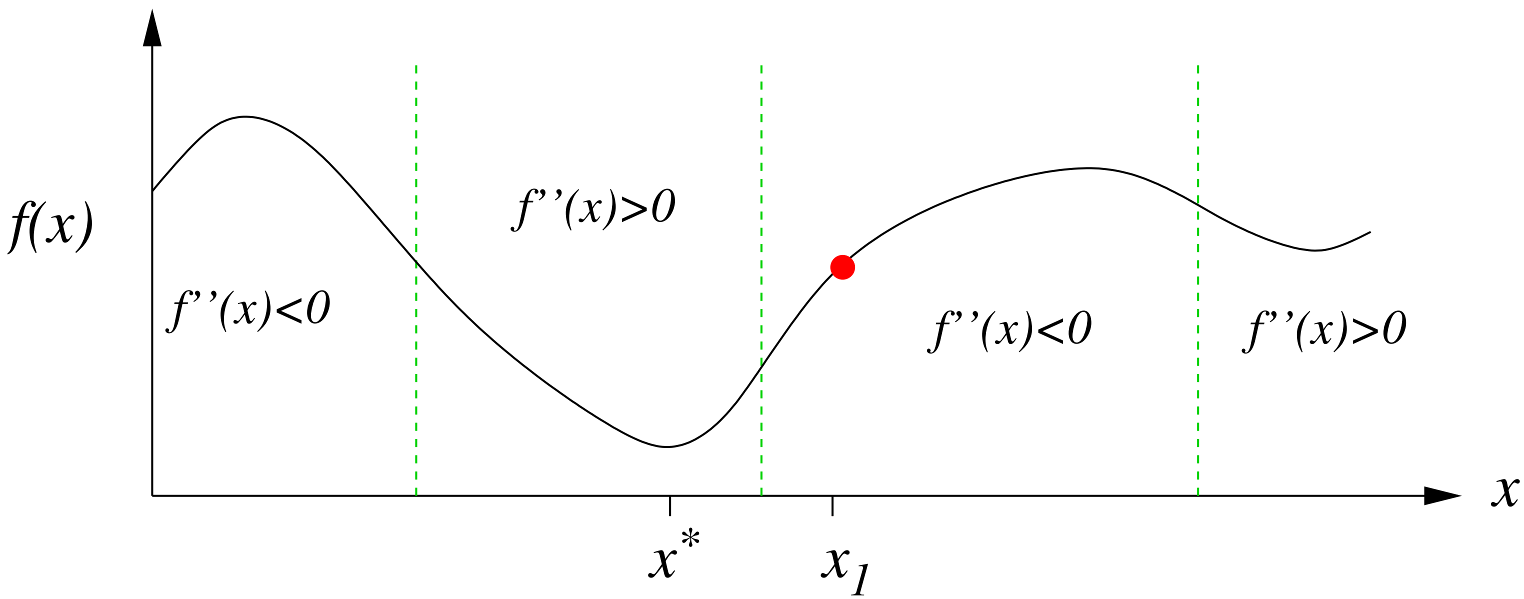

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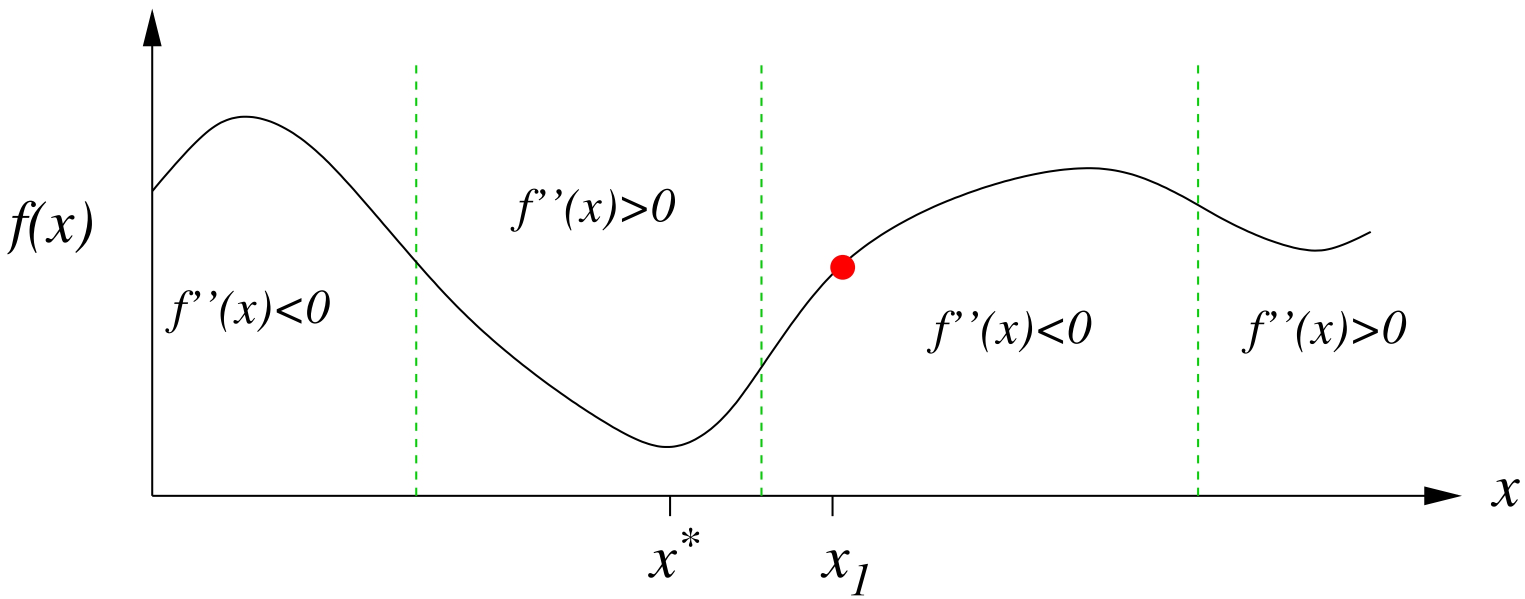

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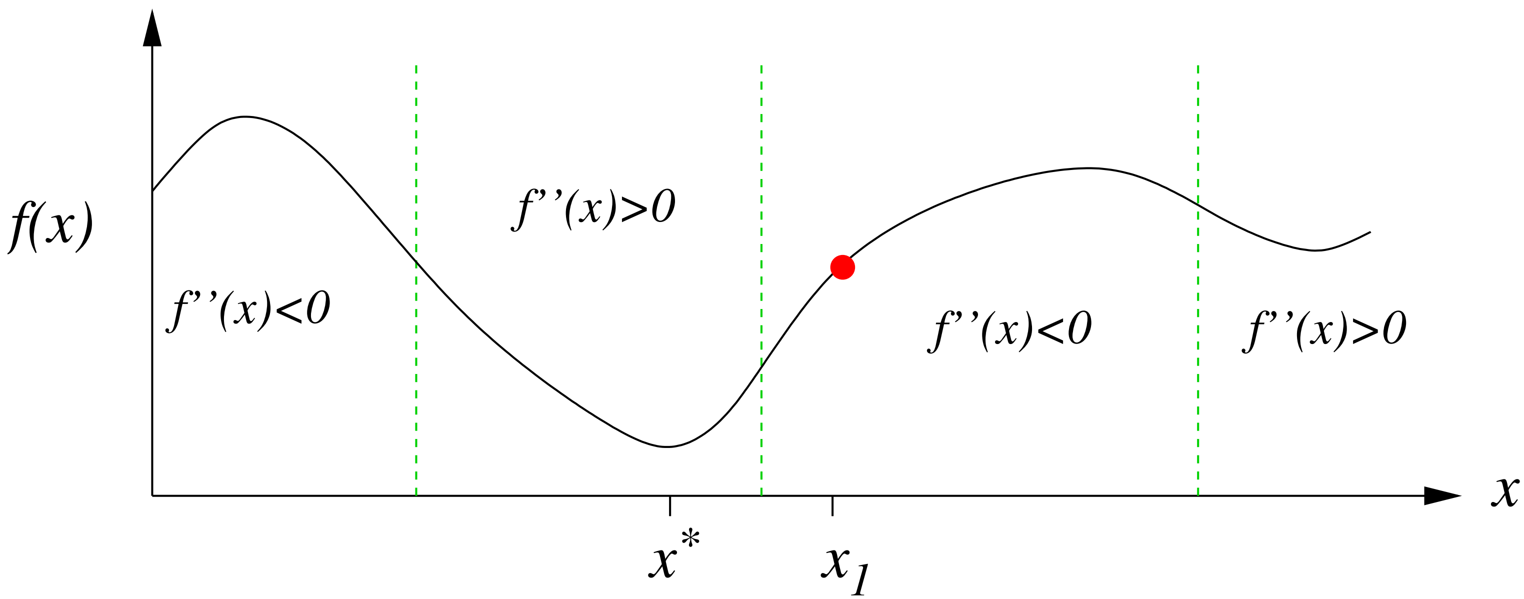

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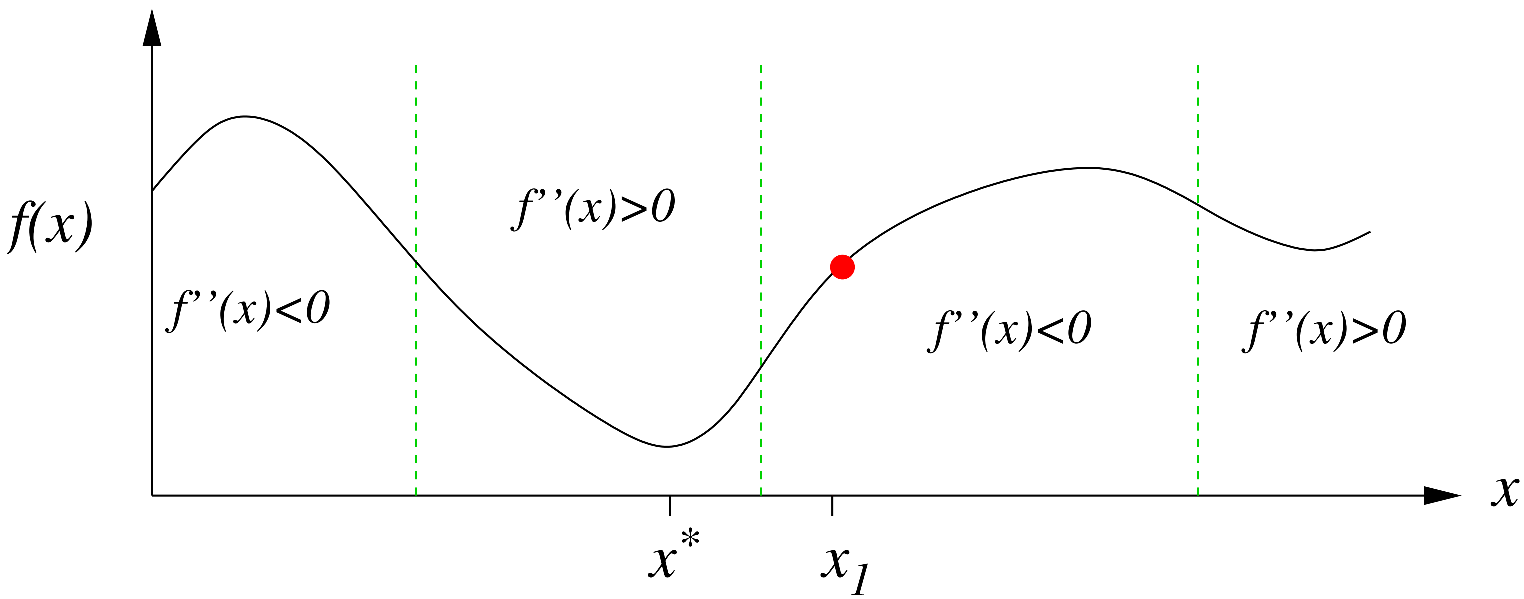
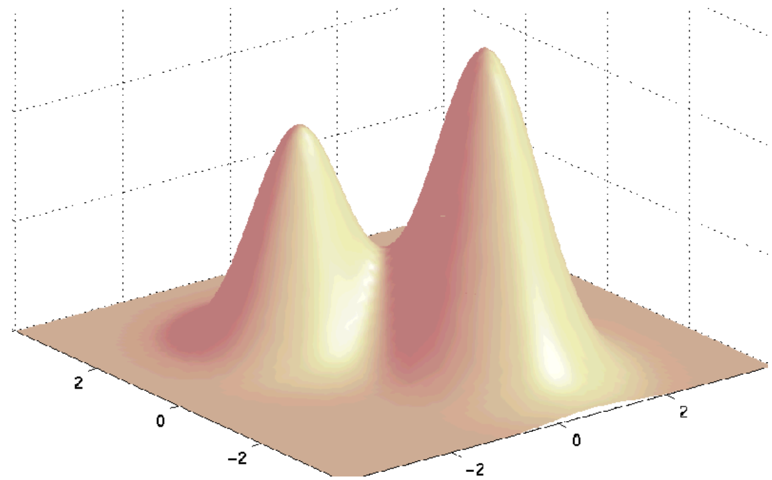


Outline

1. Motivation
2. Gradient Descent
3. **Why Gradient Descent is Difficult**



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$$\boldsymbol{x}' = \boldsymbol{x} - r\,\boldsymbol{\nabla} f(\boldsymbol{x})$$

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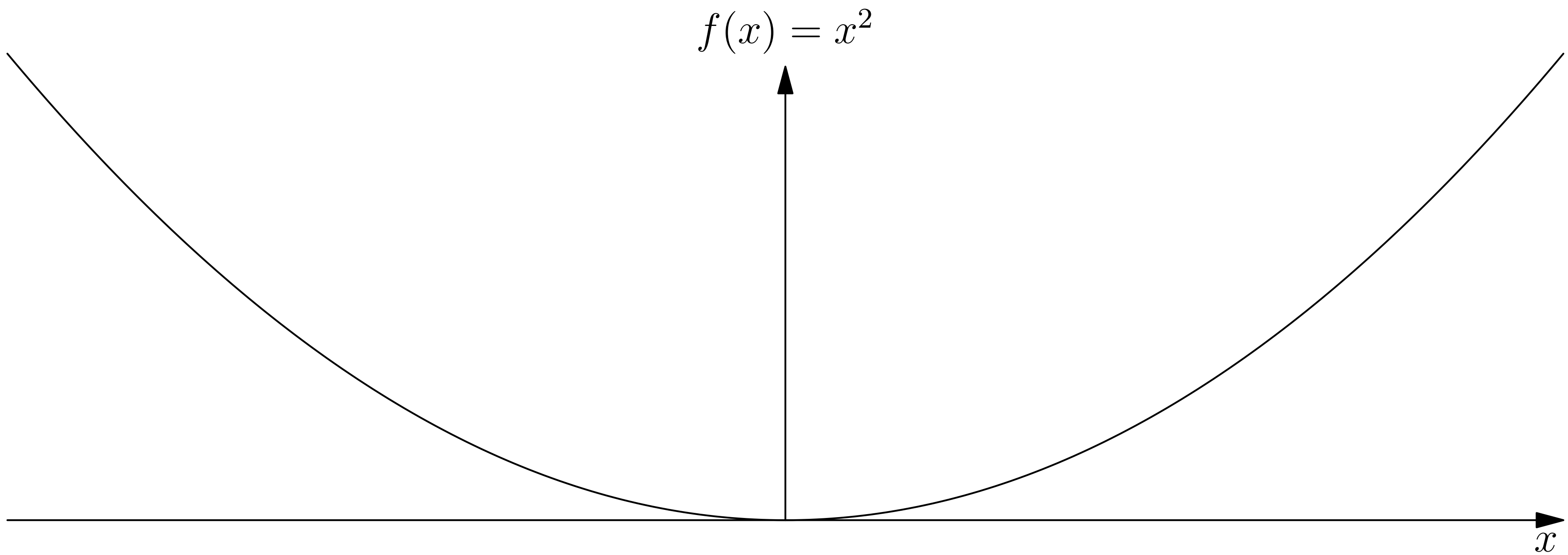

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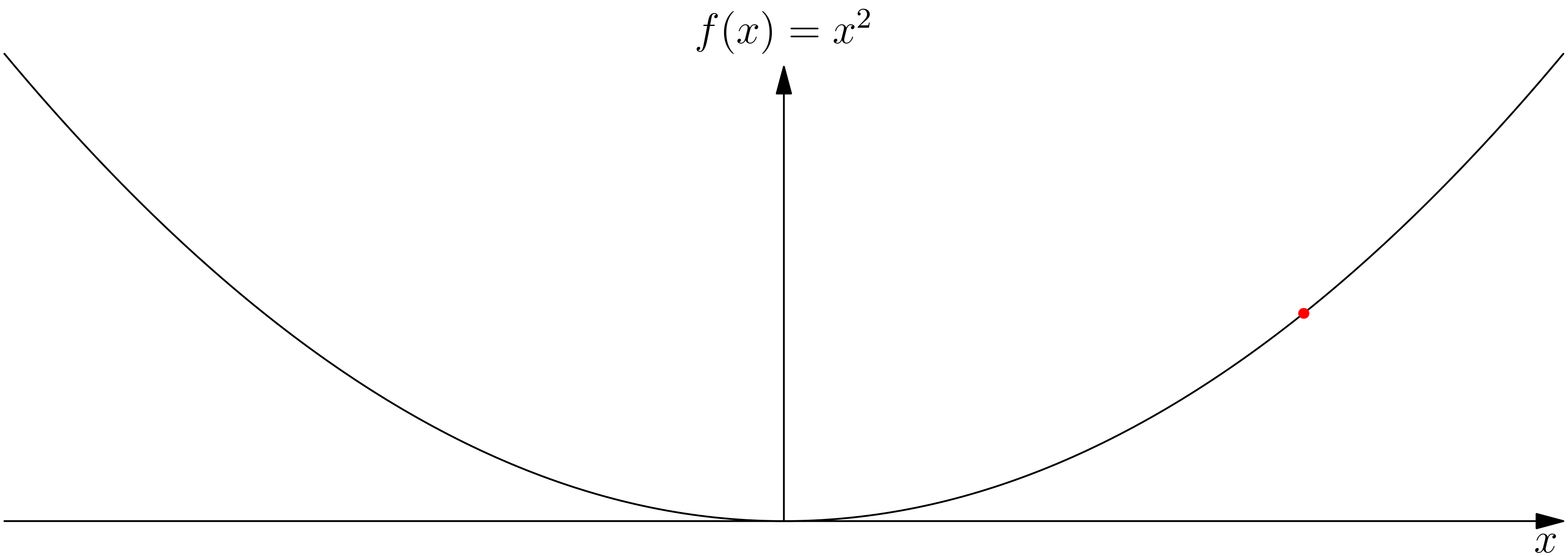

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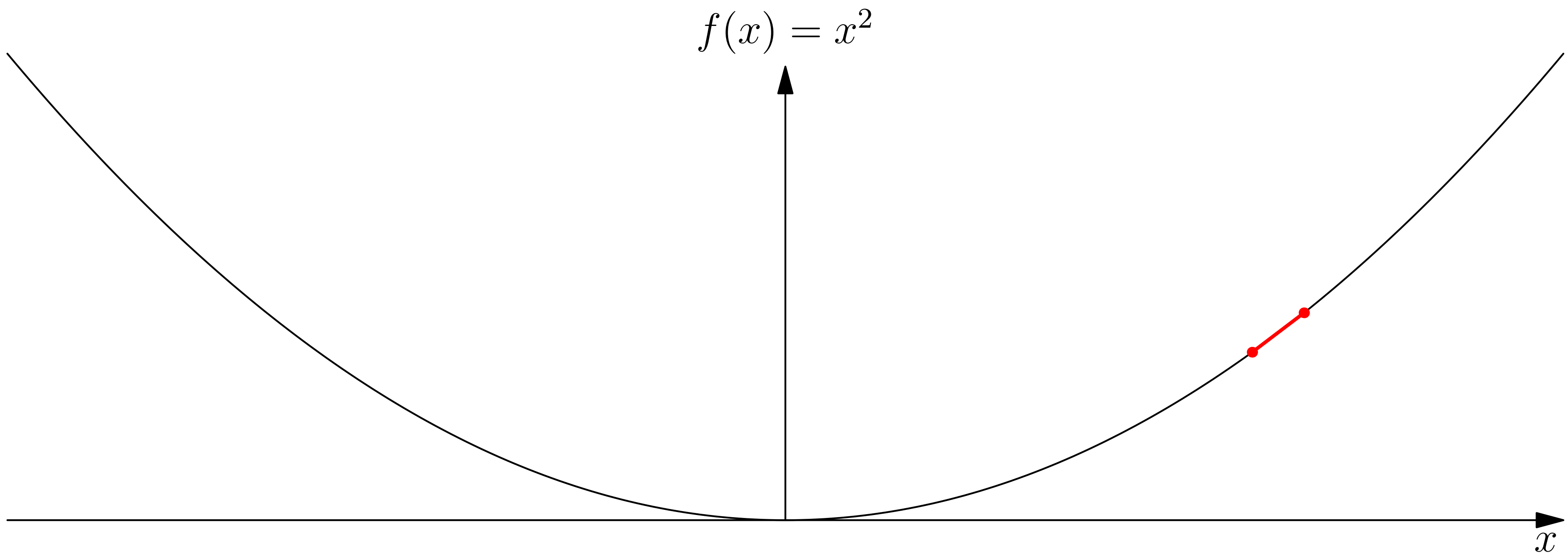

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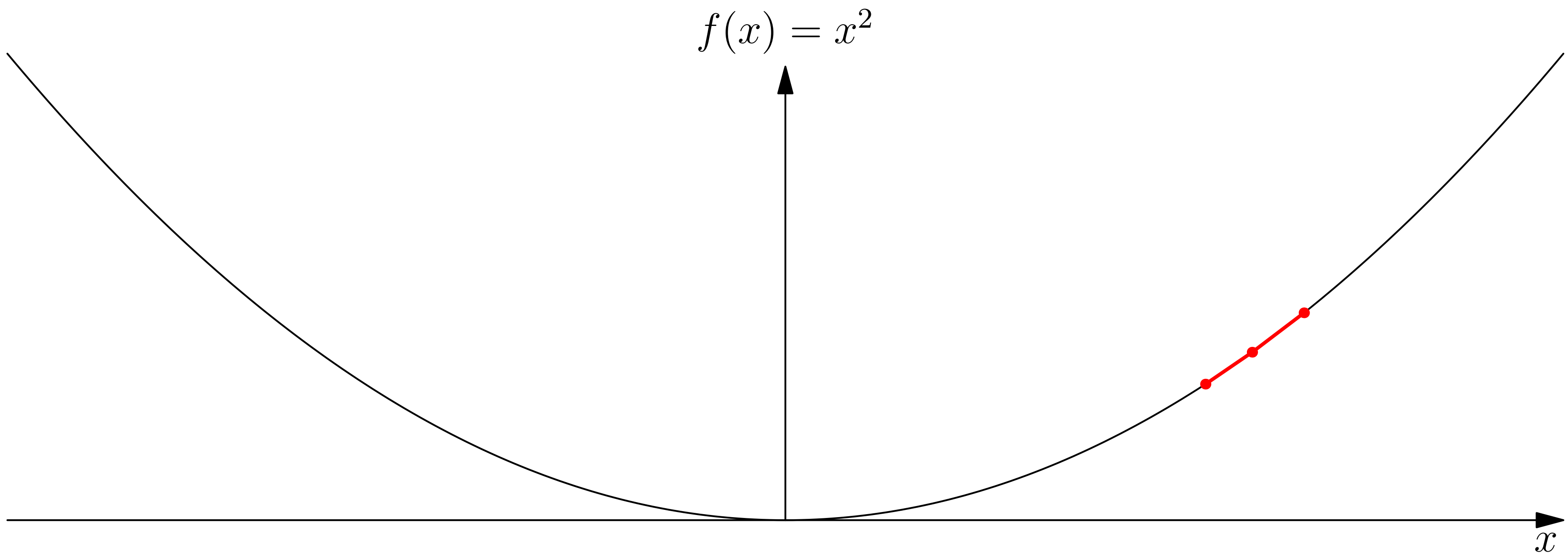

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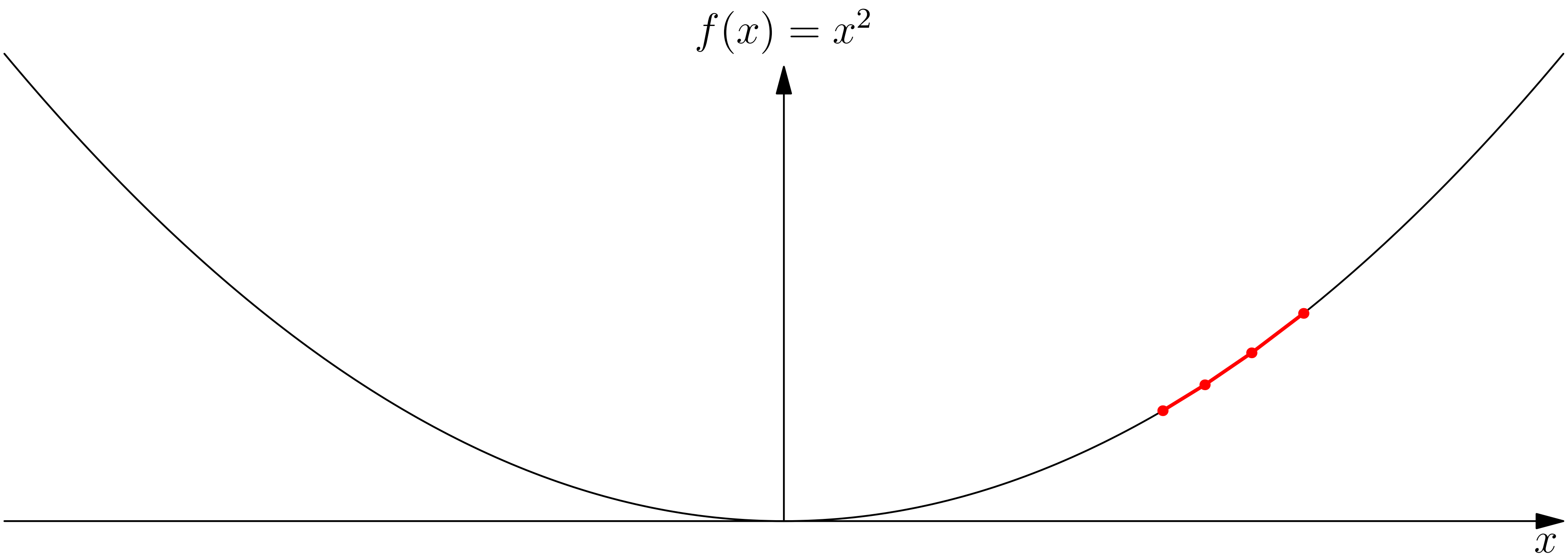

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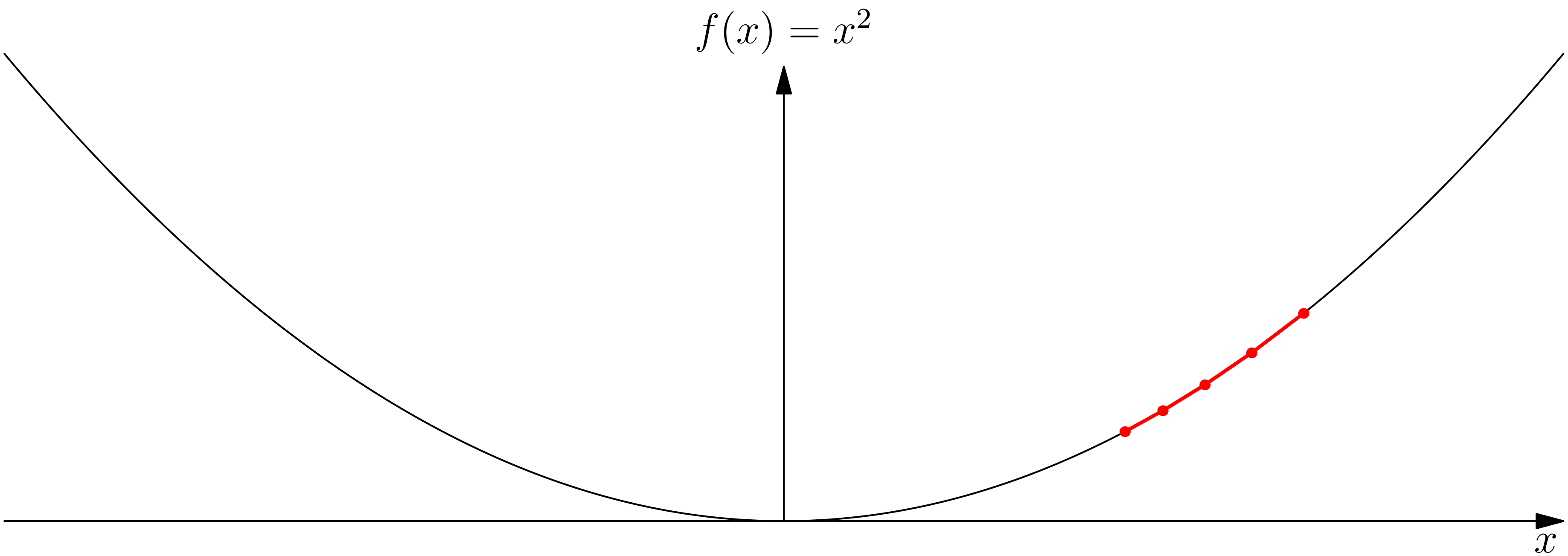

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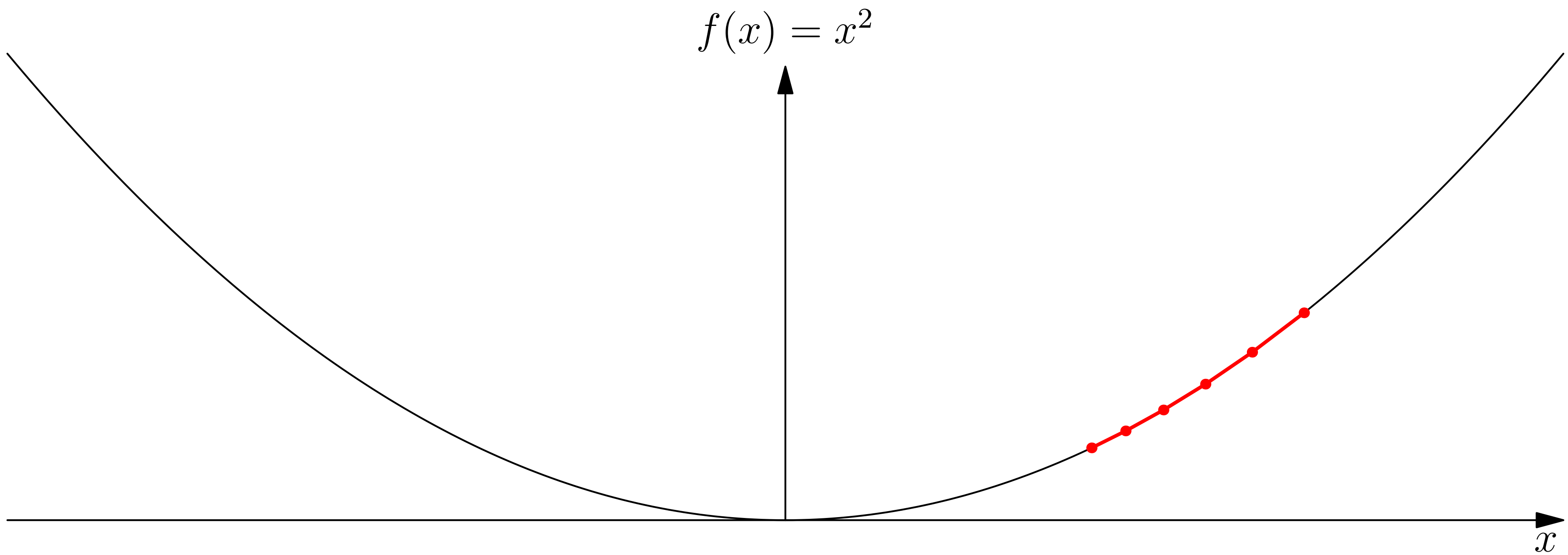

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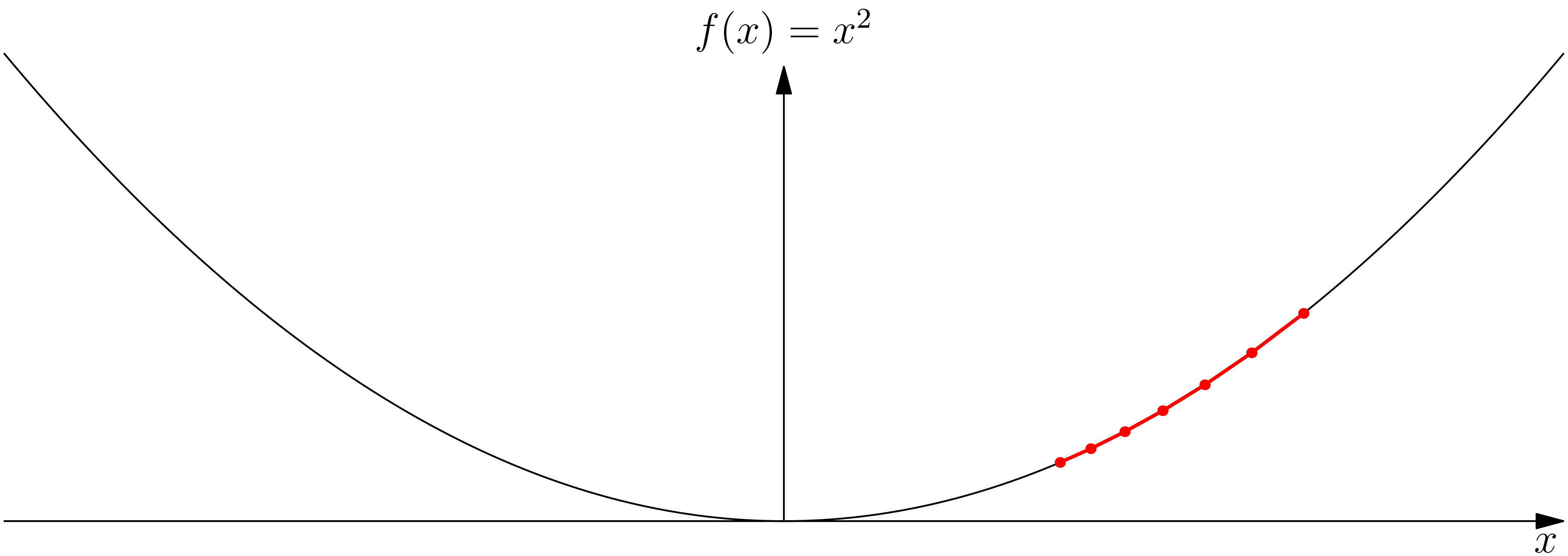

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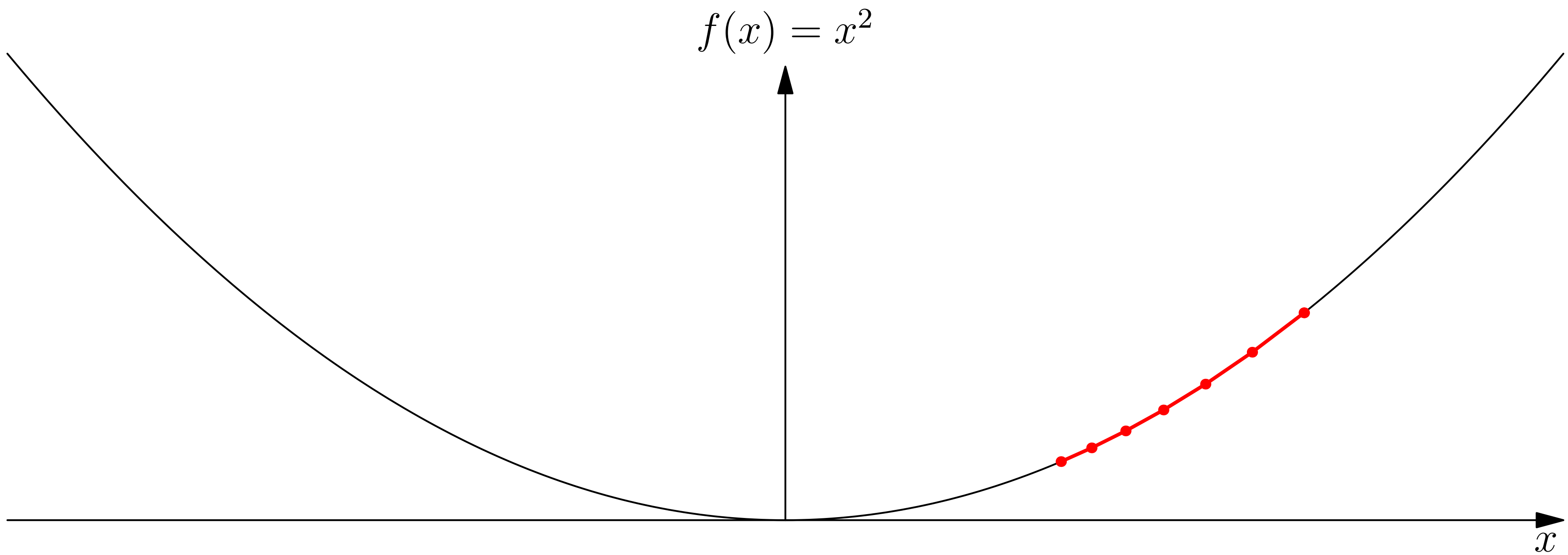

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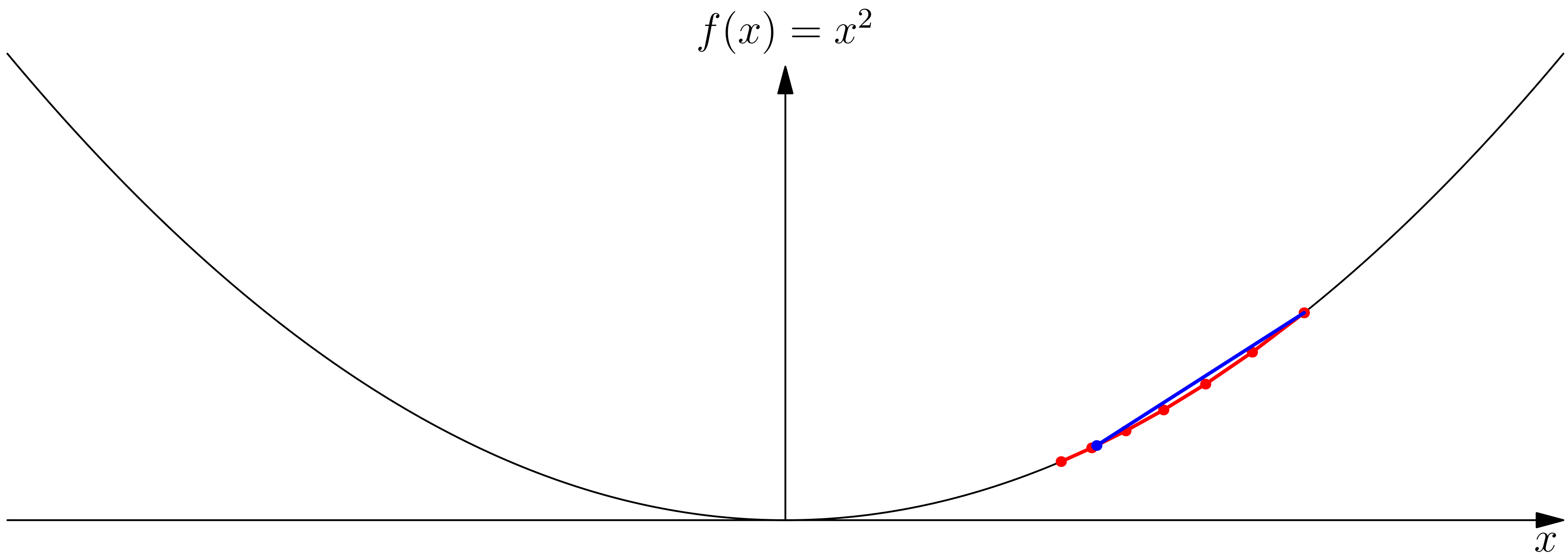

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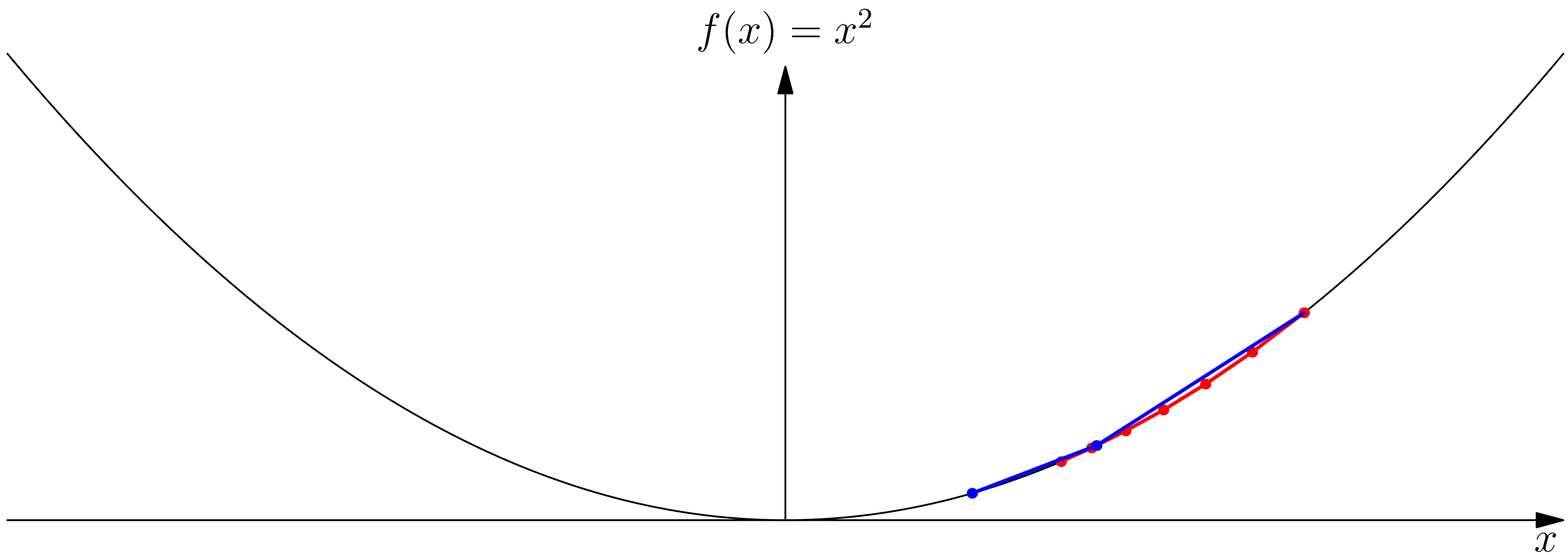

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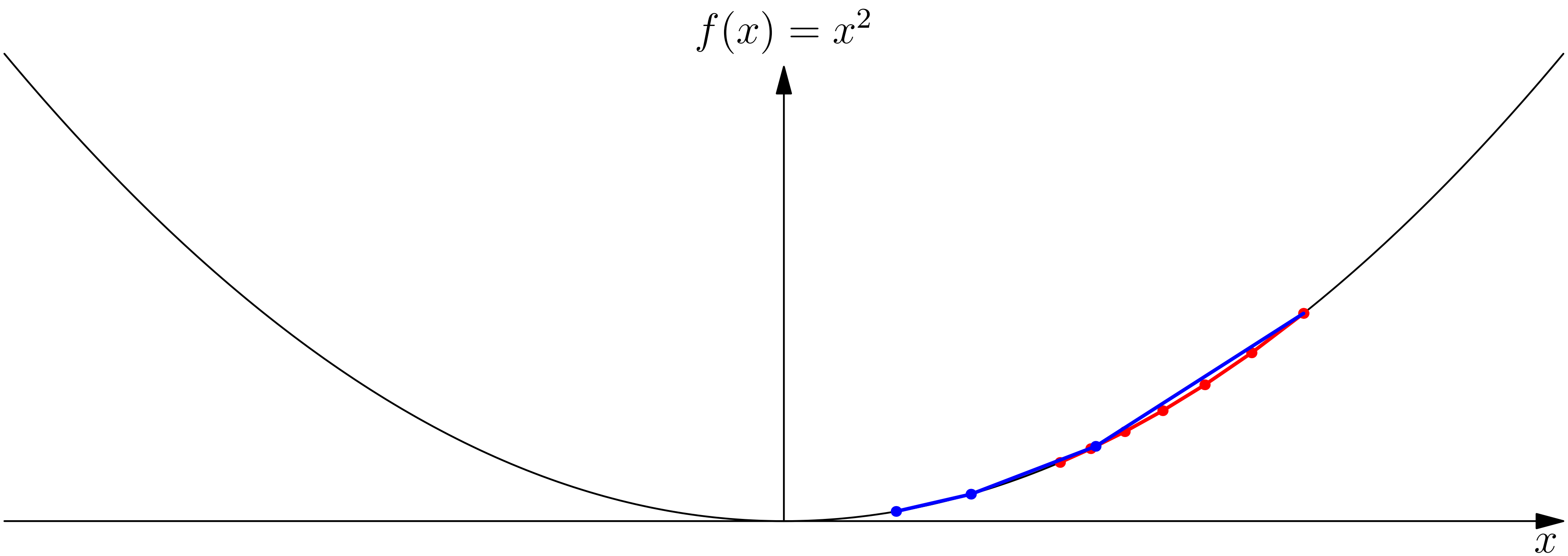

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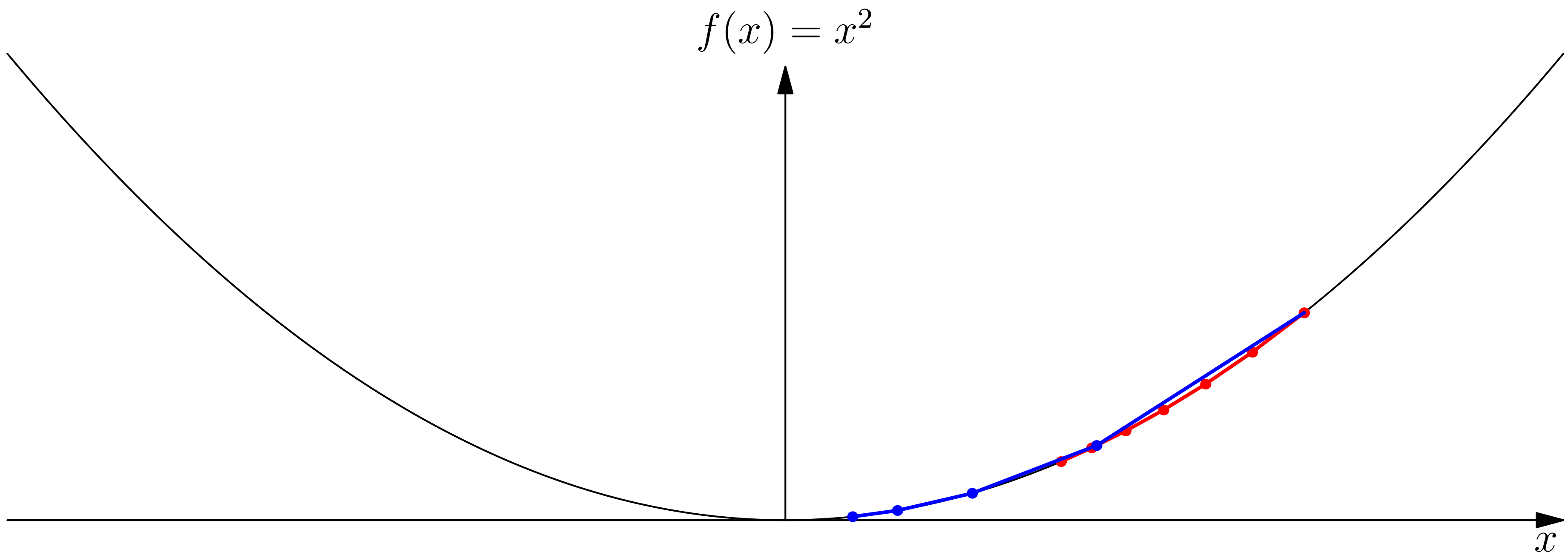

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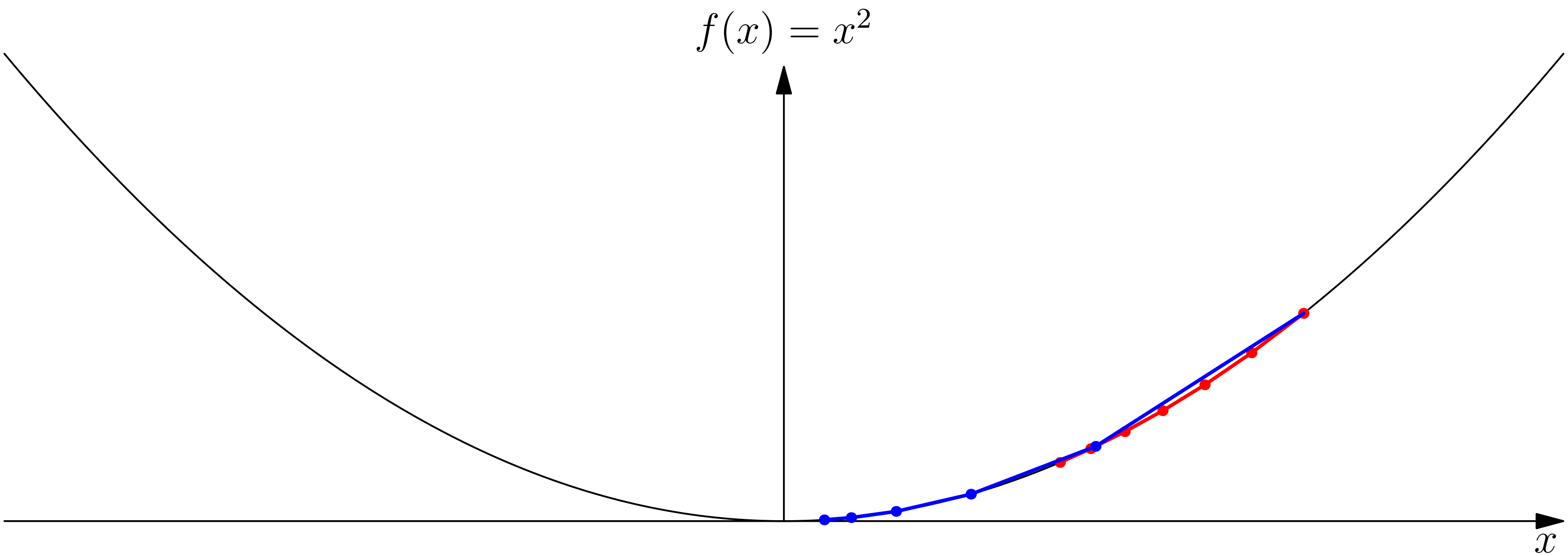

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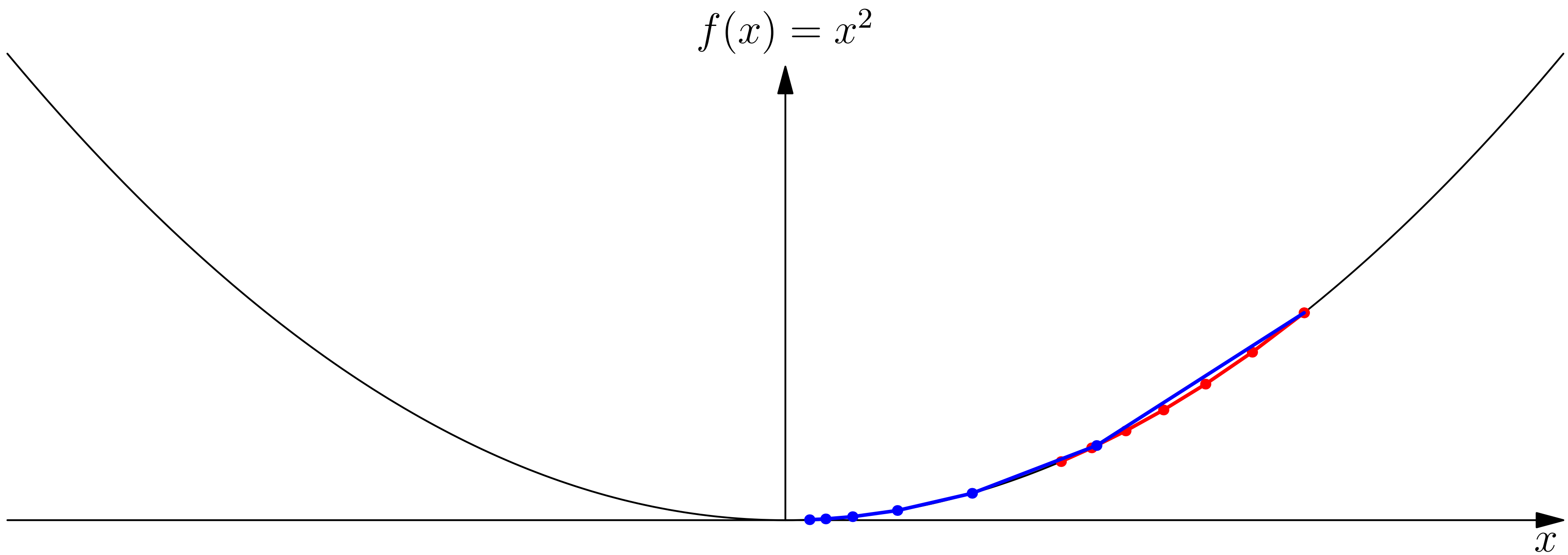

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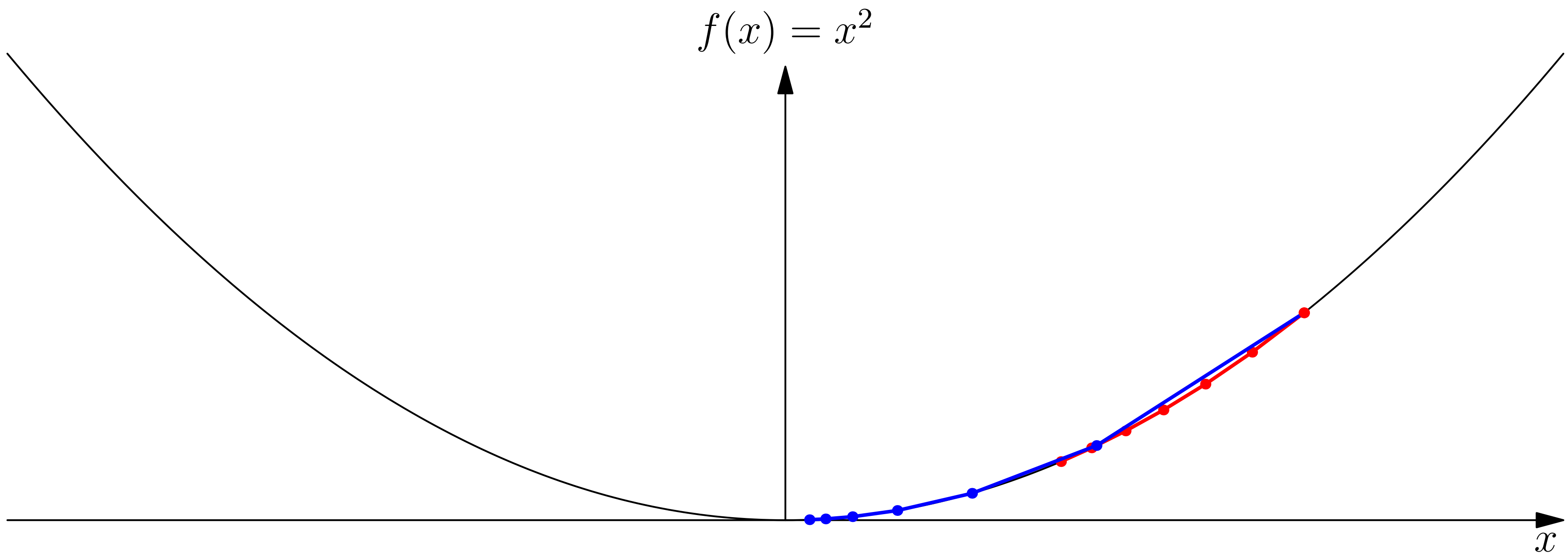

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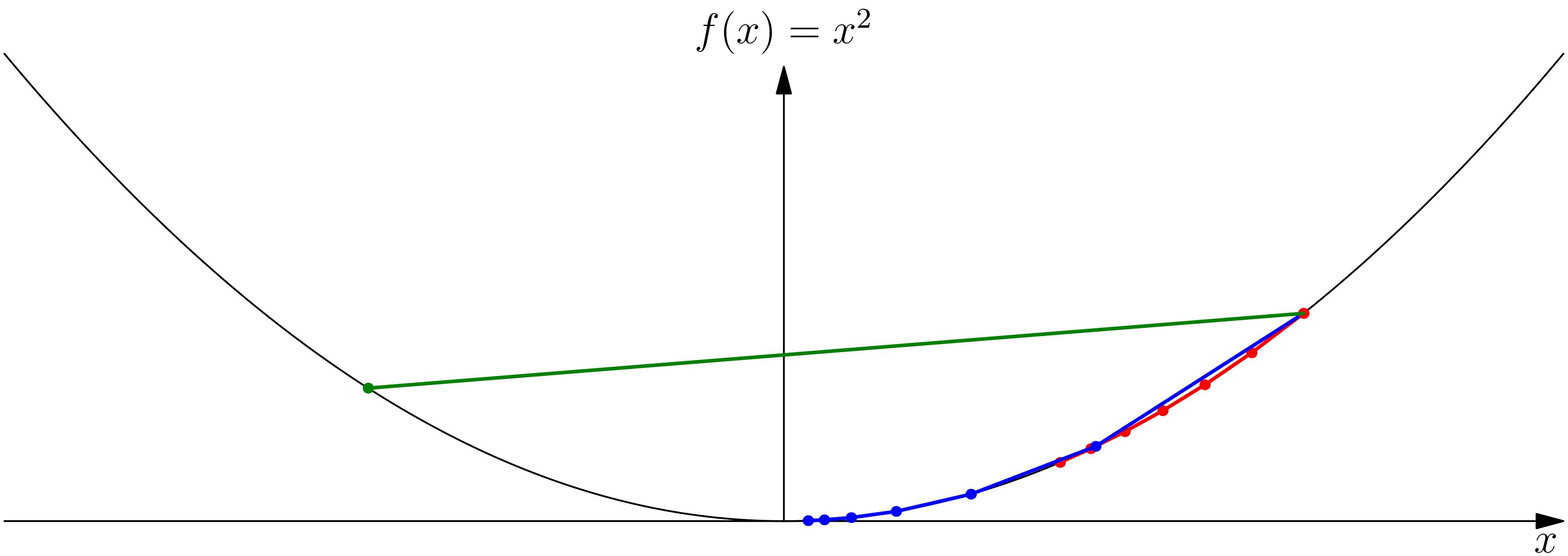

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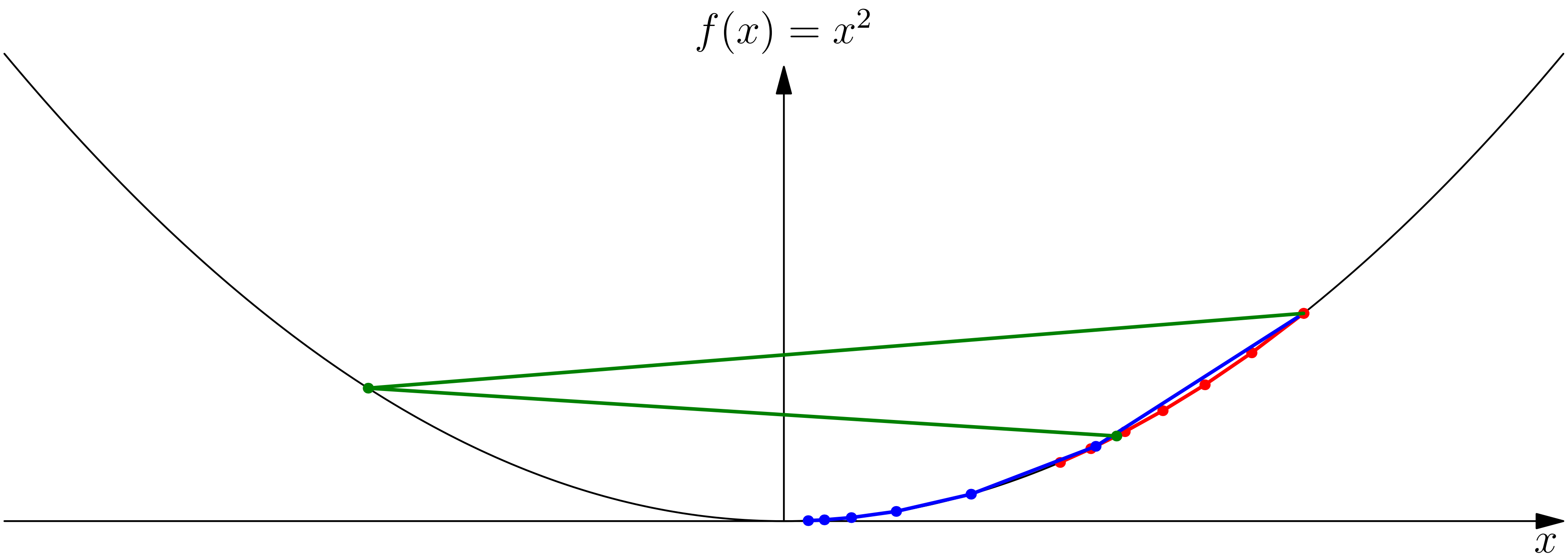

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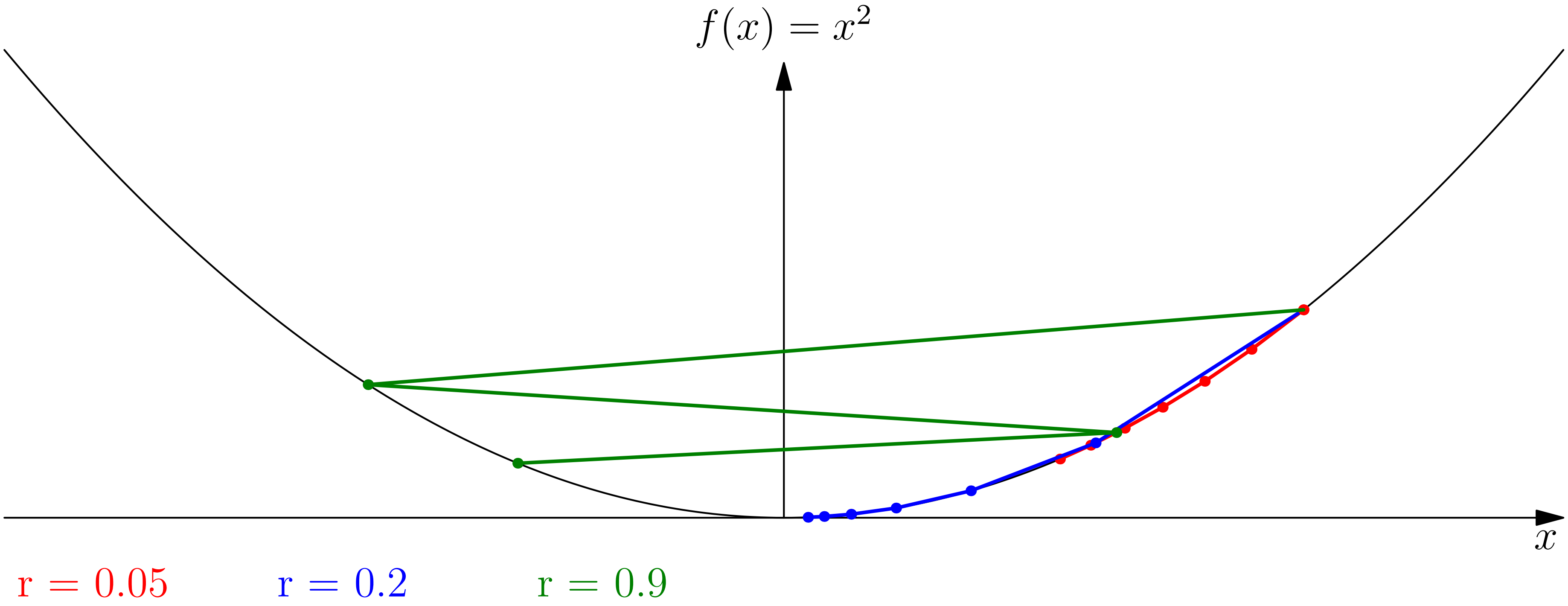

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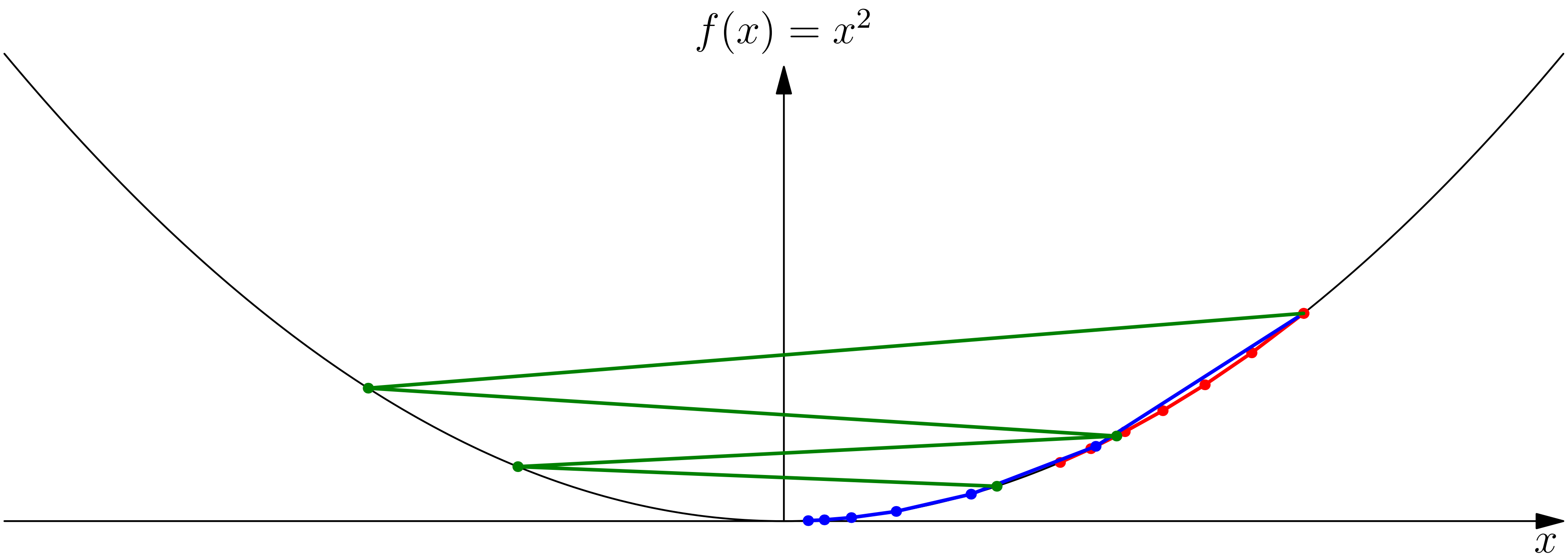

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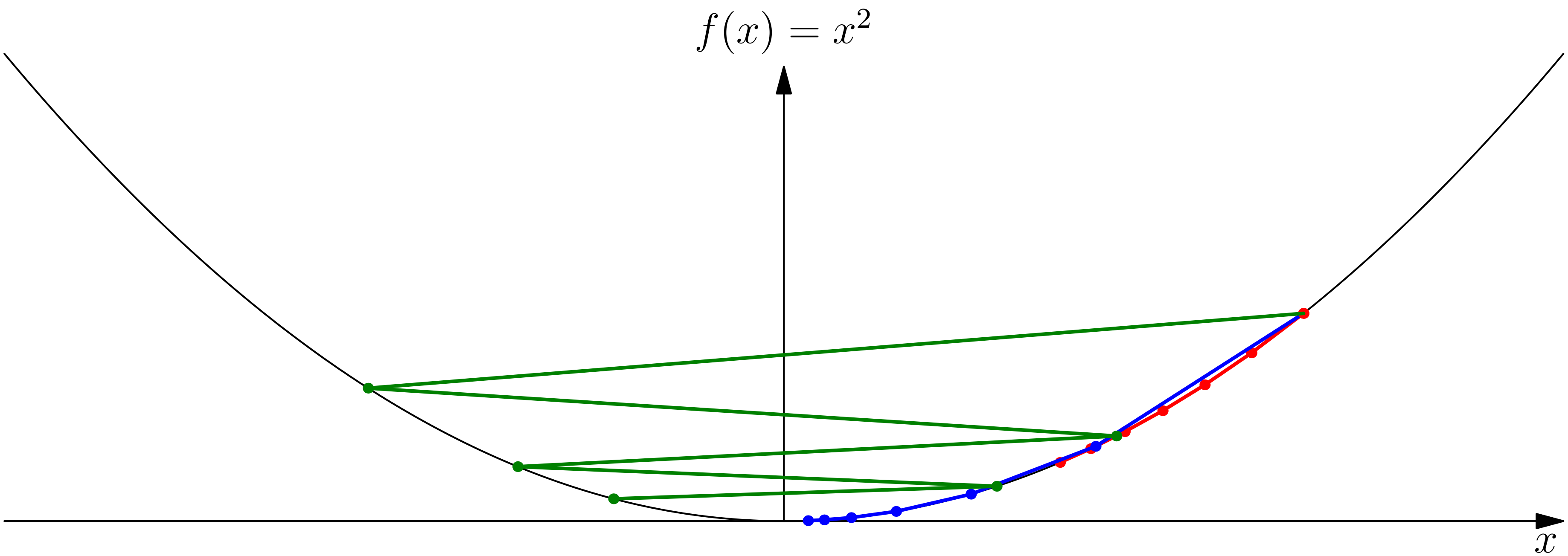

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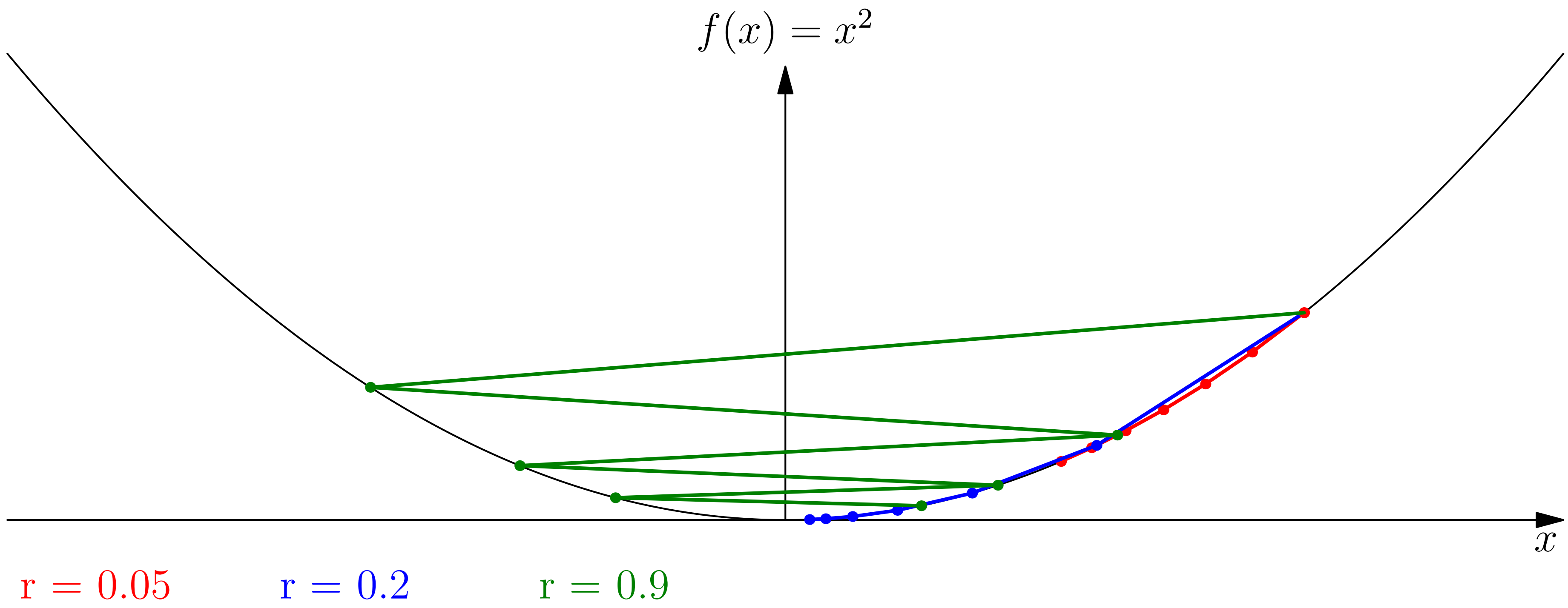

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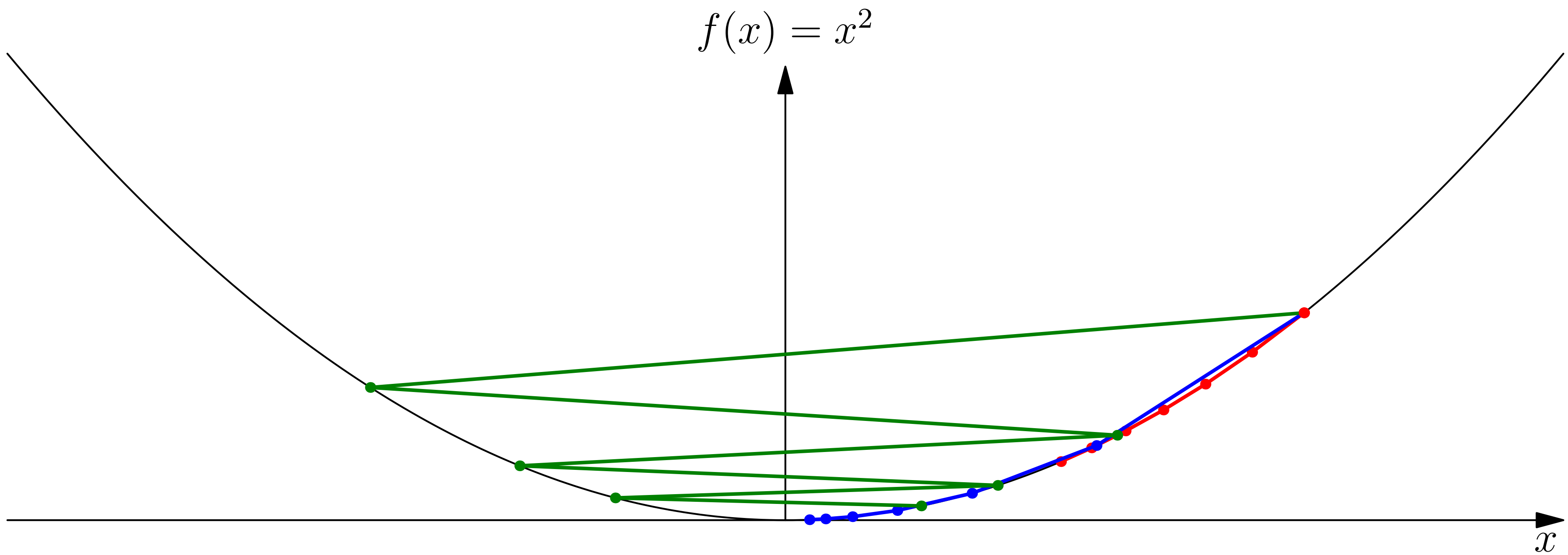

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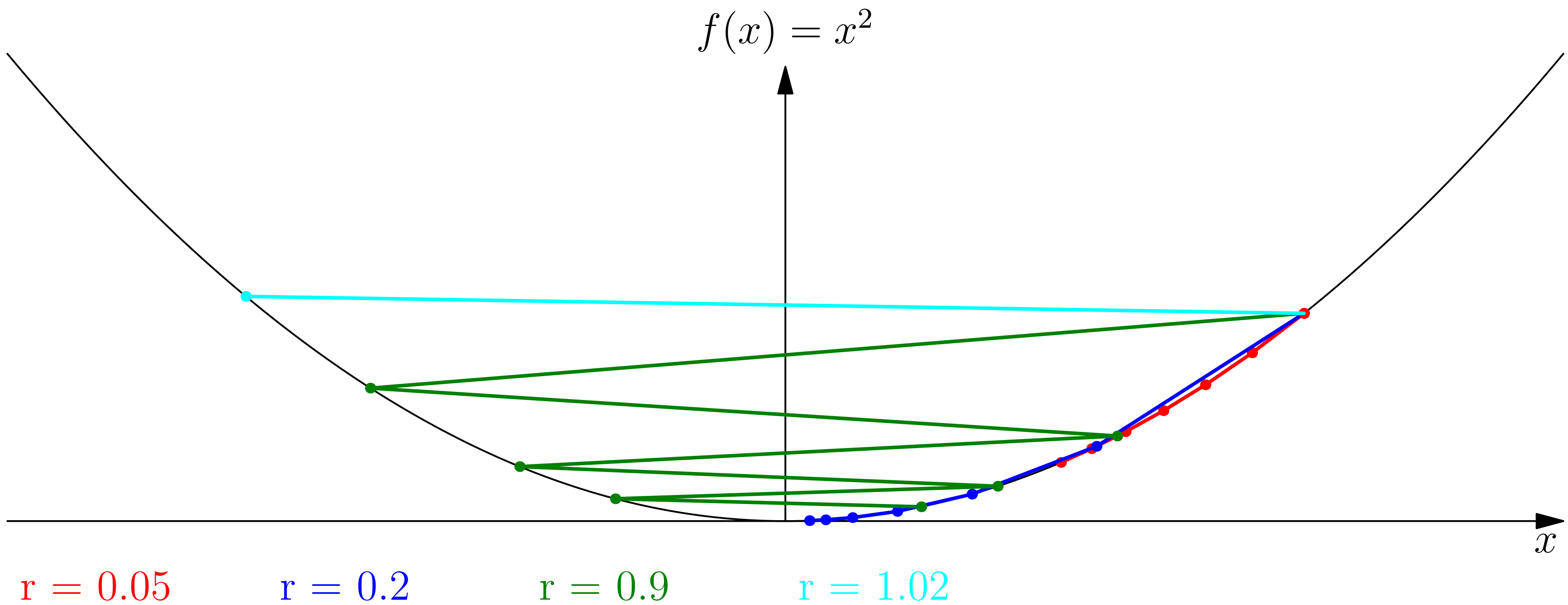

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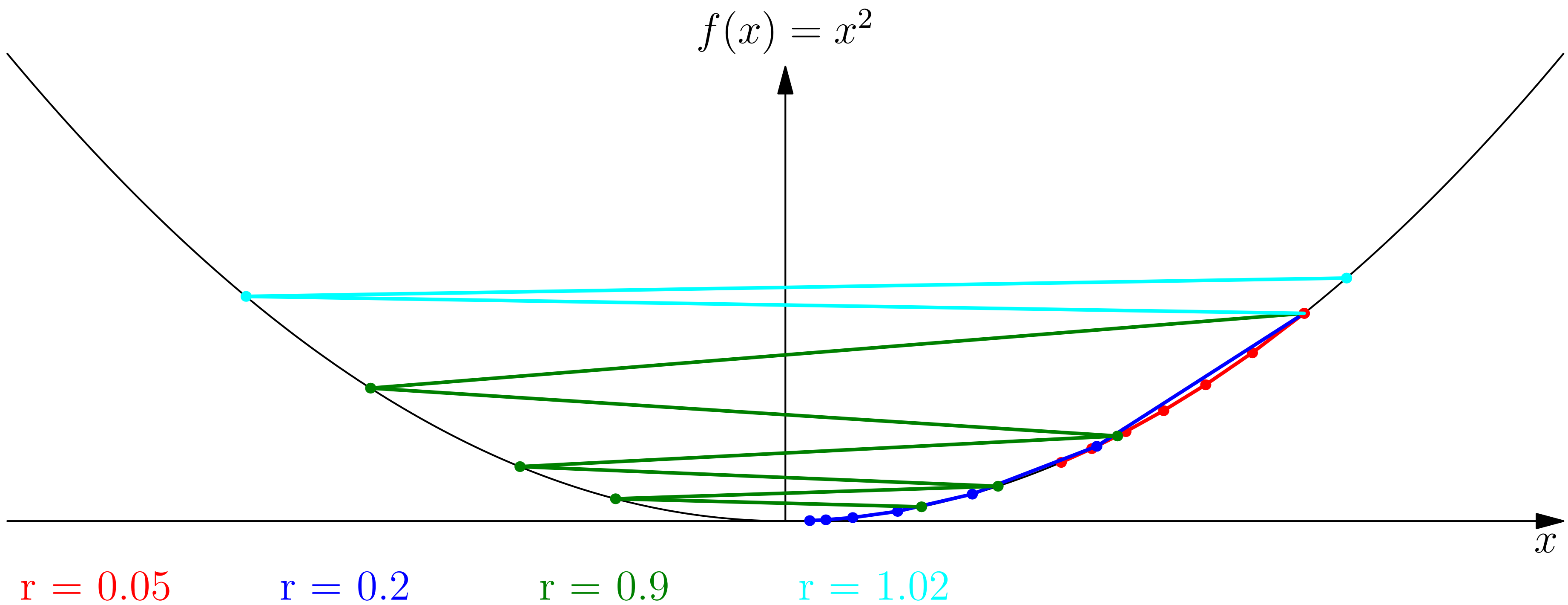

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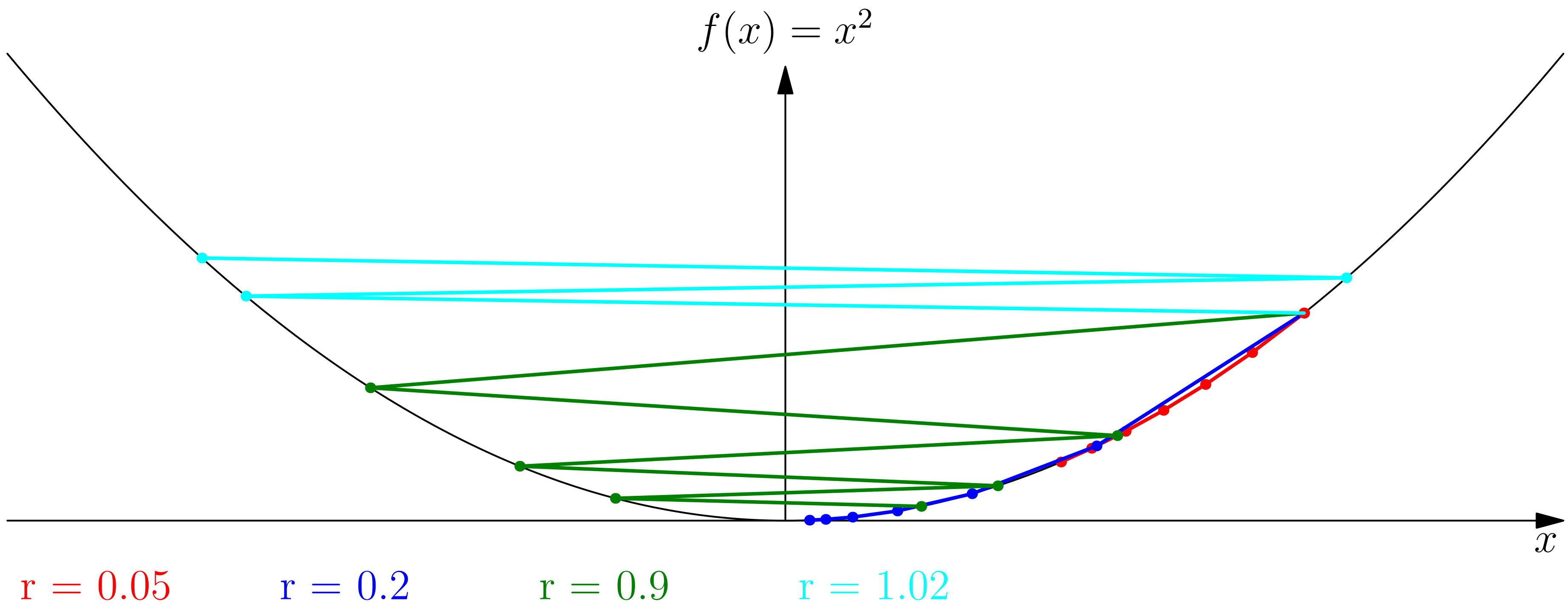

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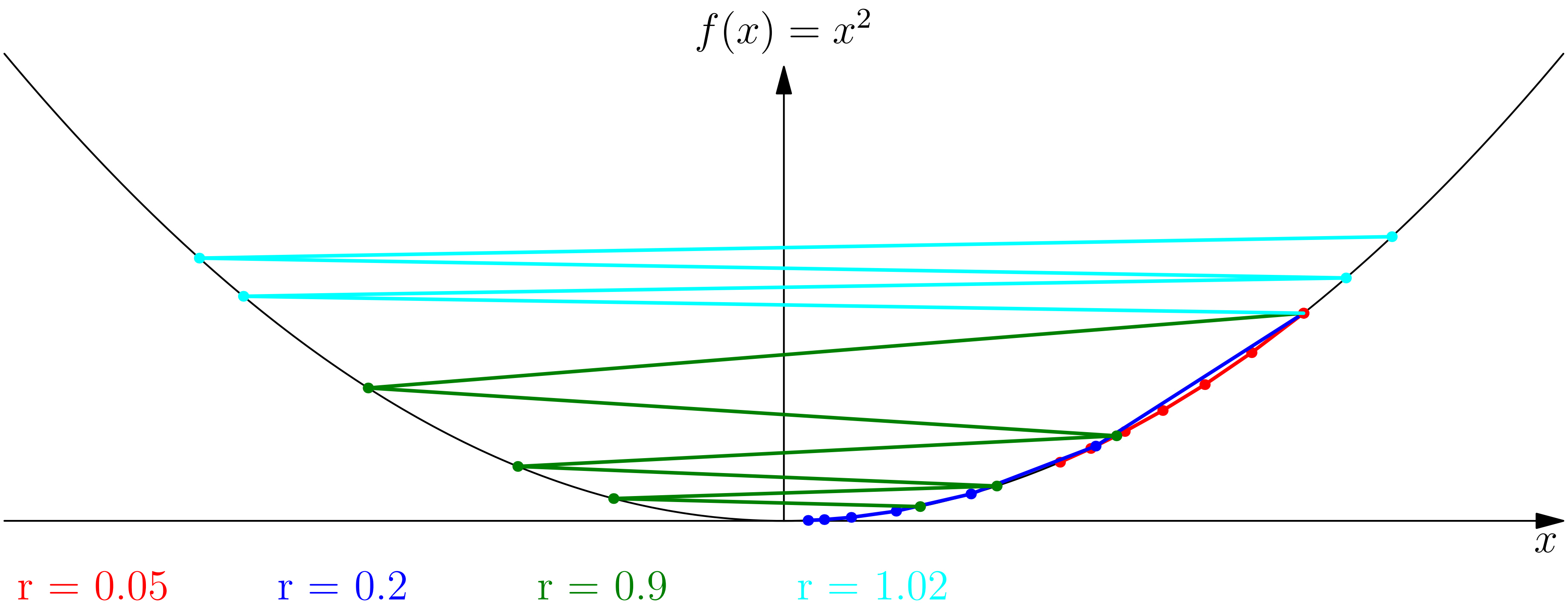

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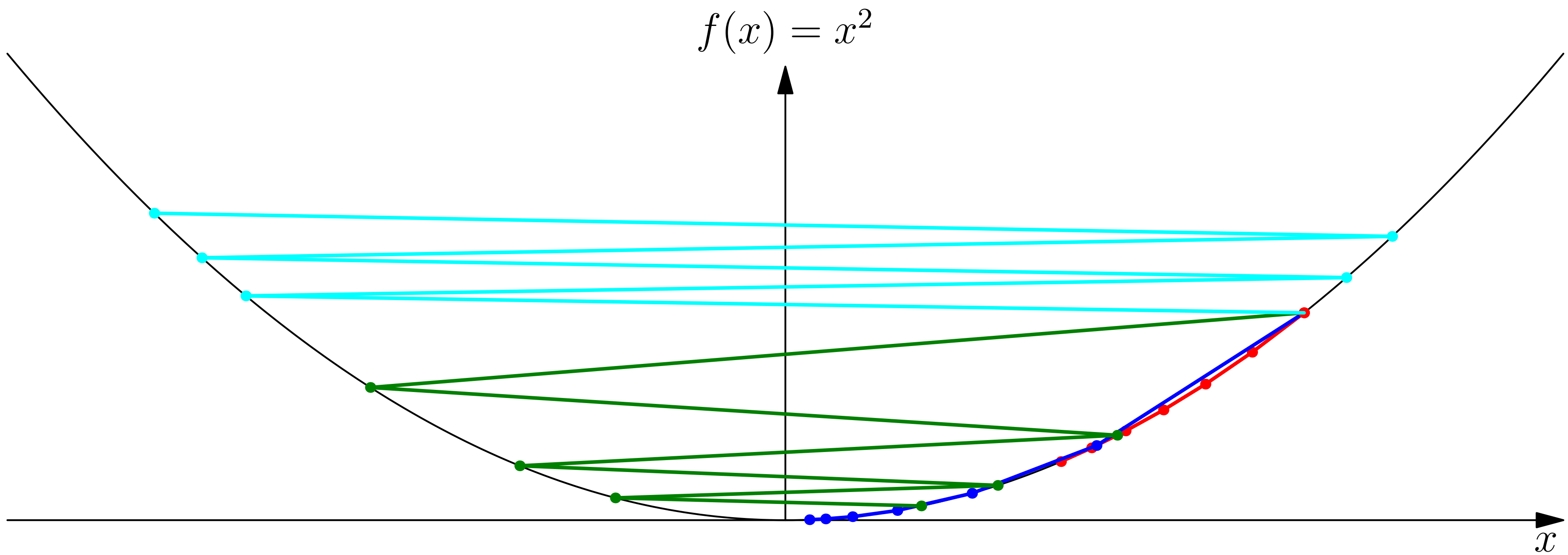

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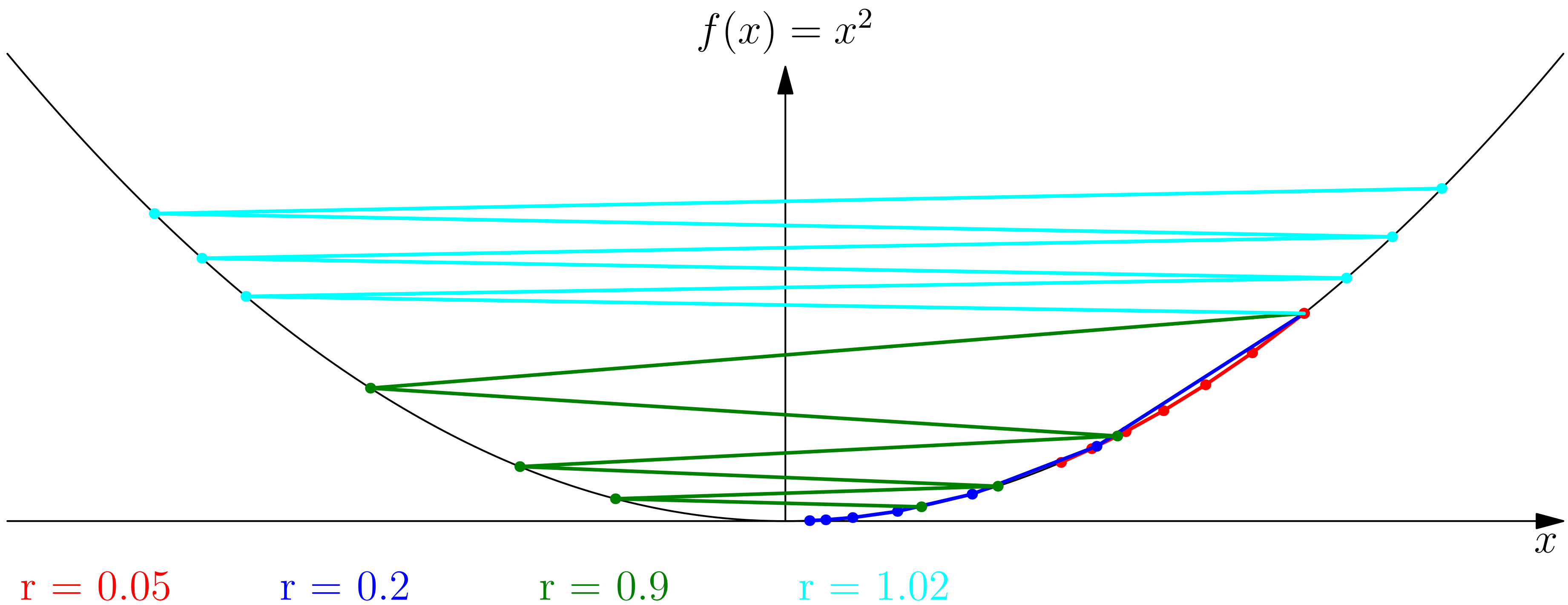

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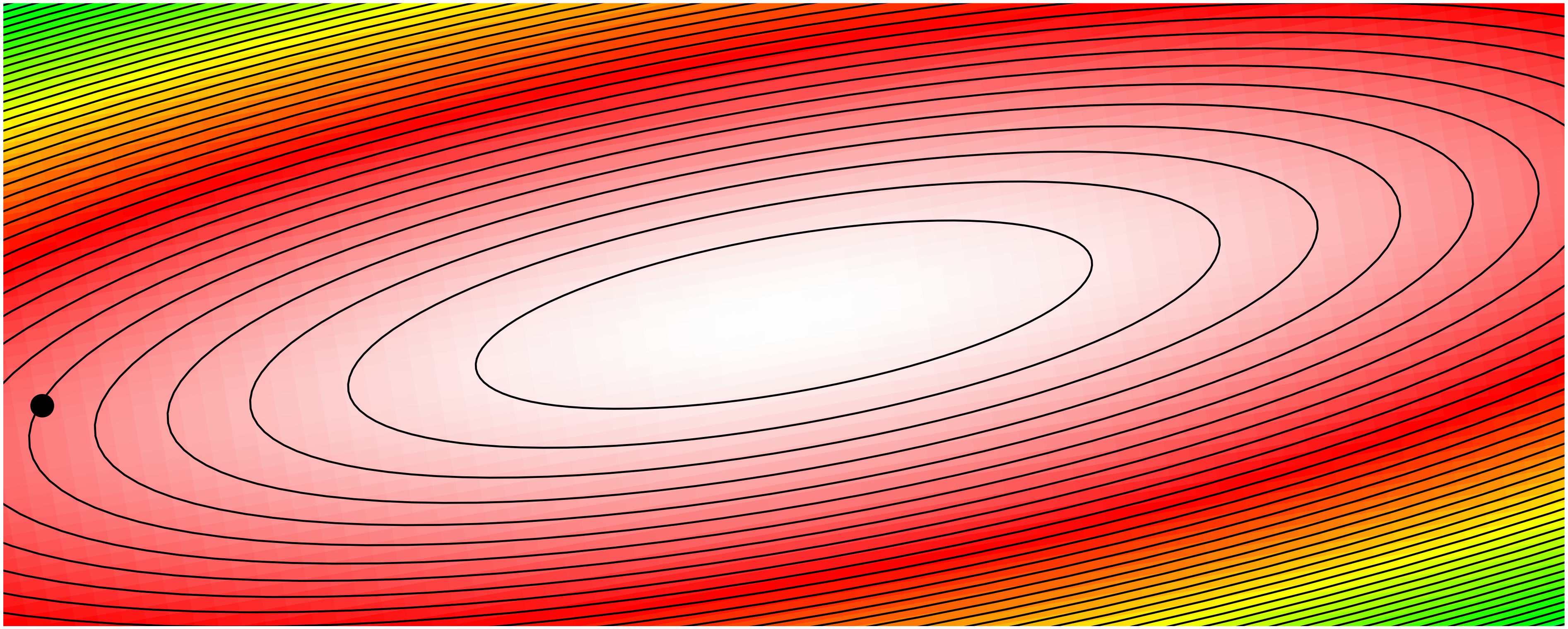

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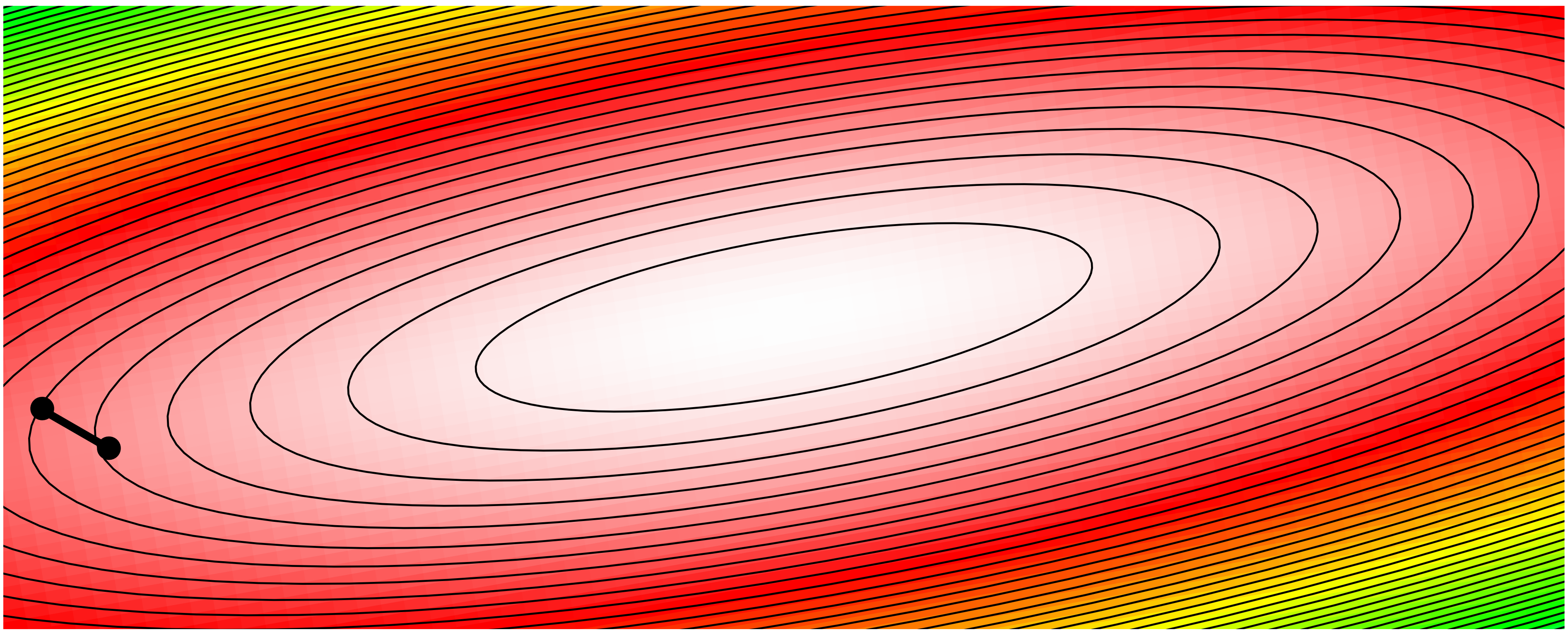

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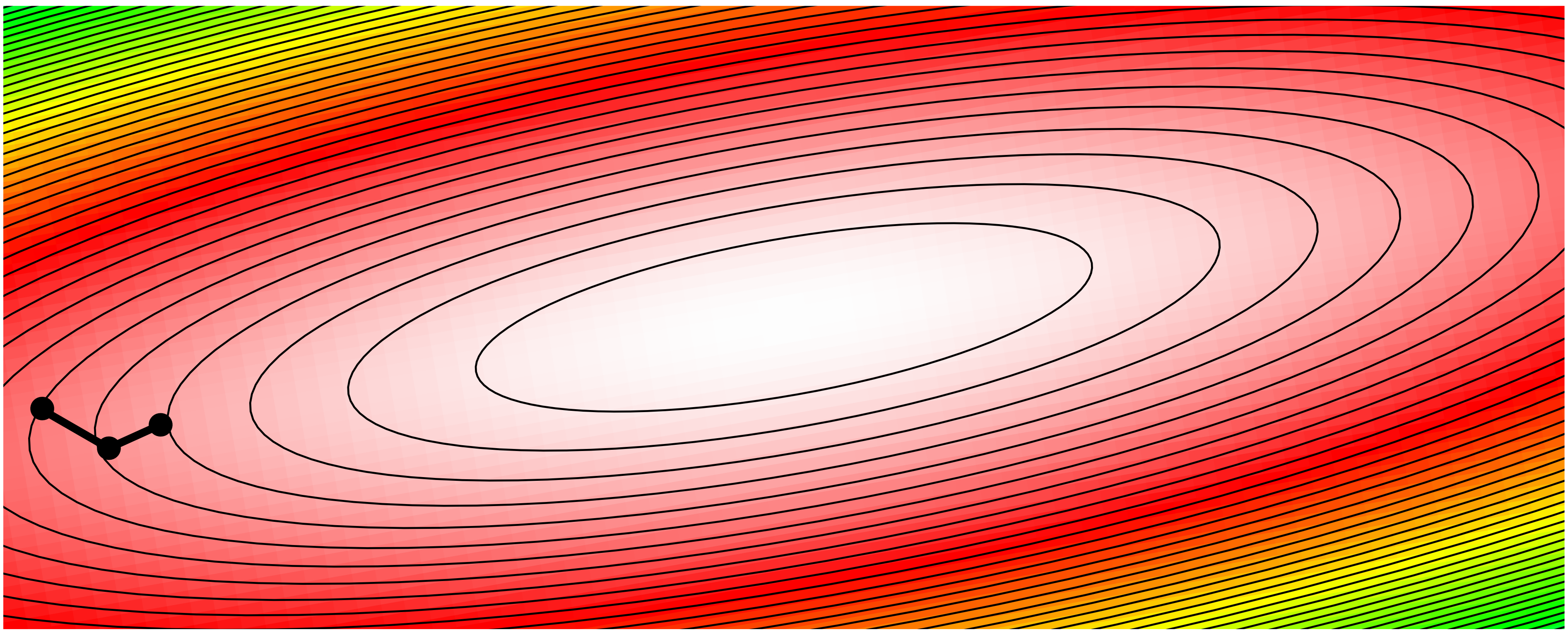

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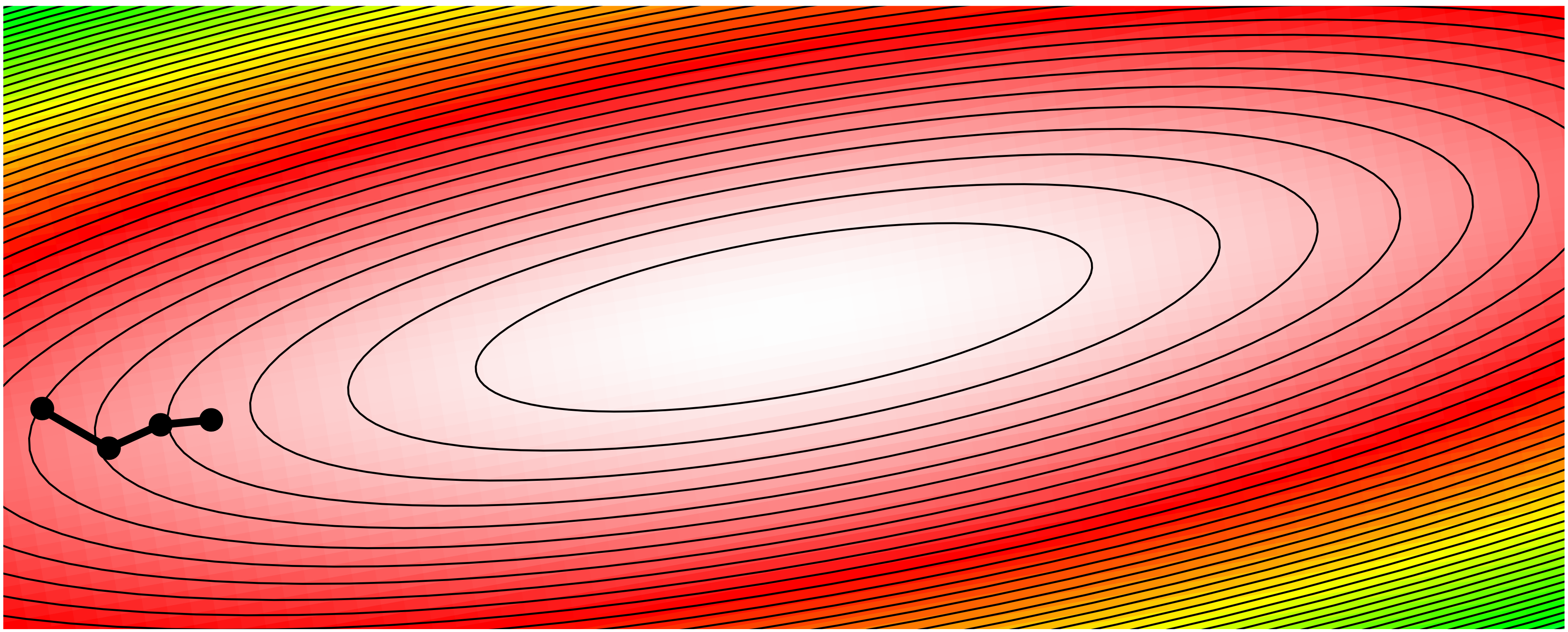

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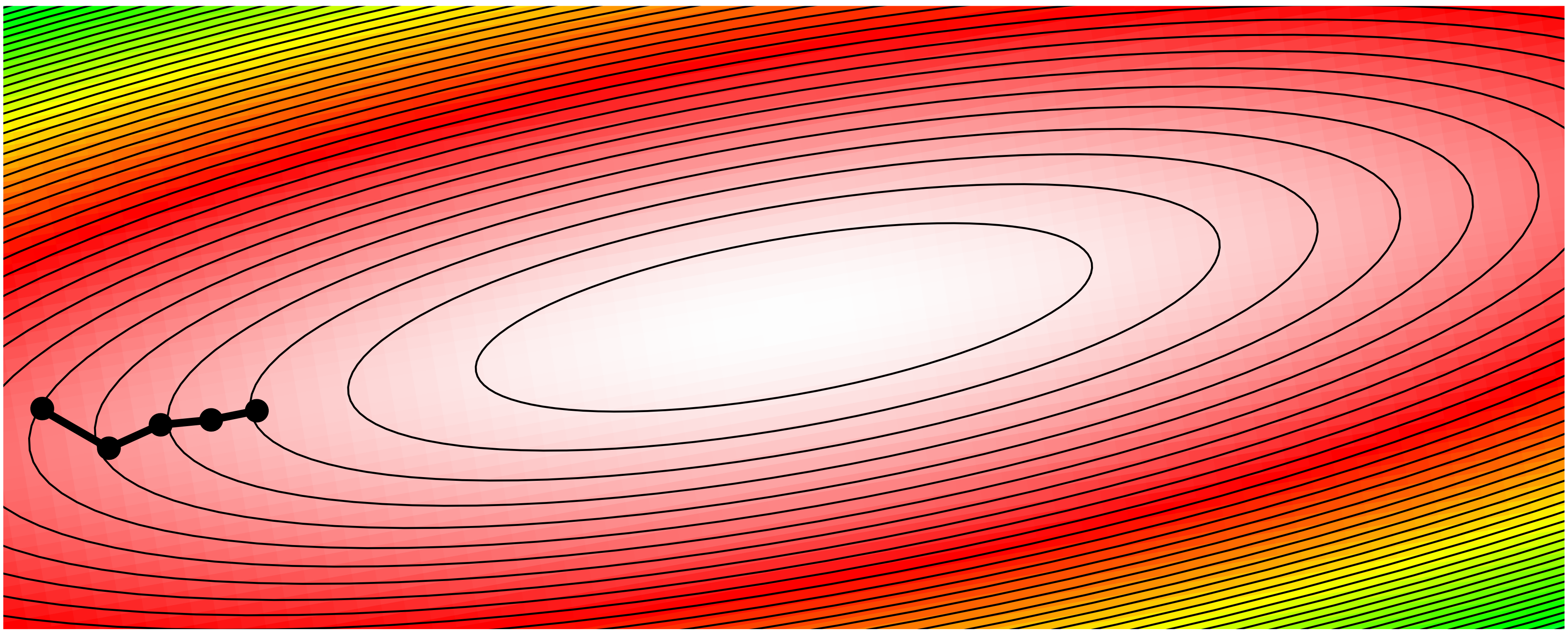

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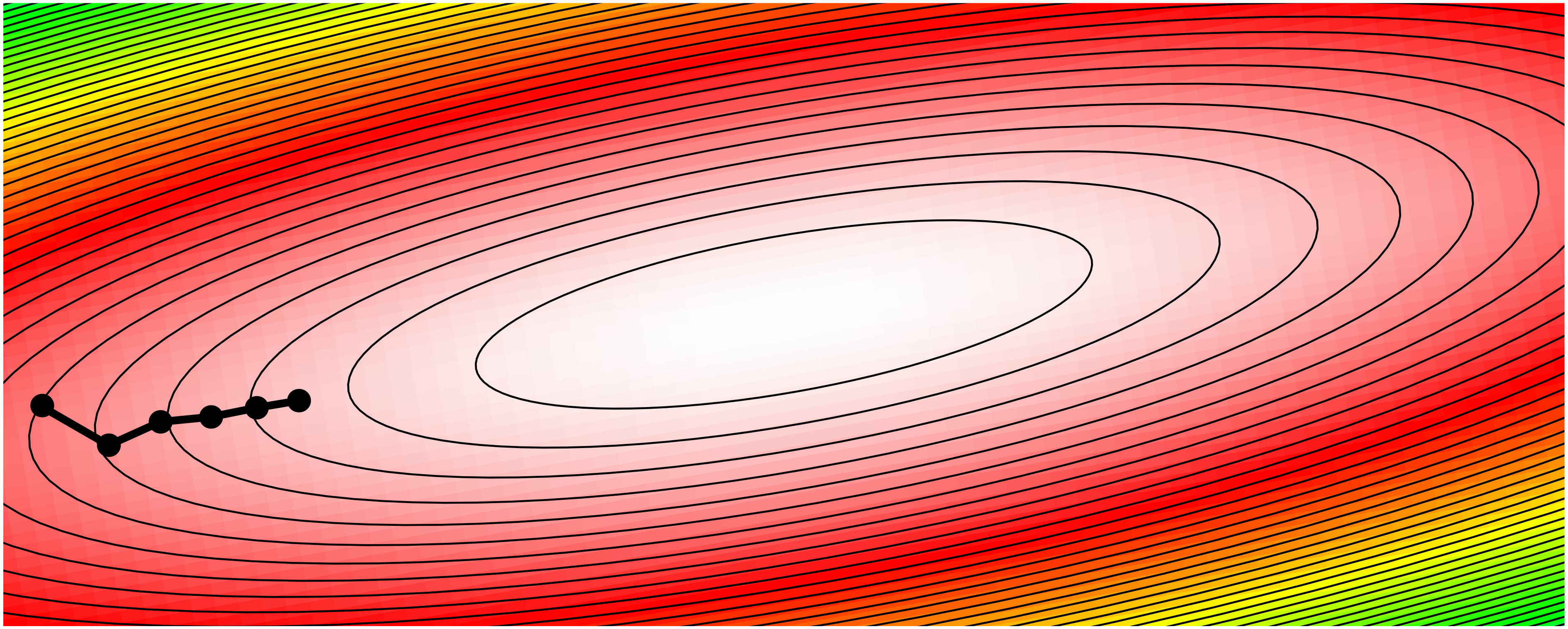

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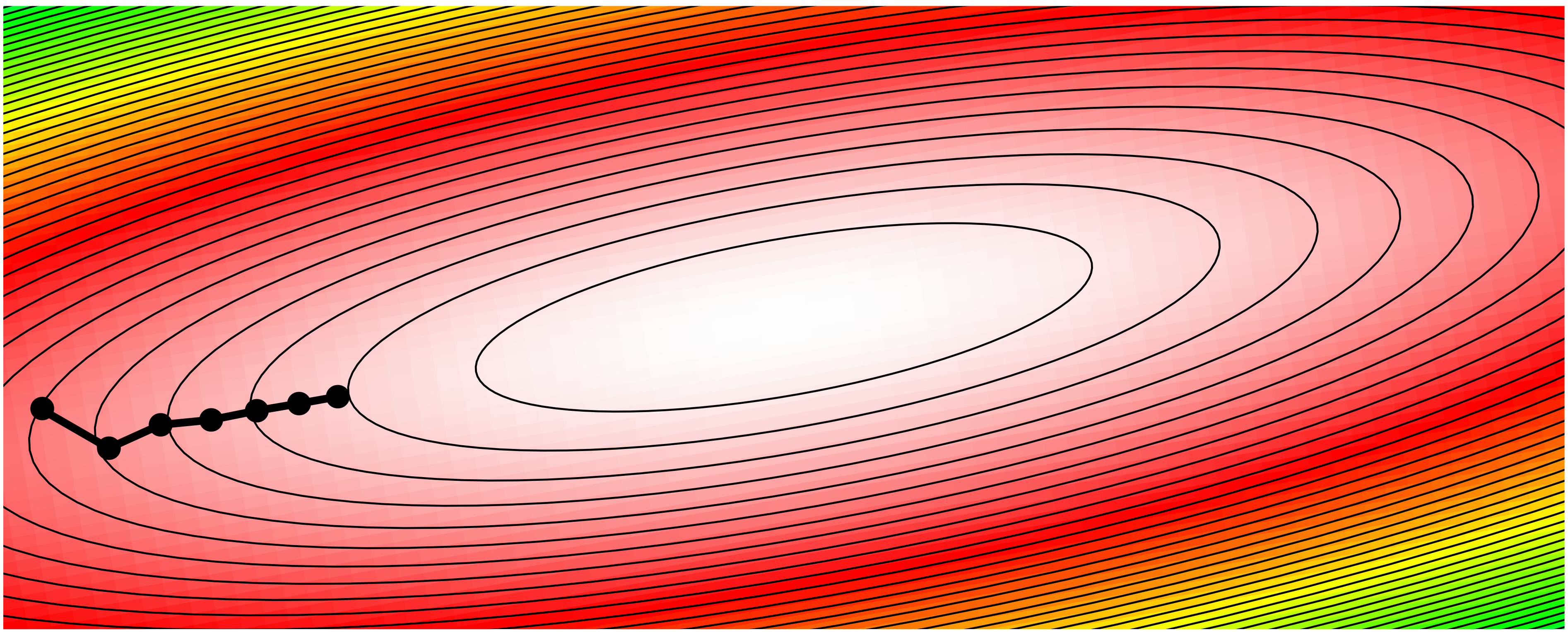

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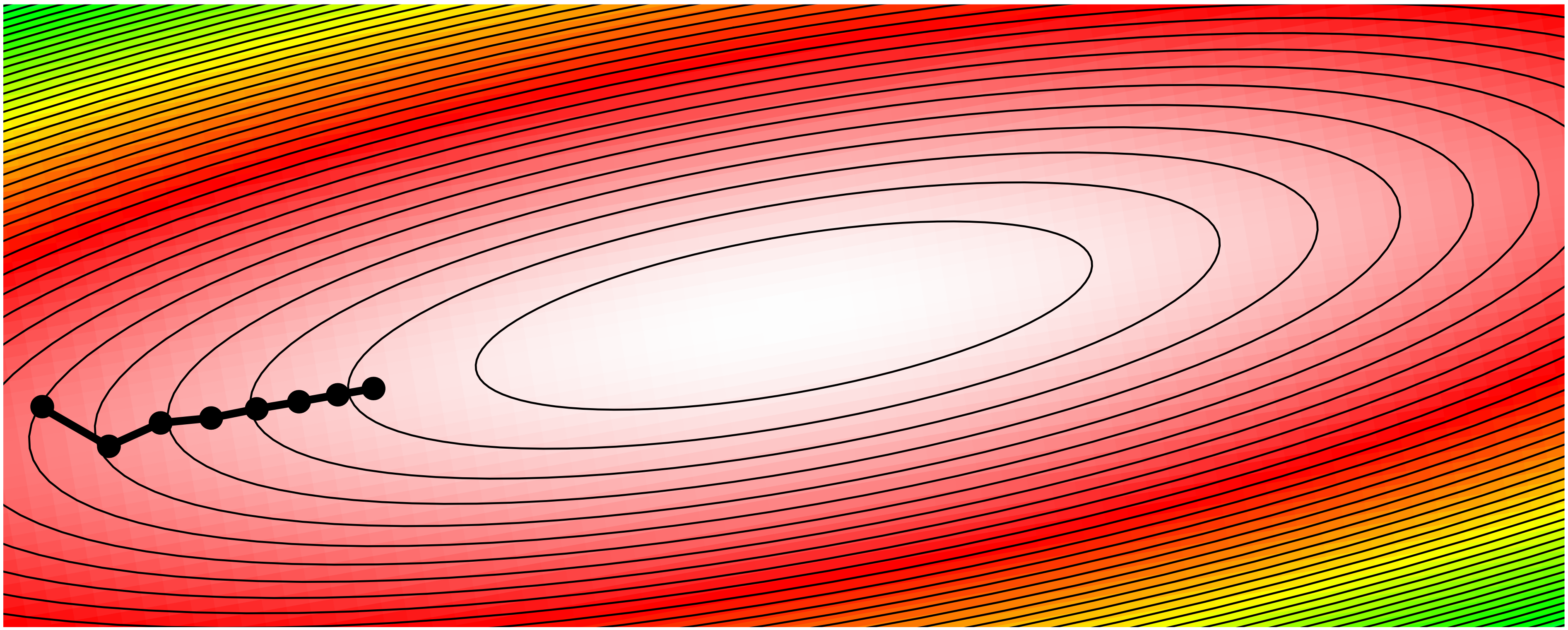

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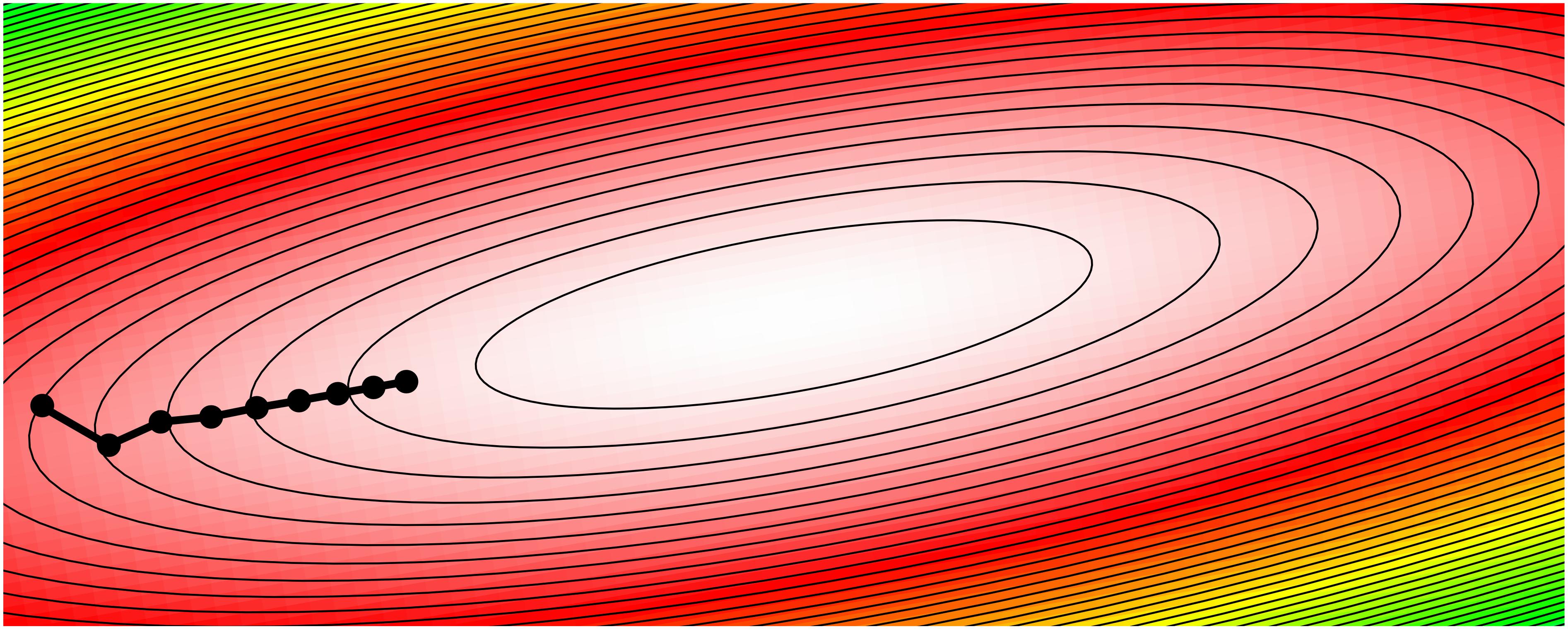

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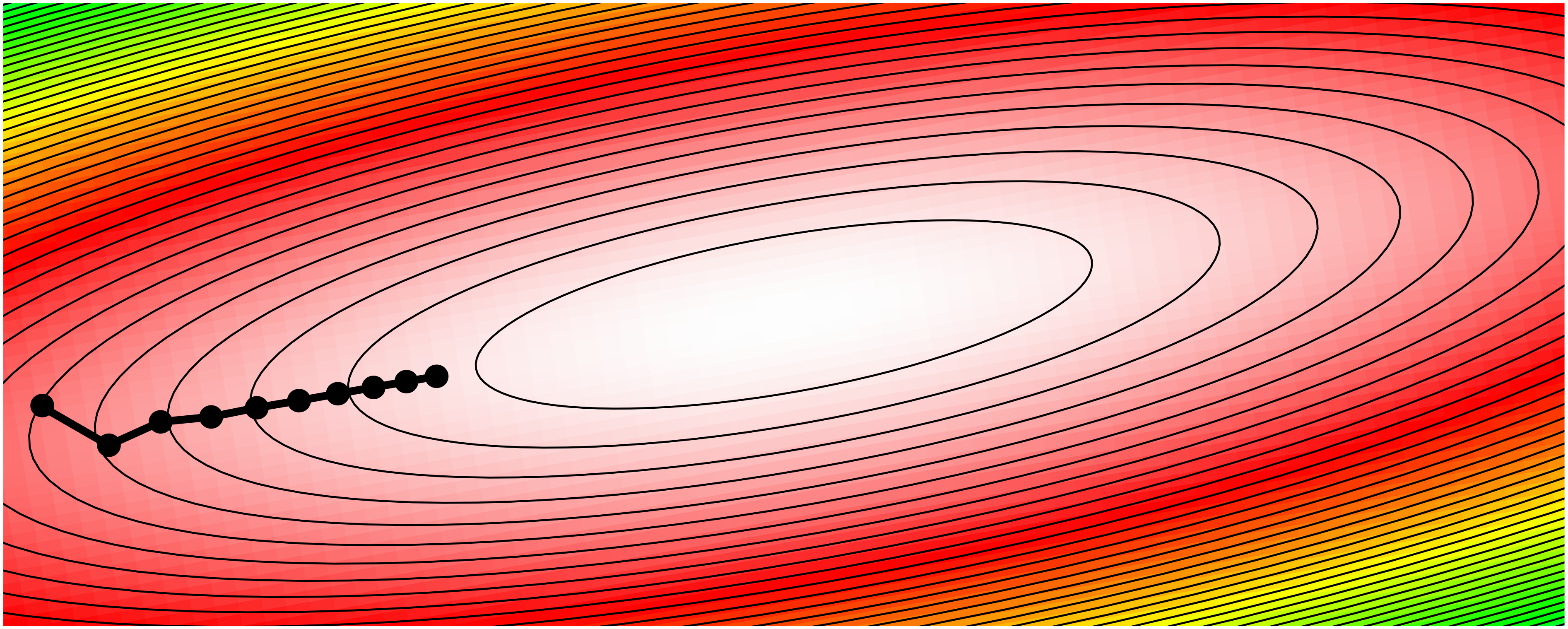

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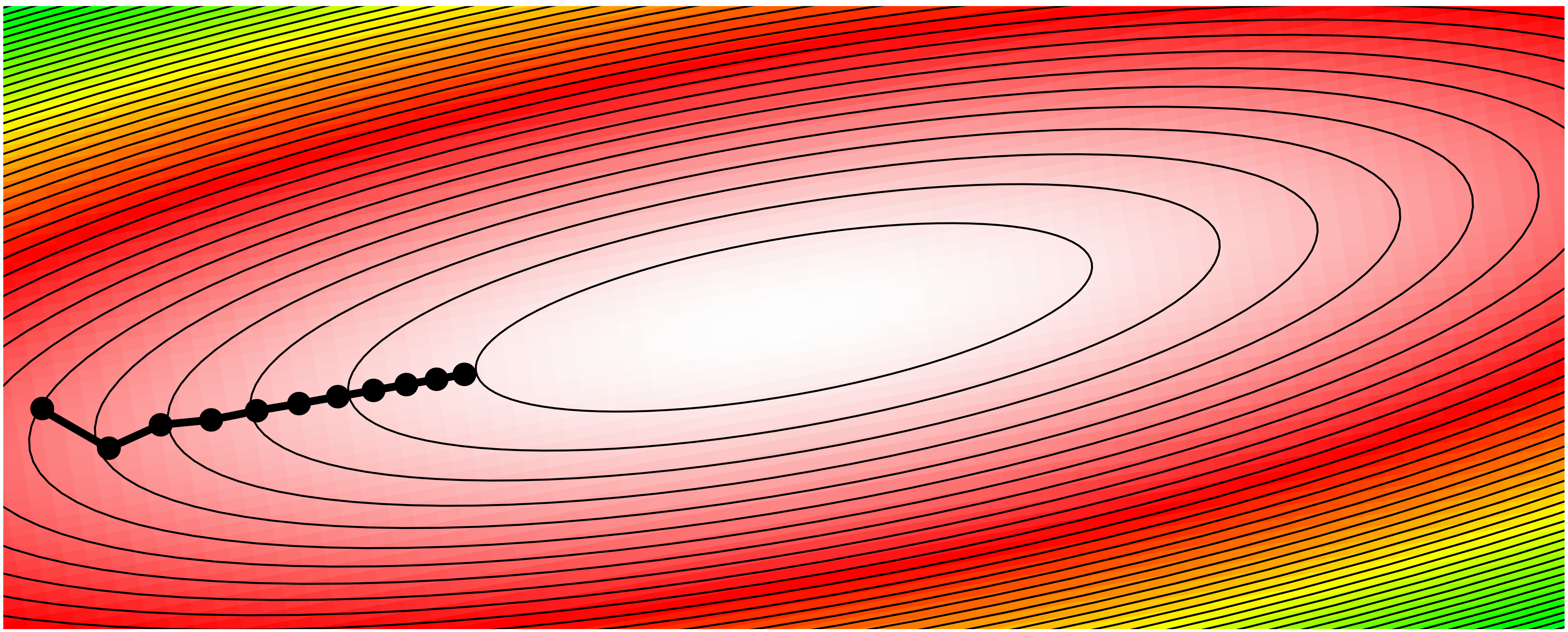

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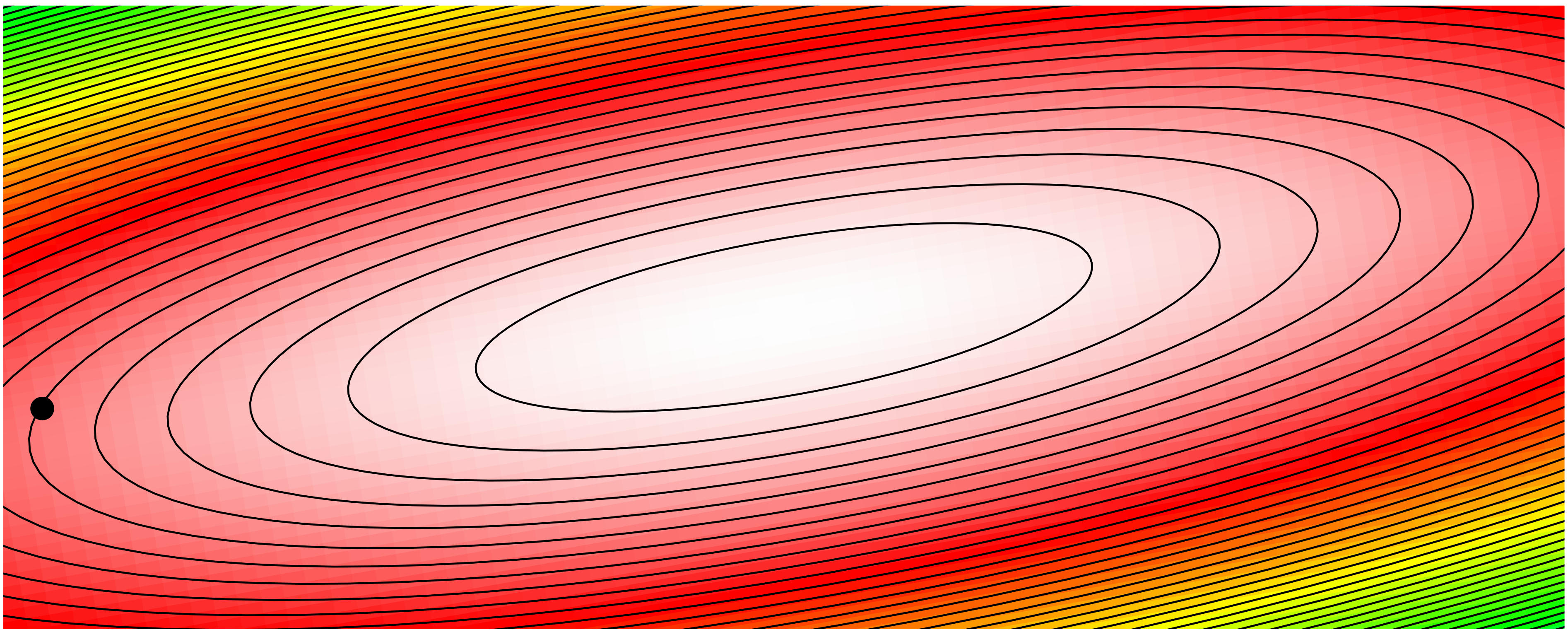

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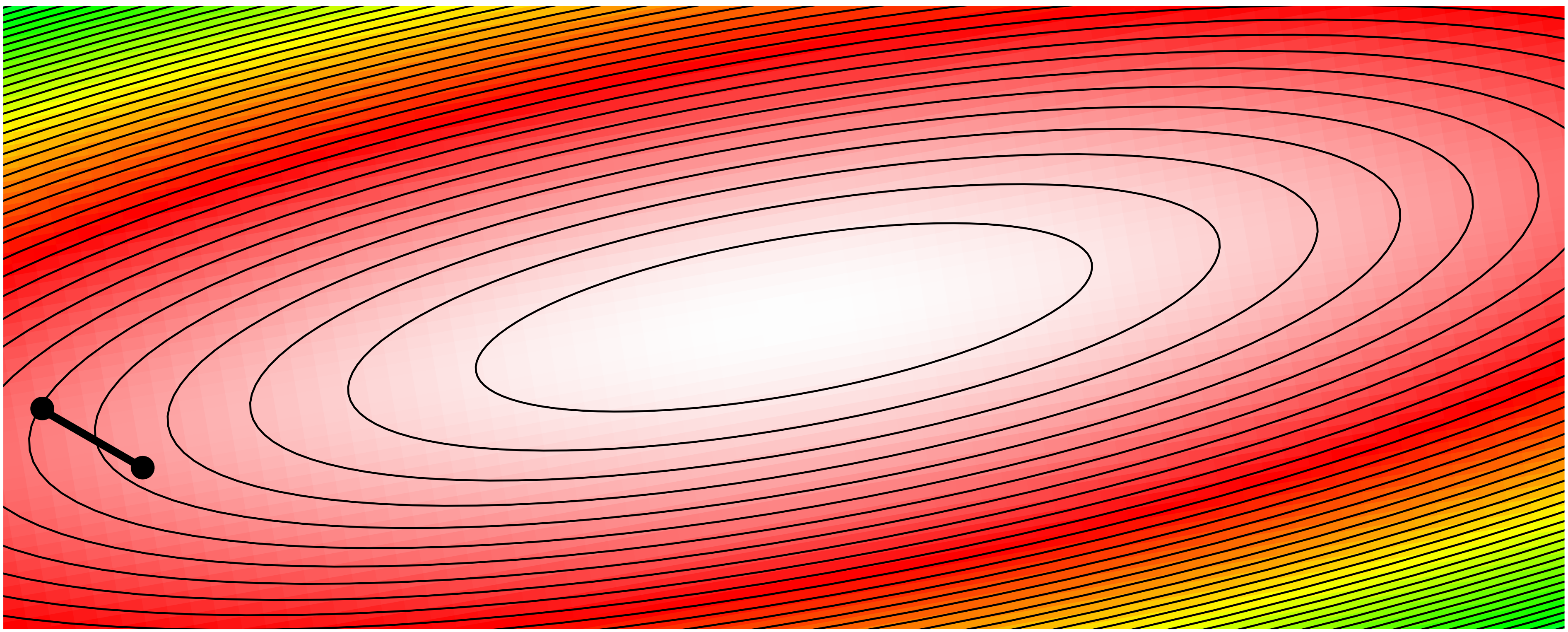

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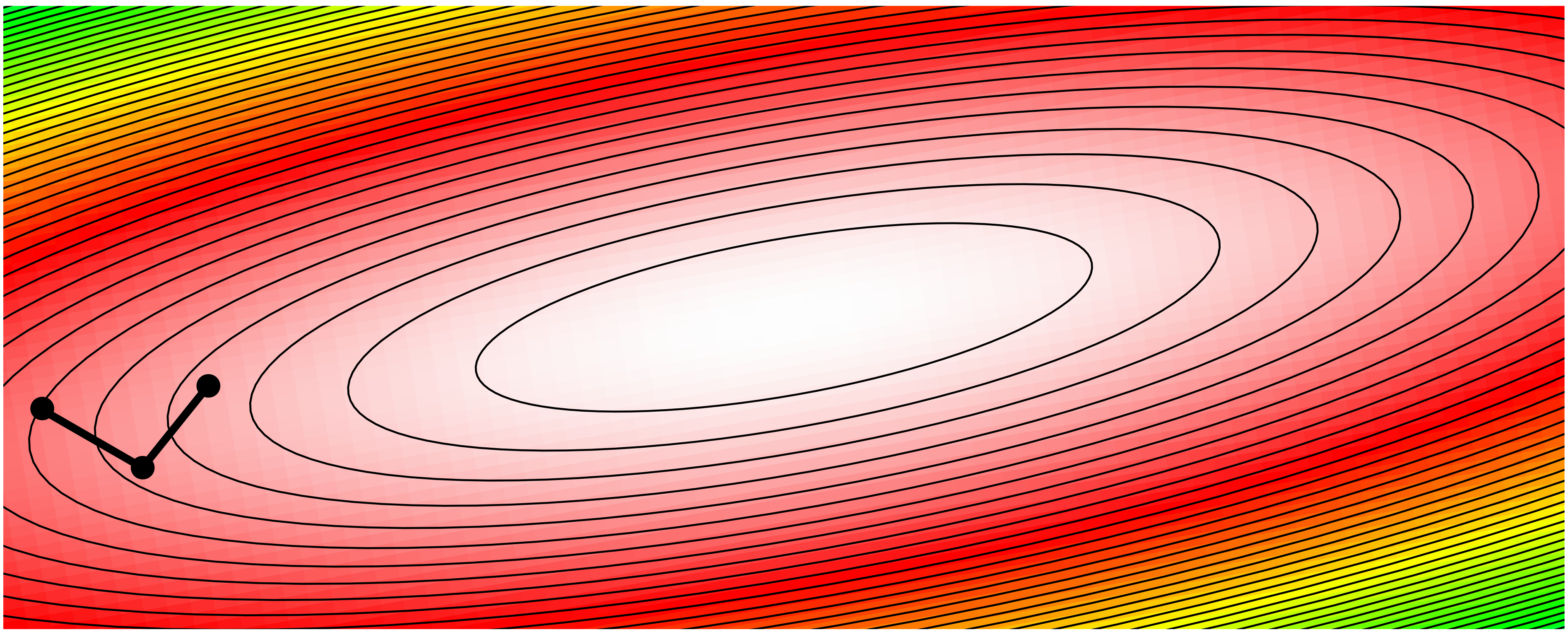

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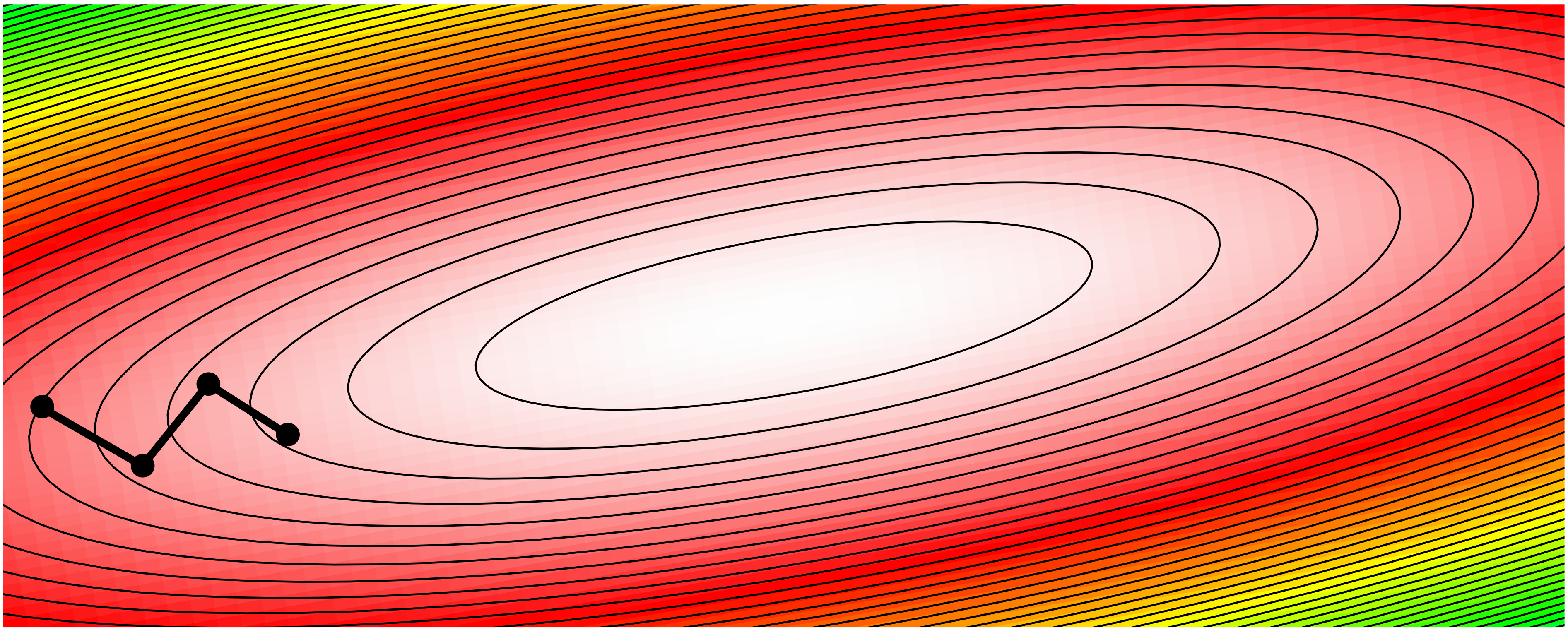

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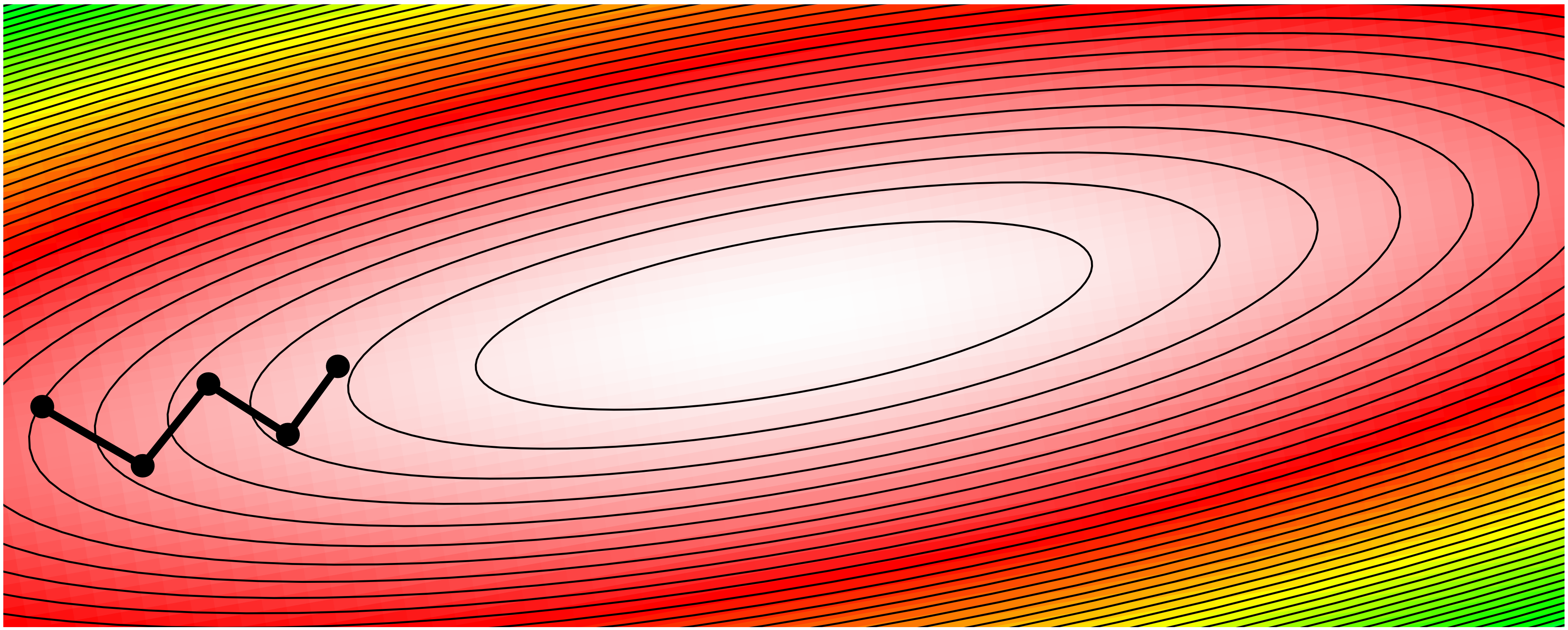

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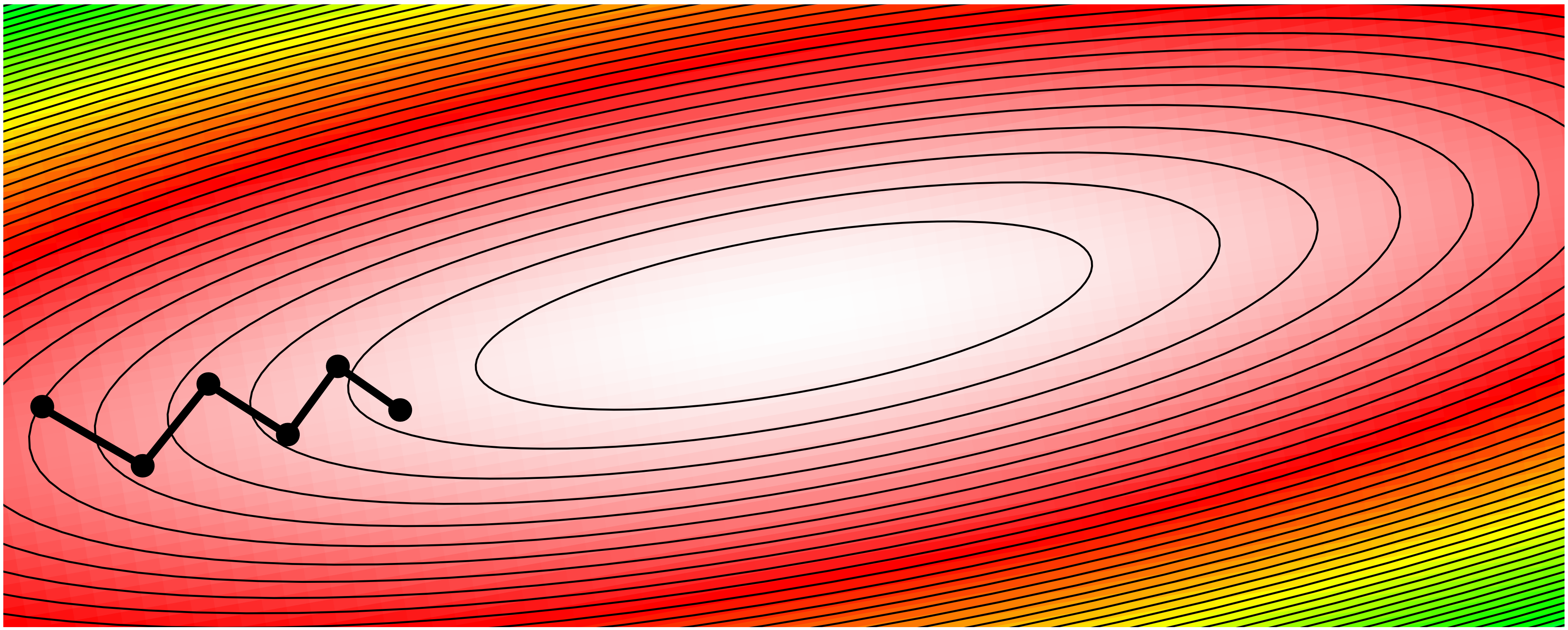

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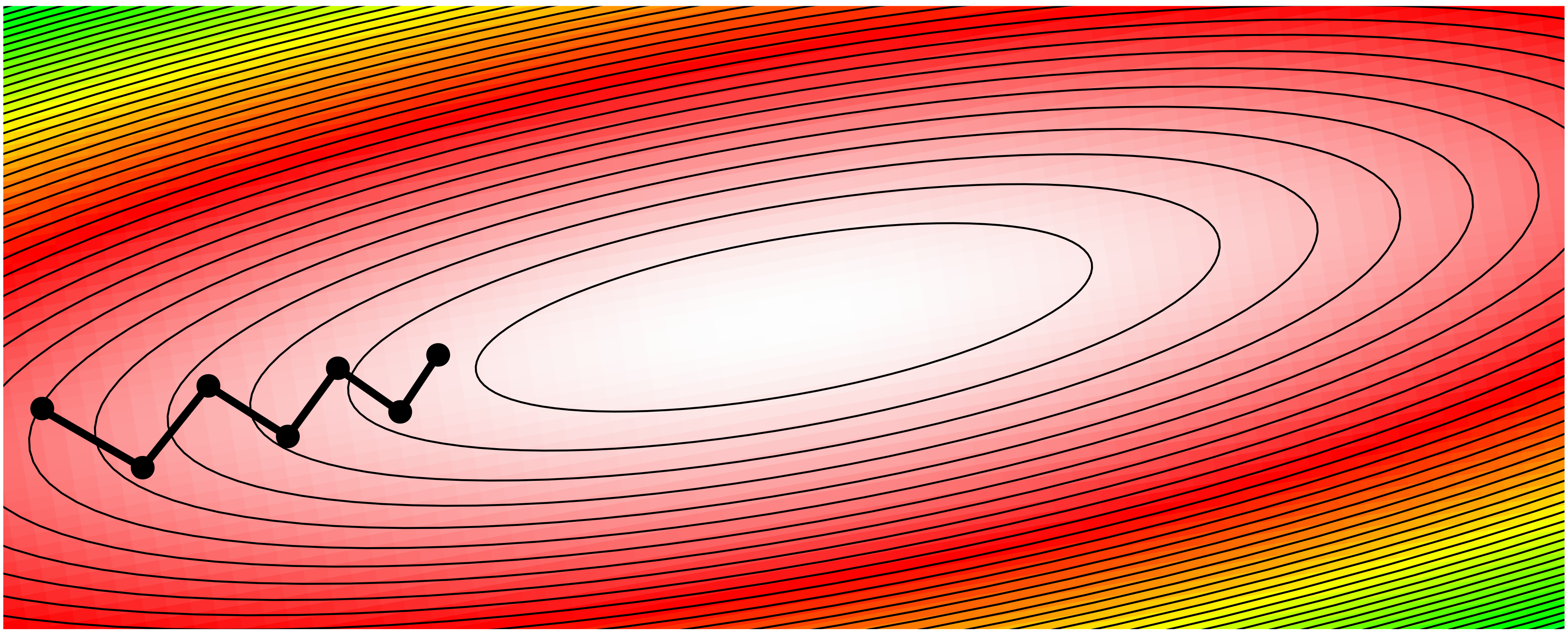

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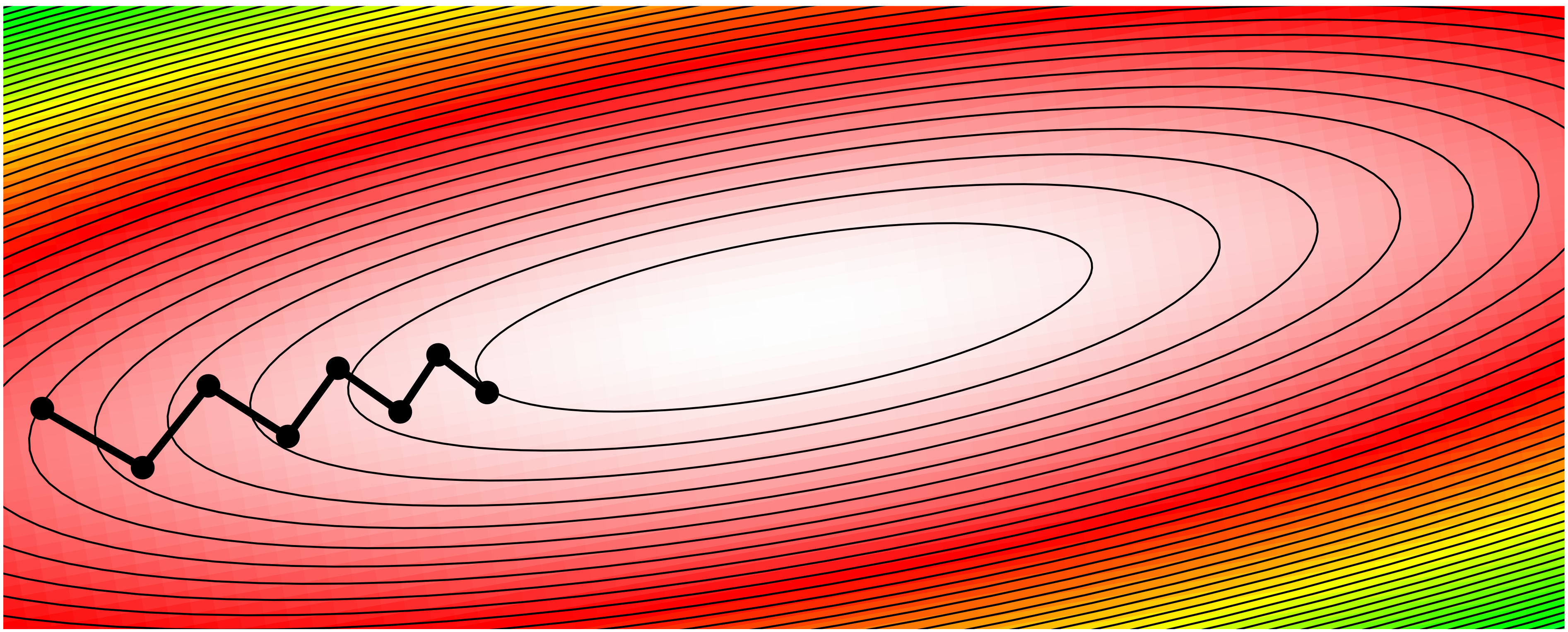

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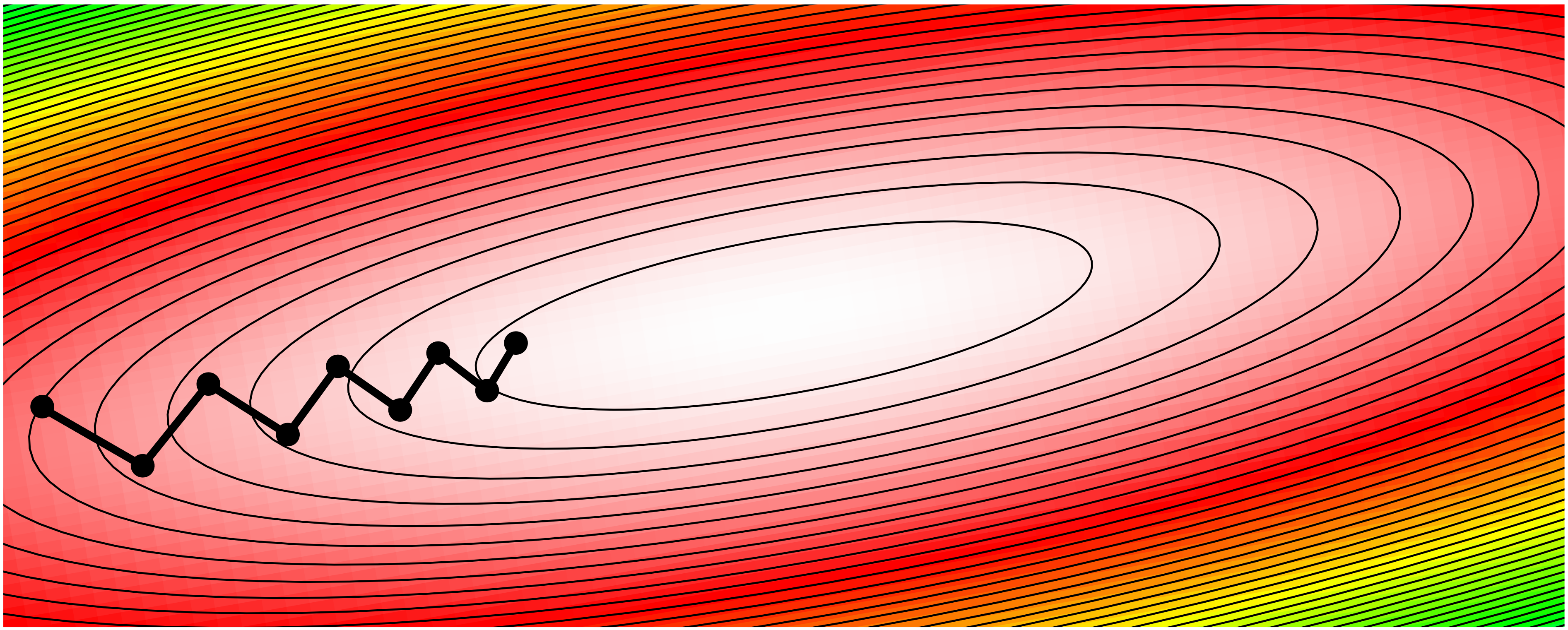

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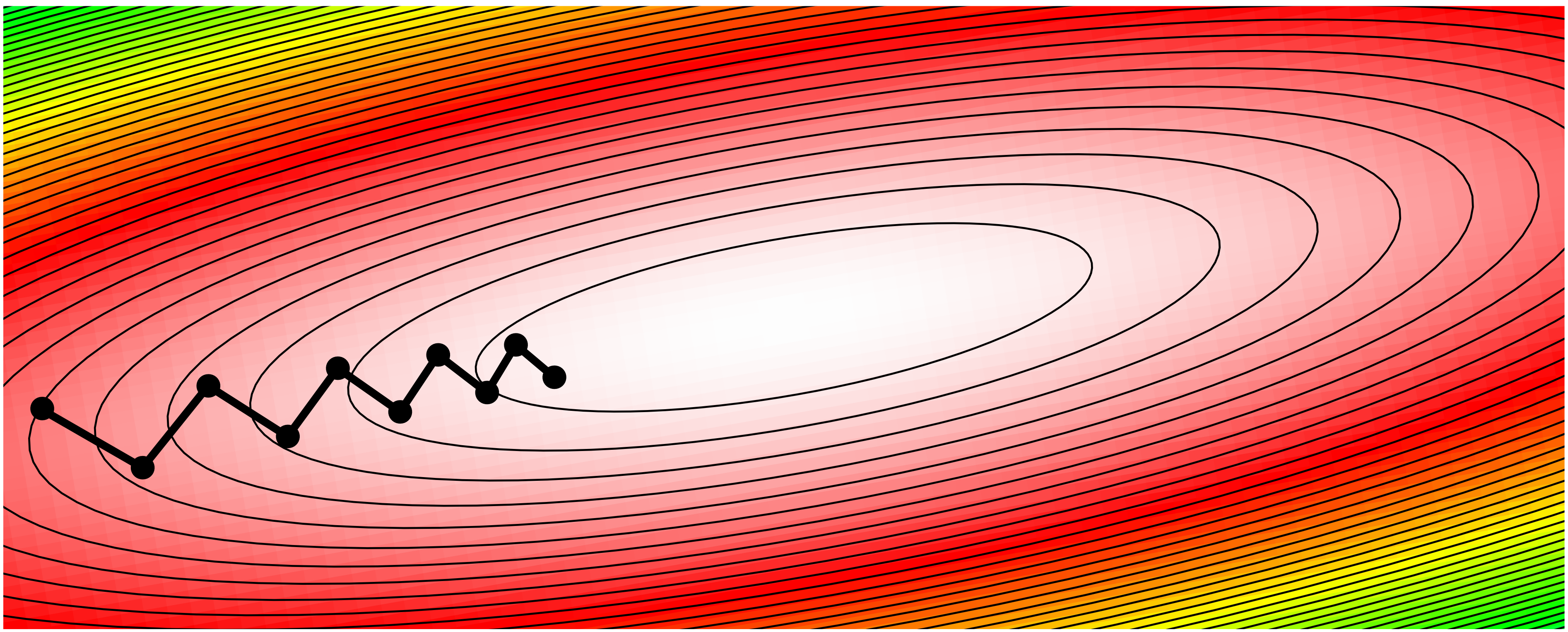

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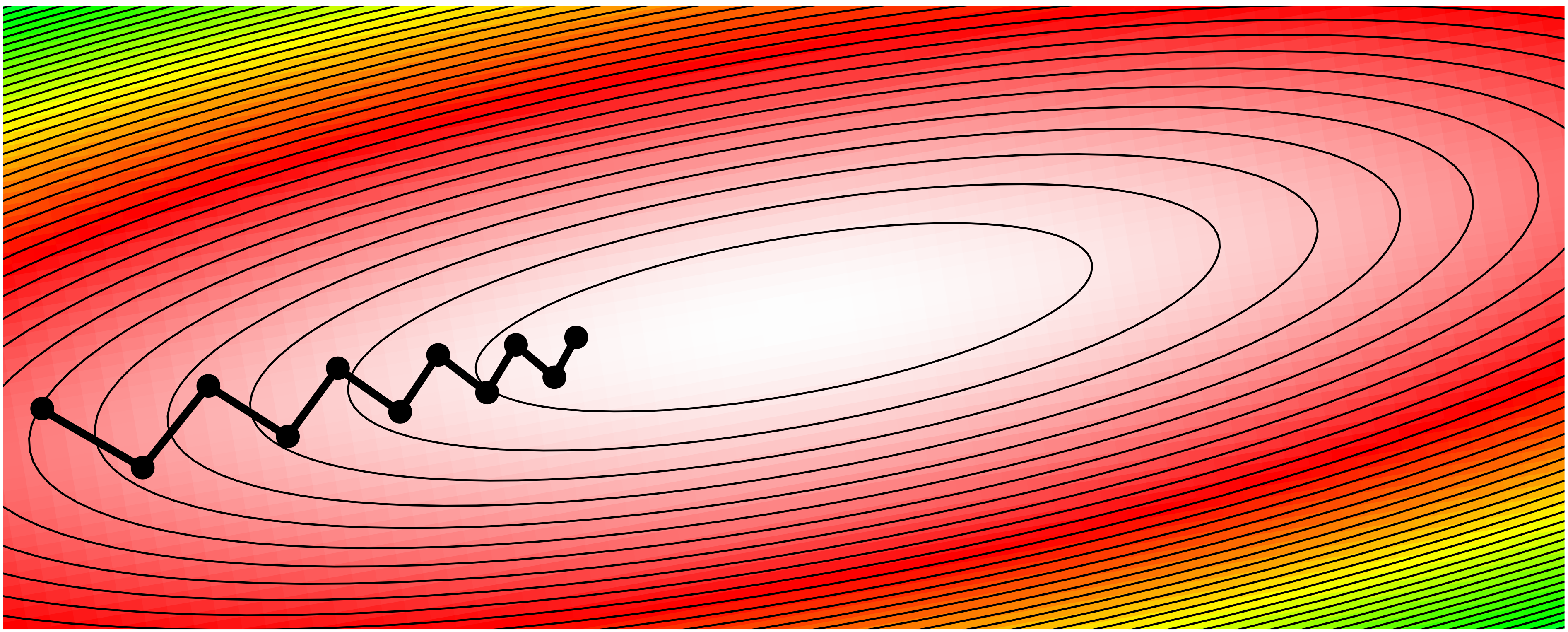

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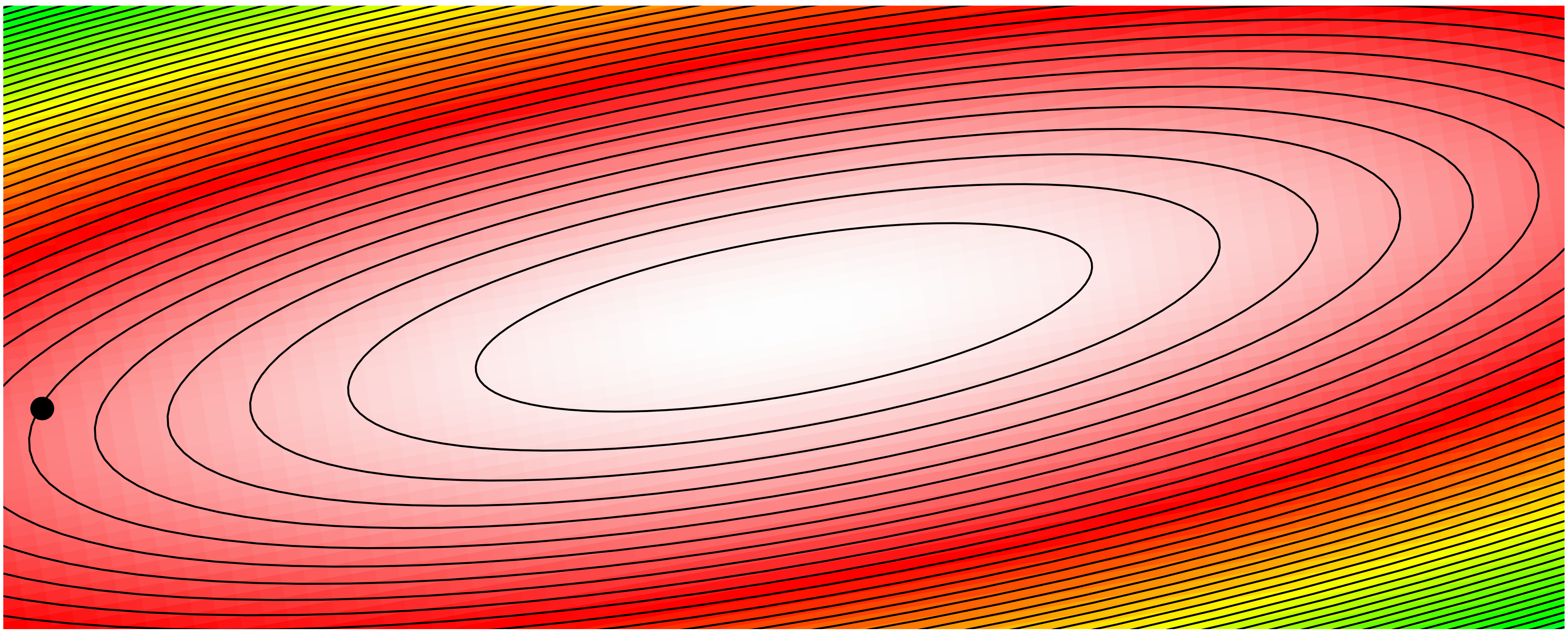

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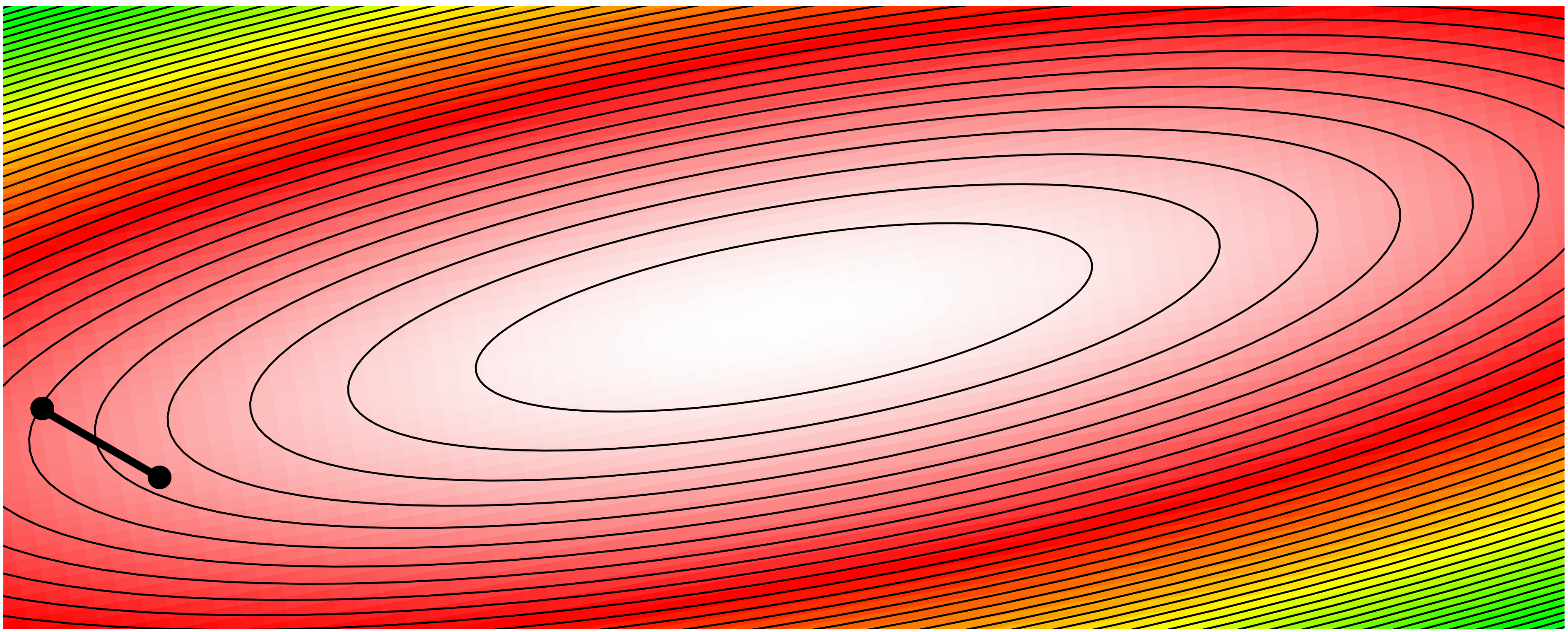

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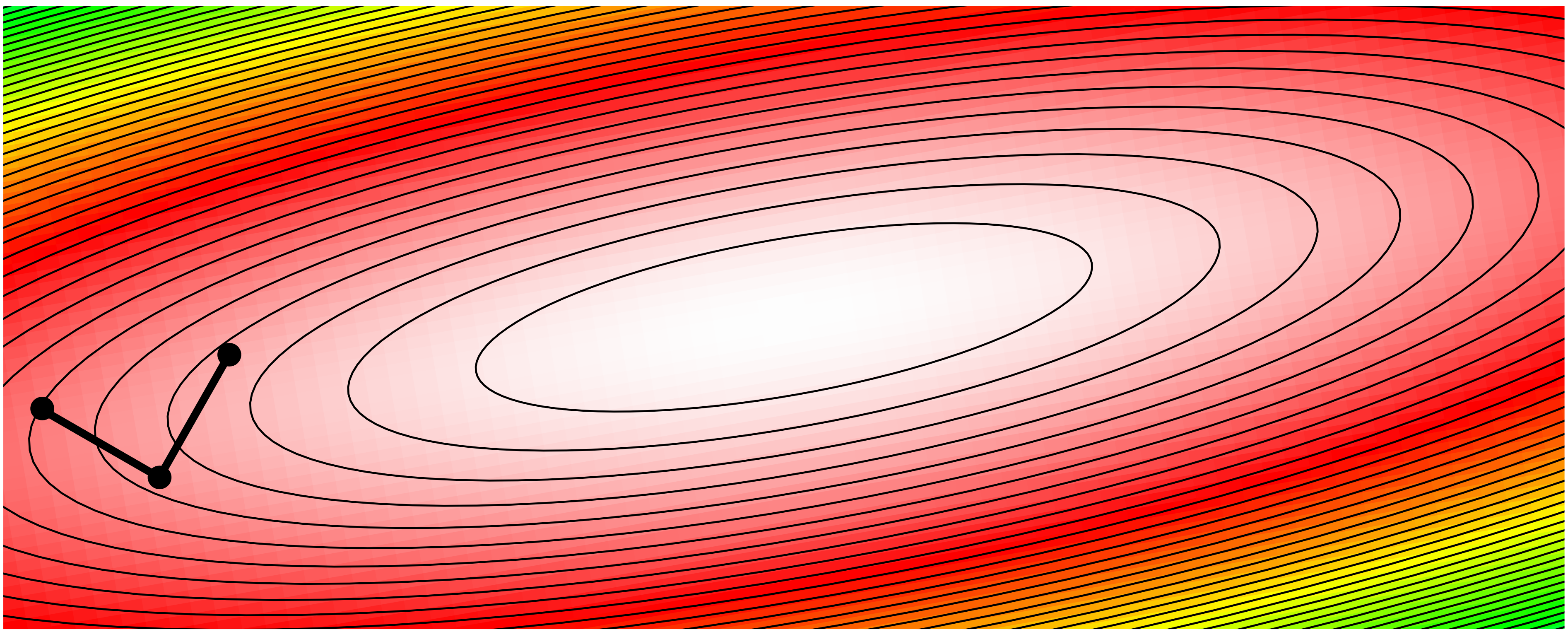

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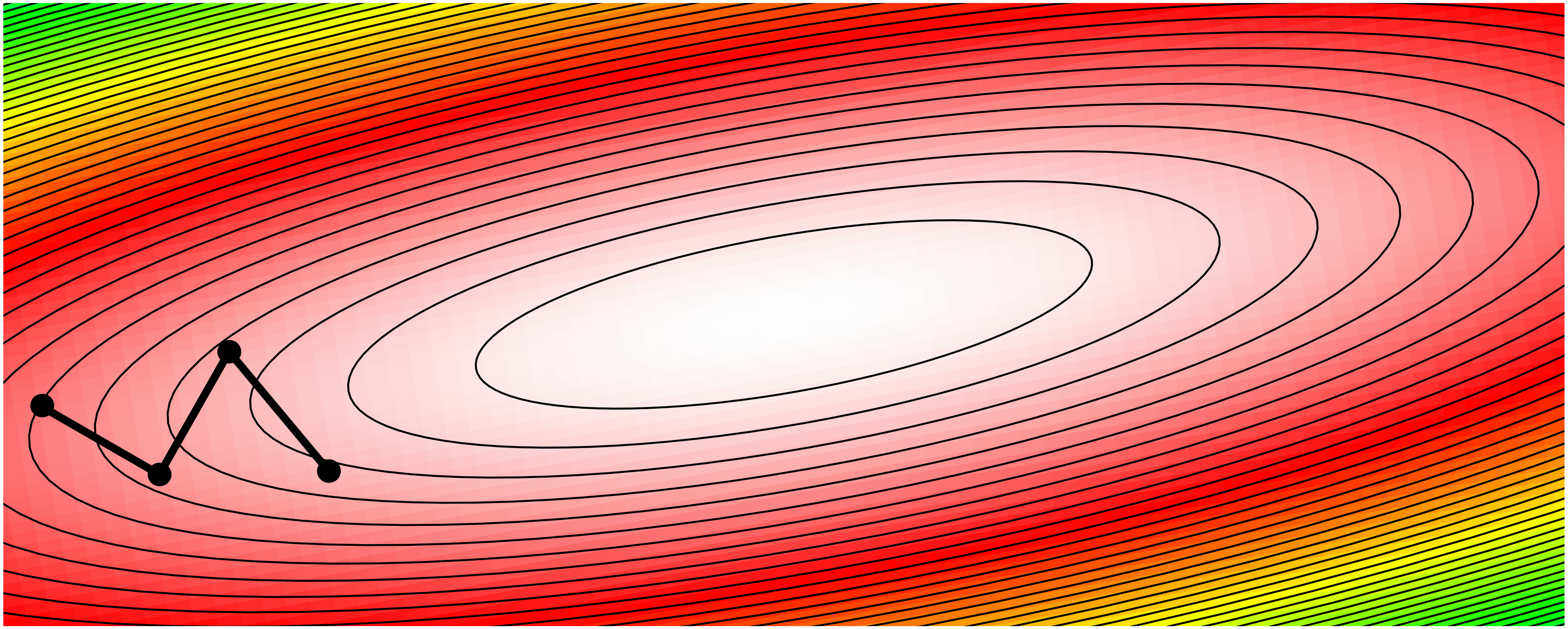

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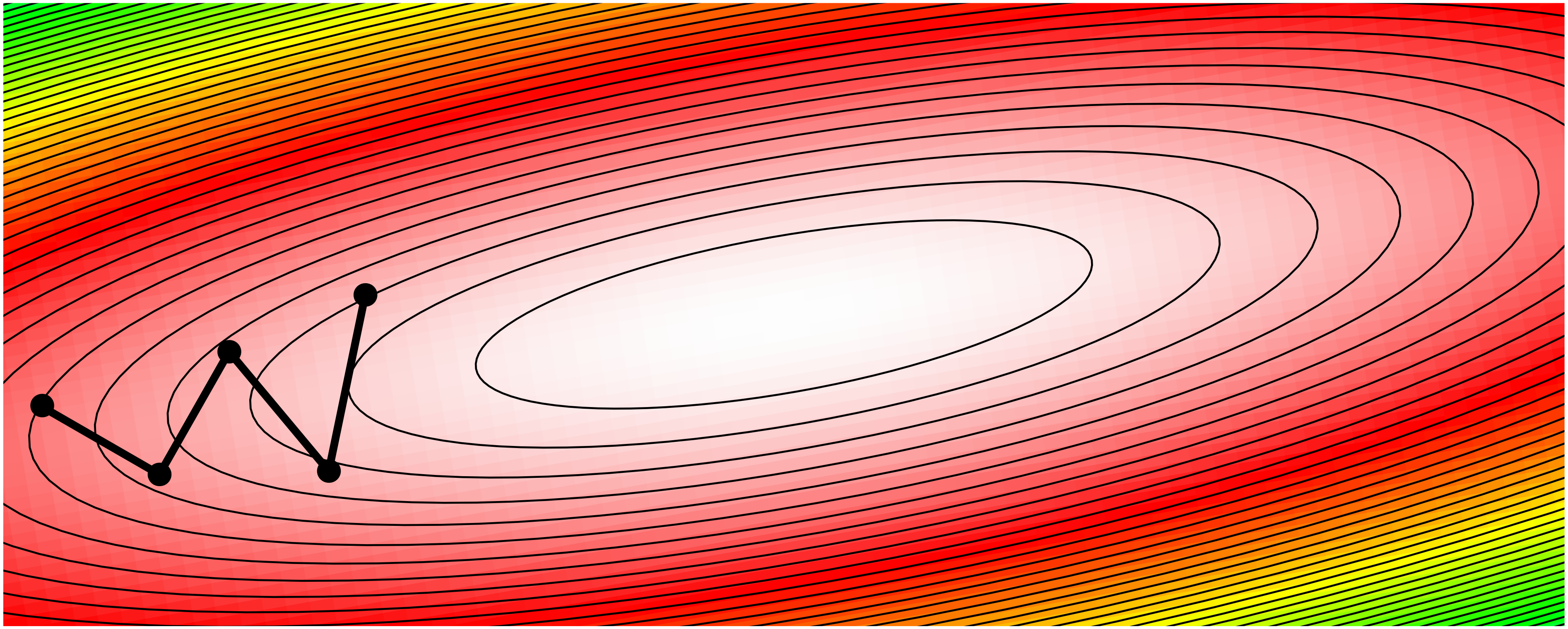

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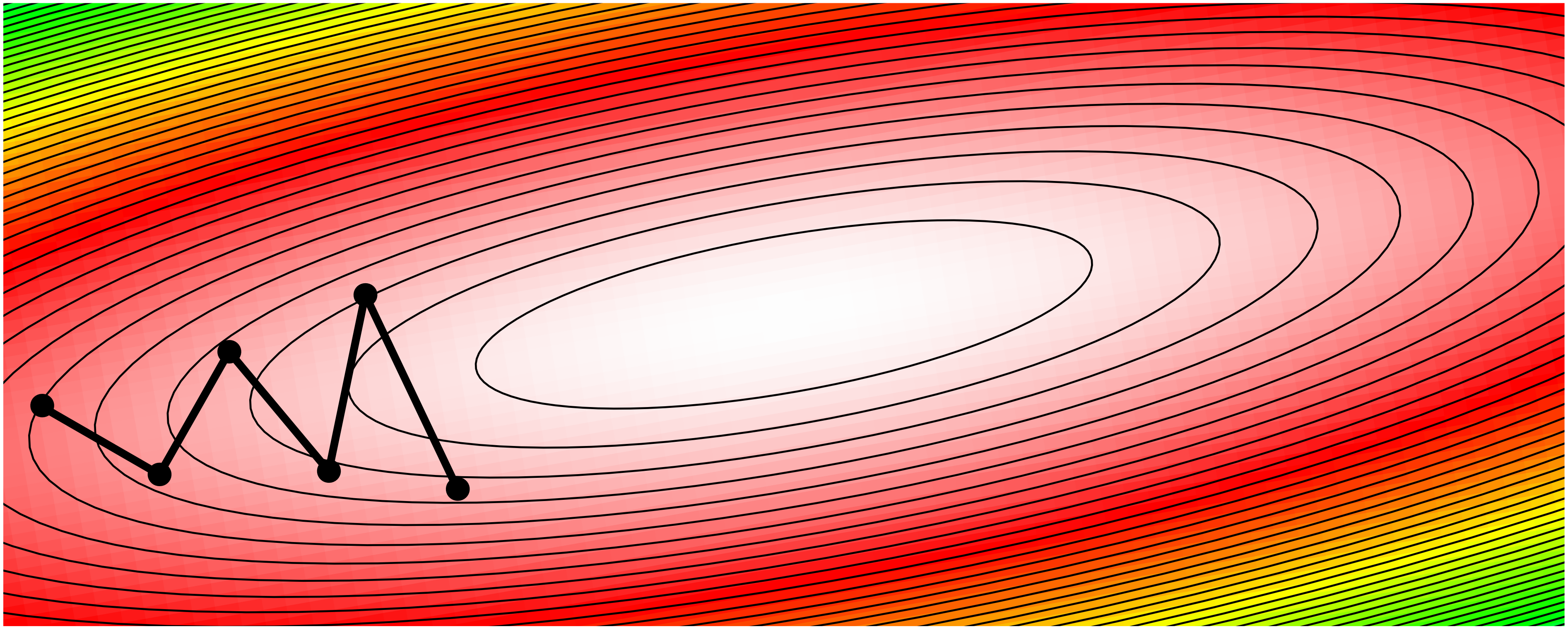

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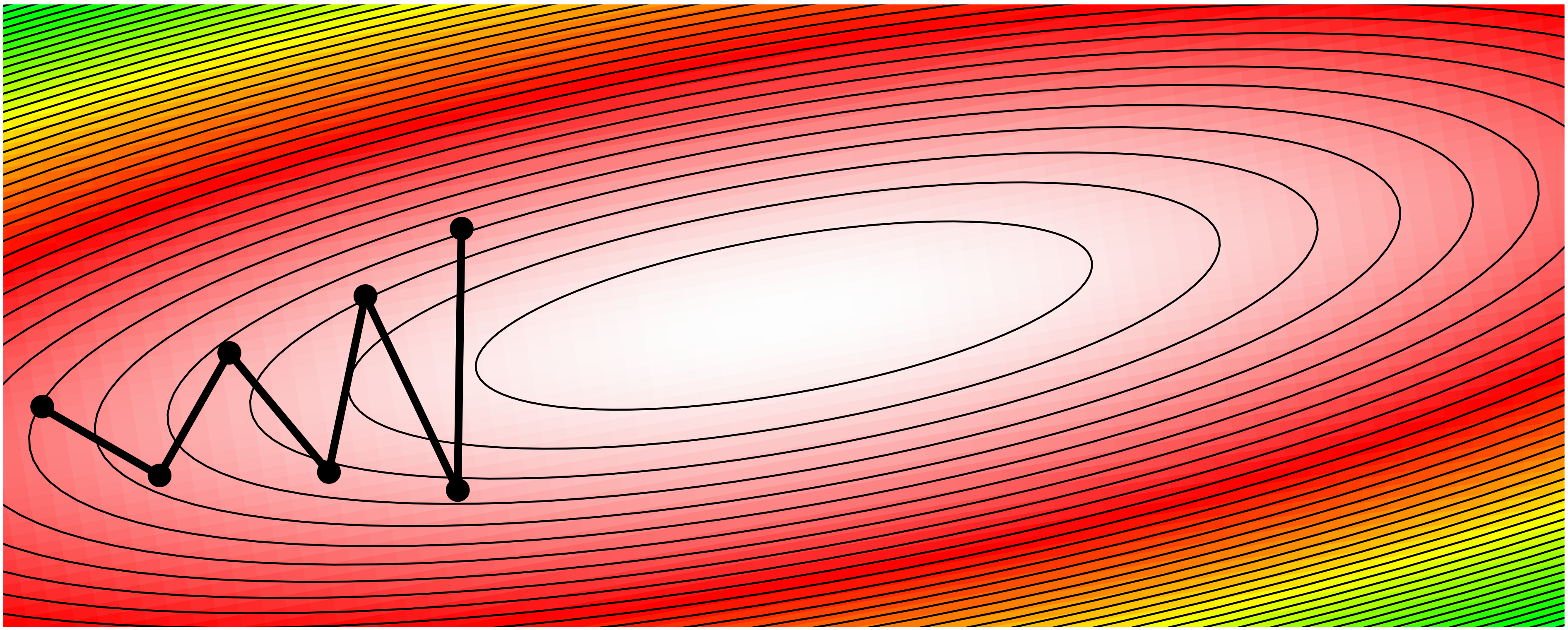

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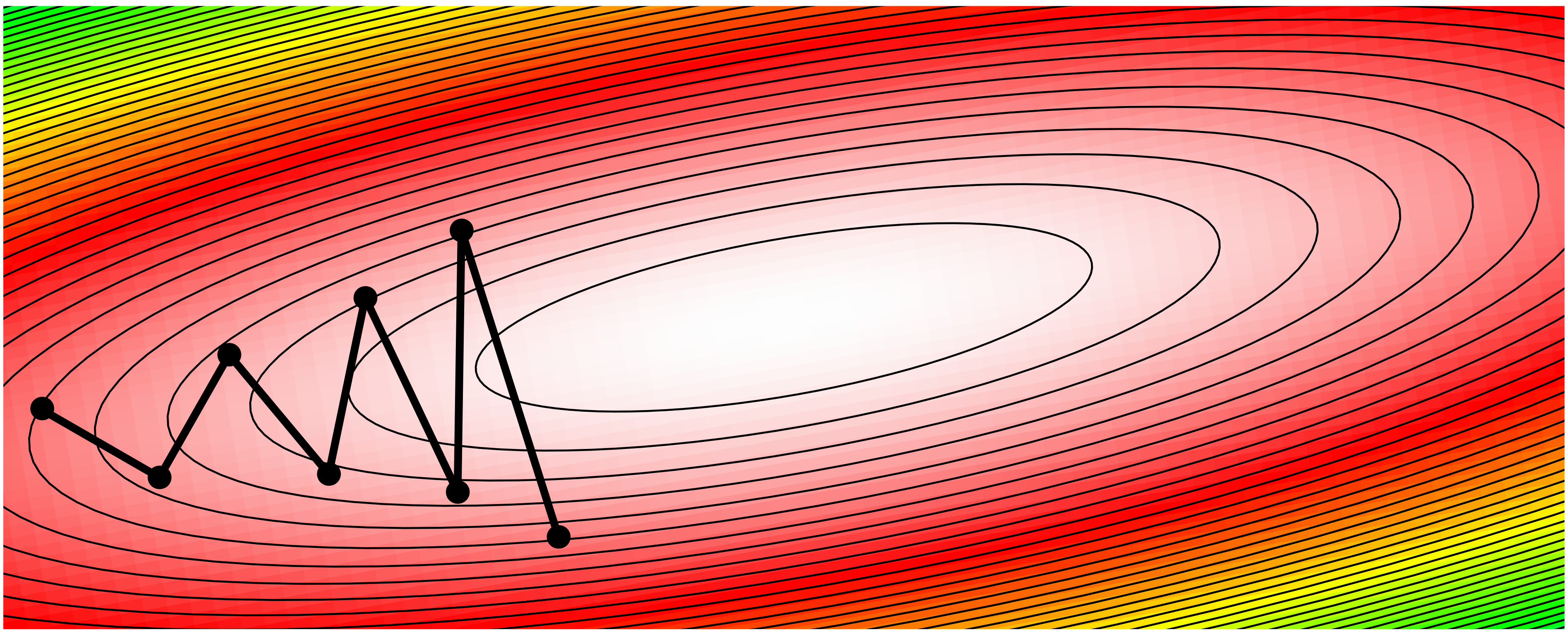

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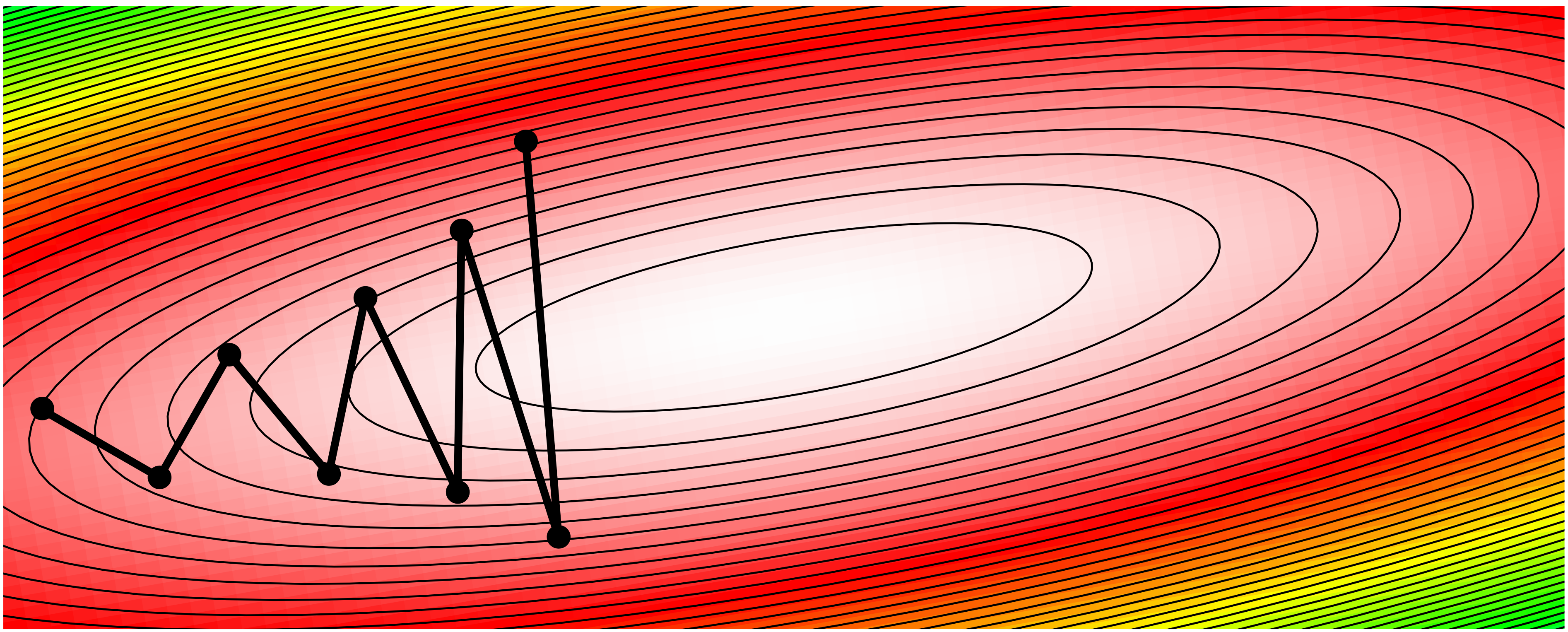

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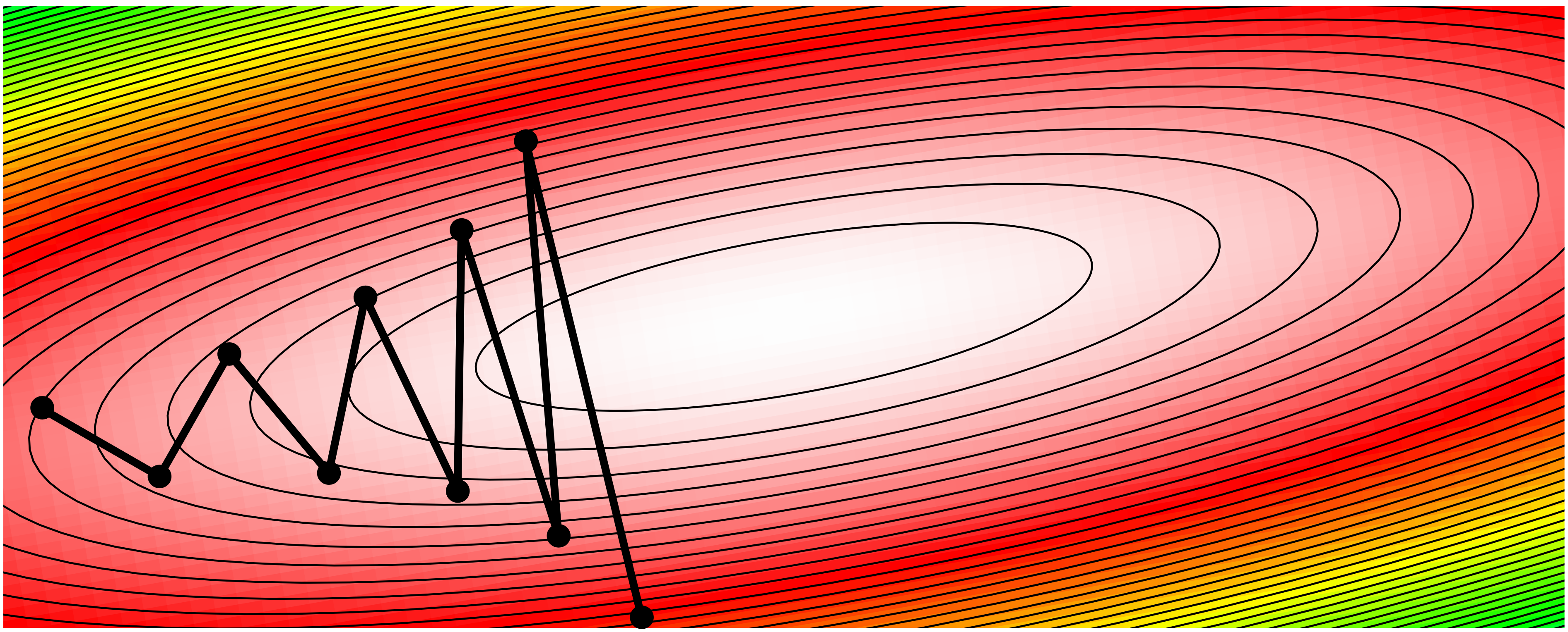

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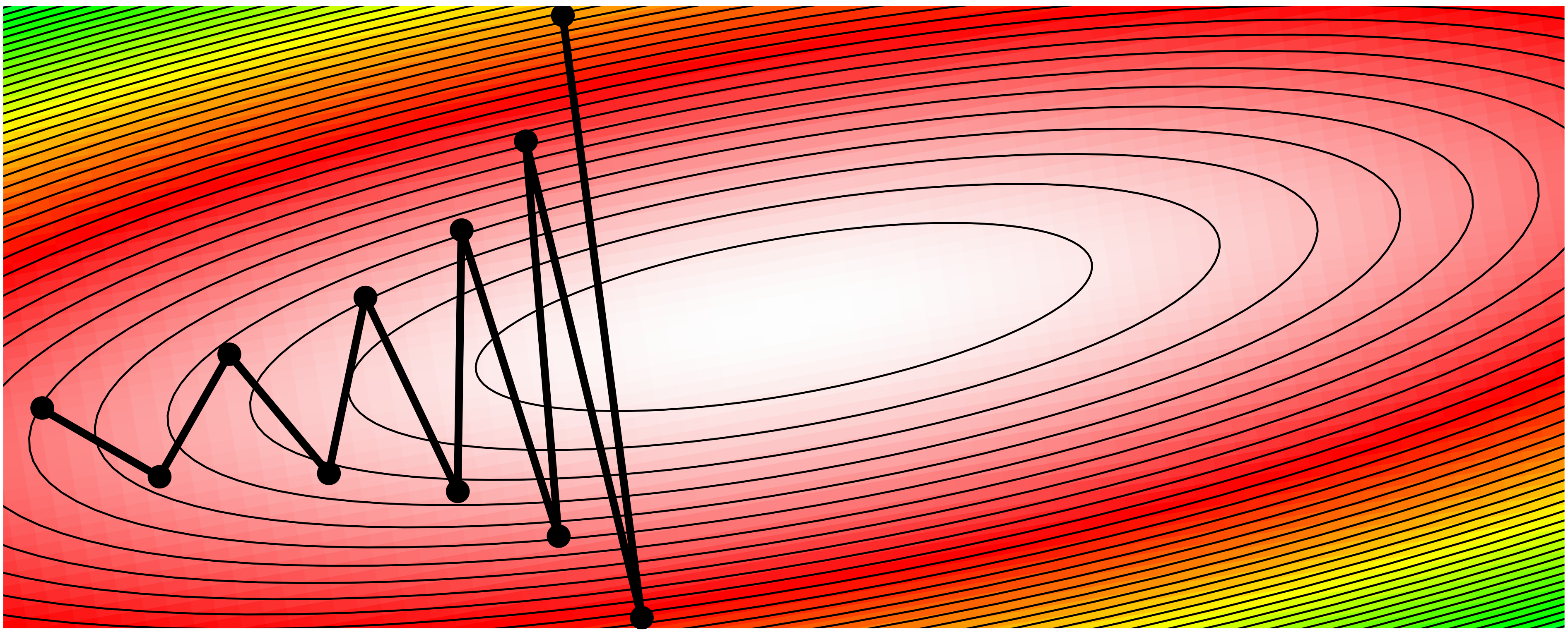

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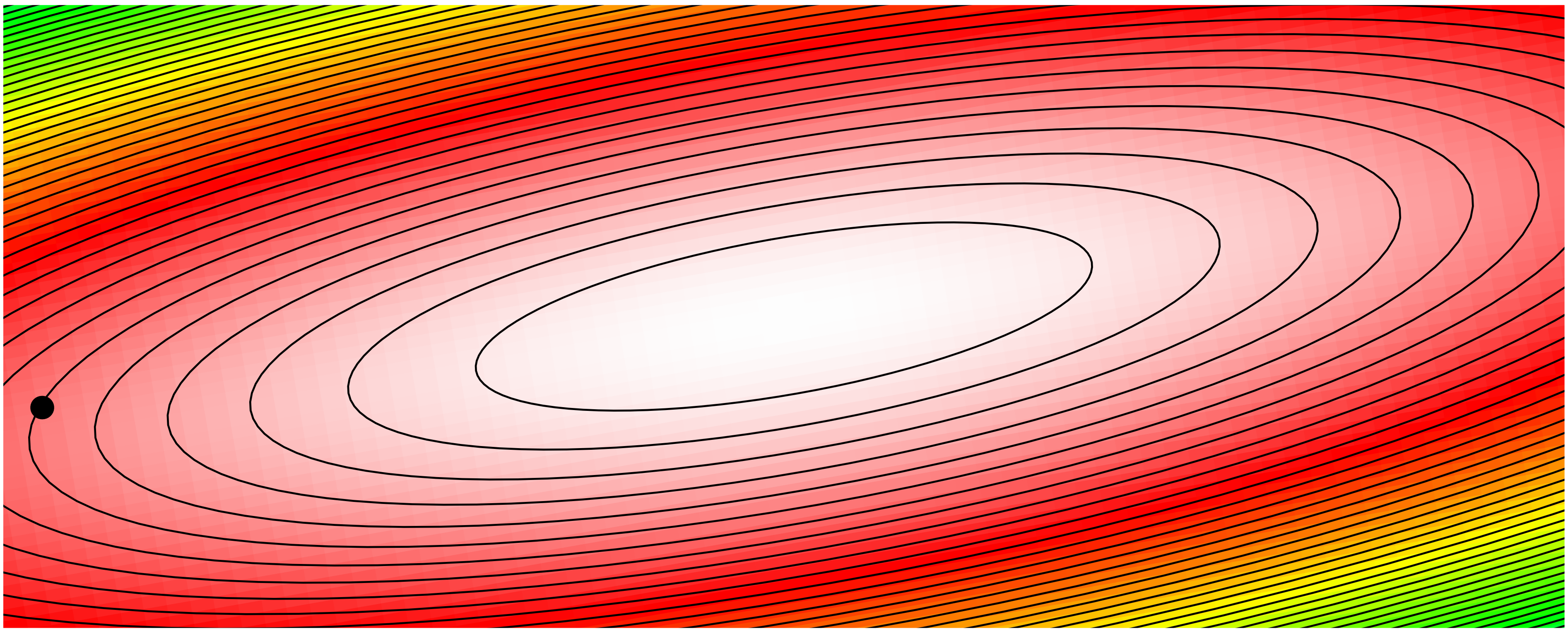

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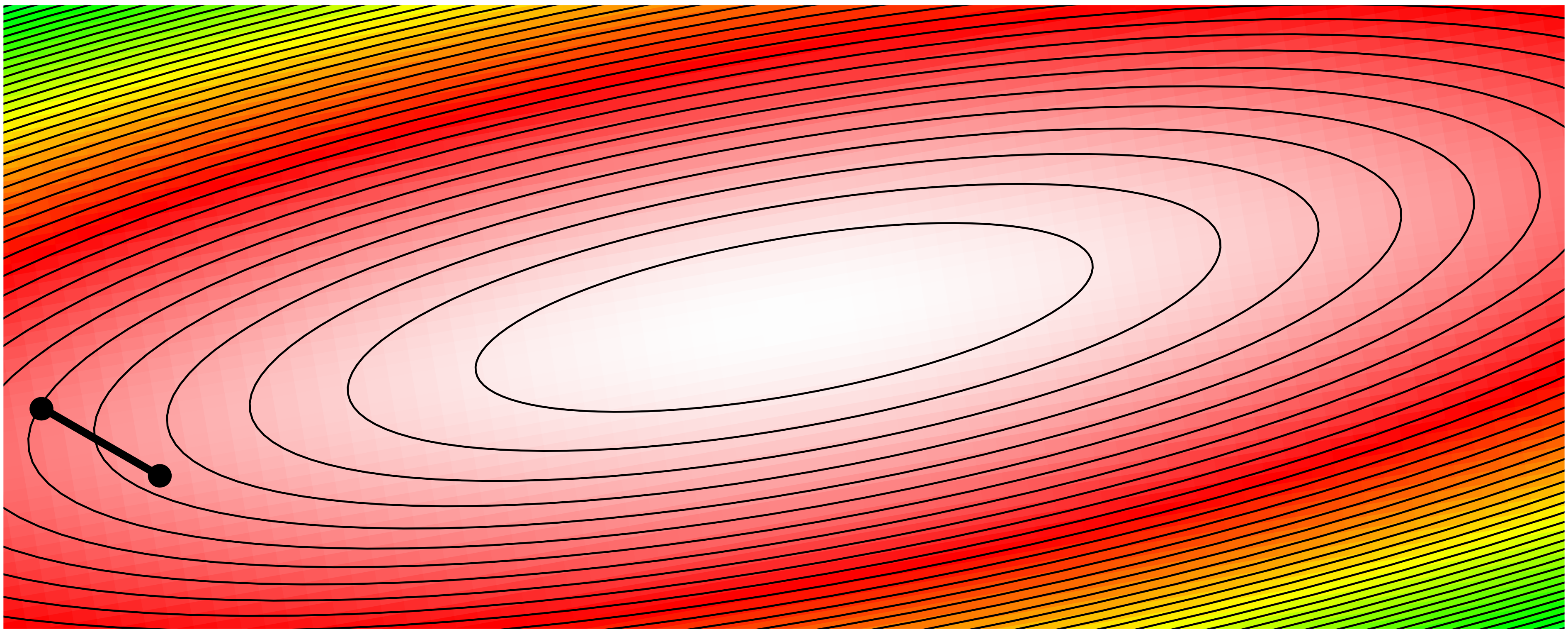

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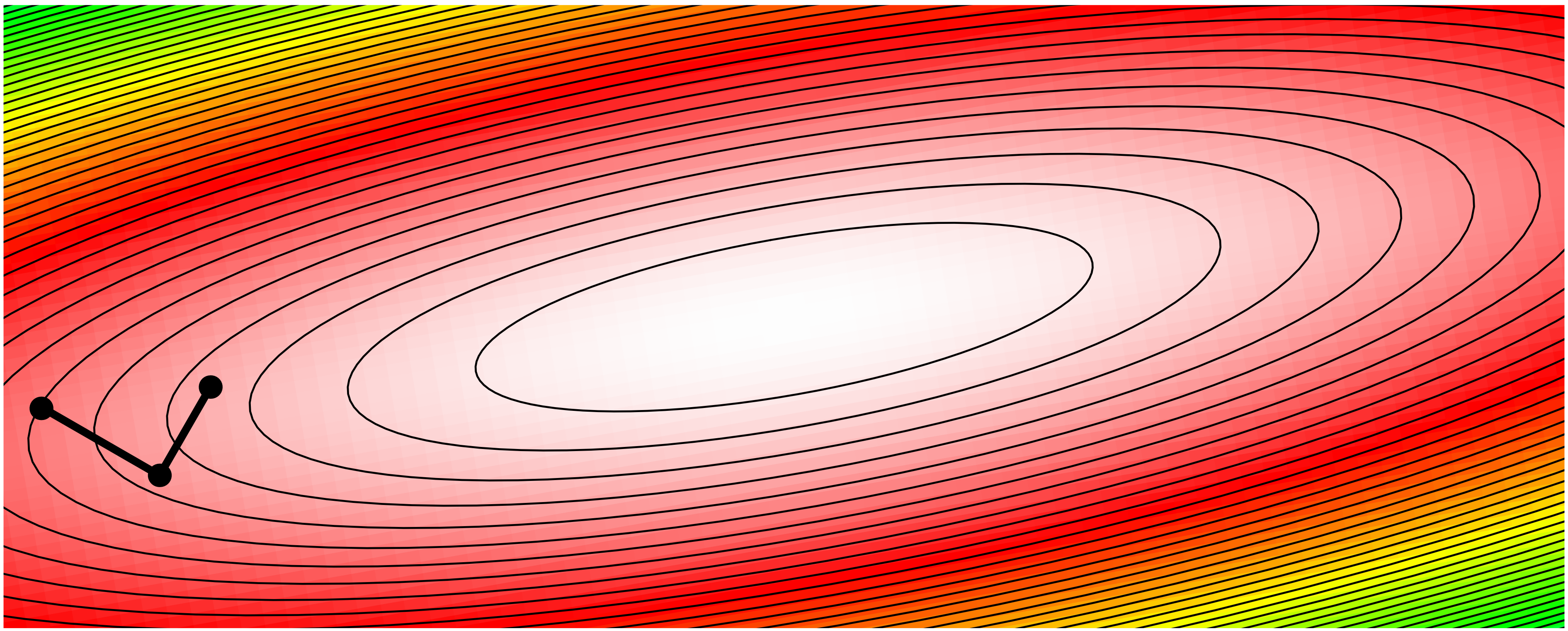

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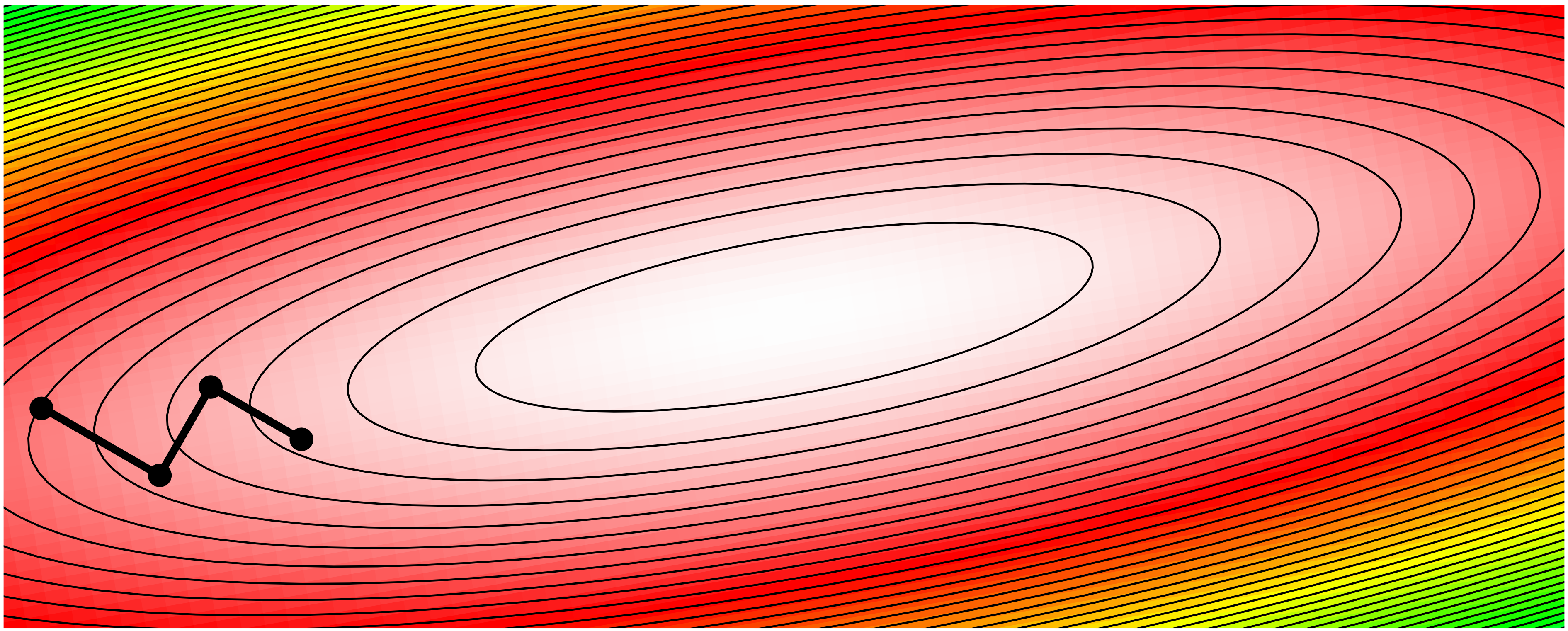

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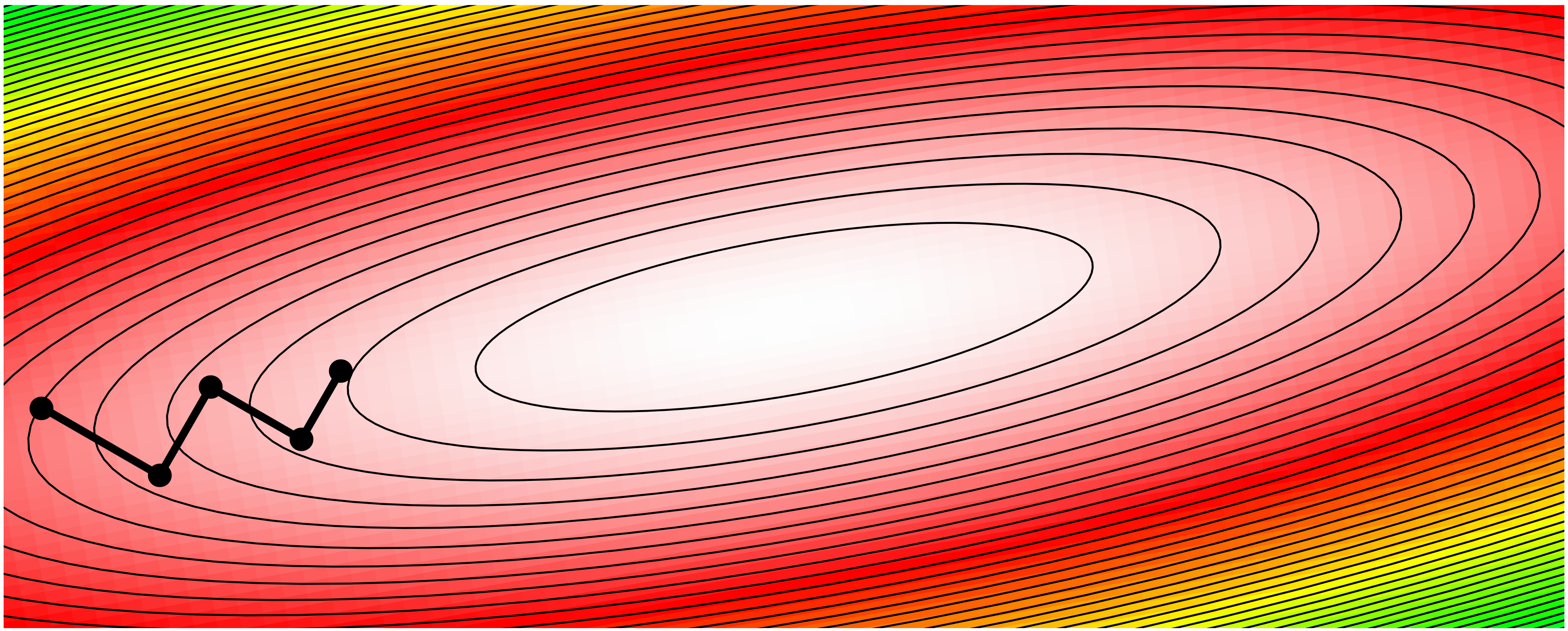

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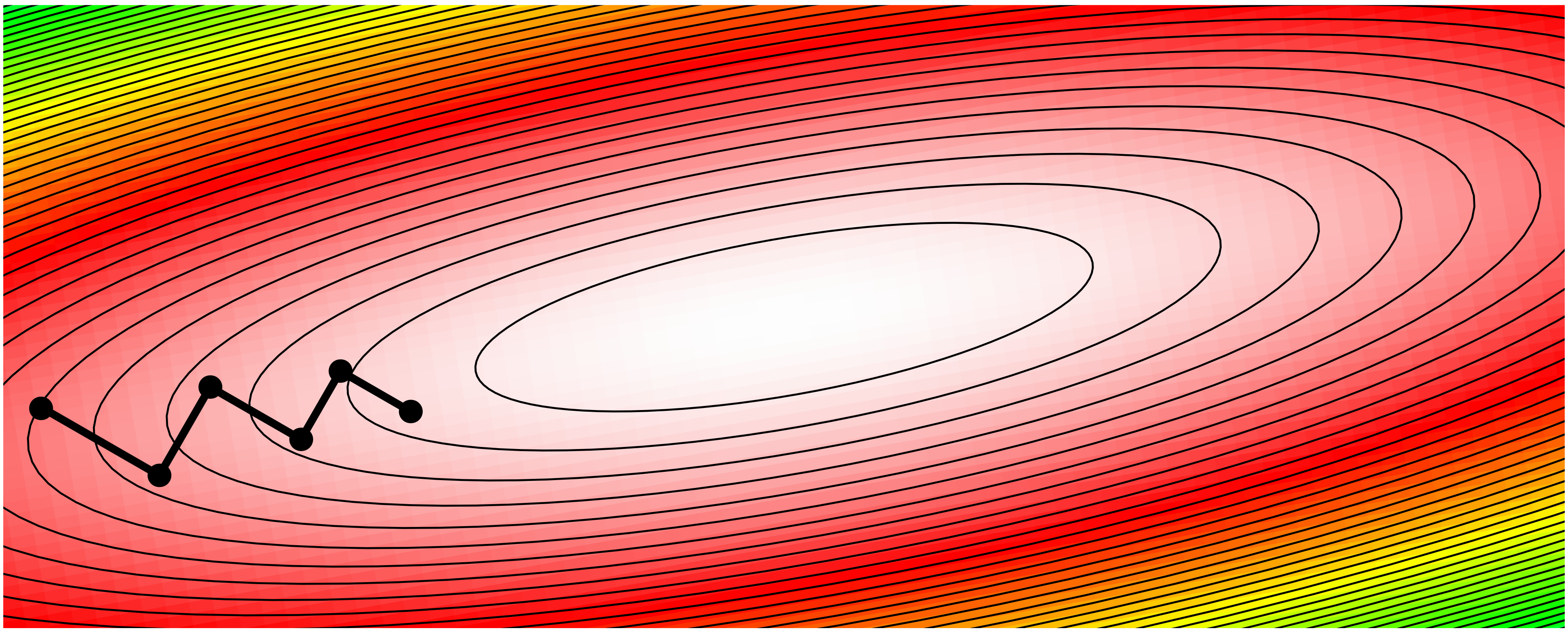

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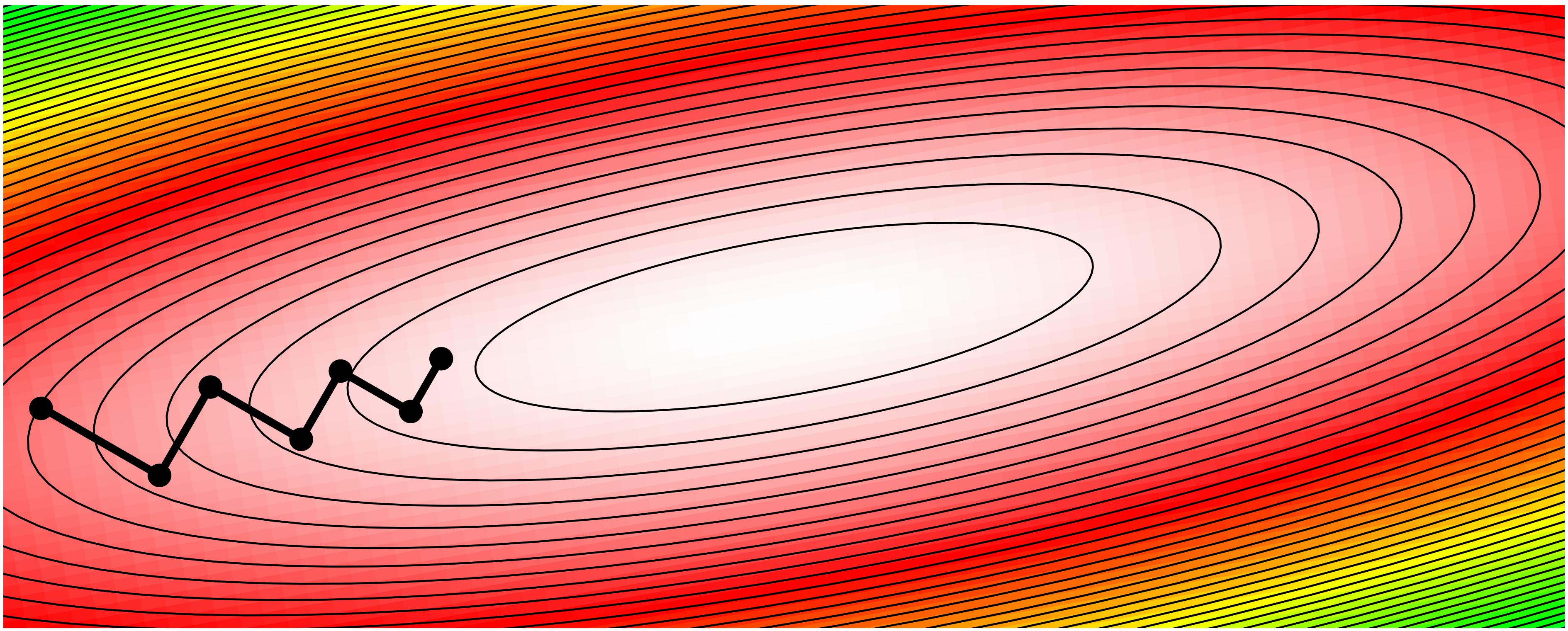

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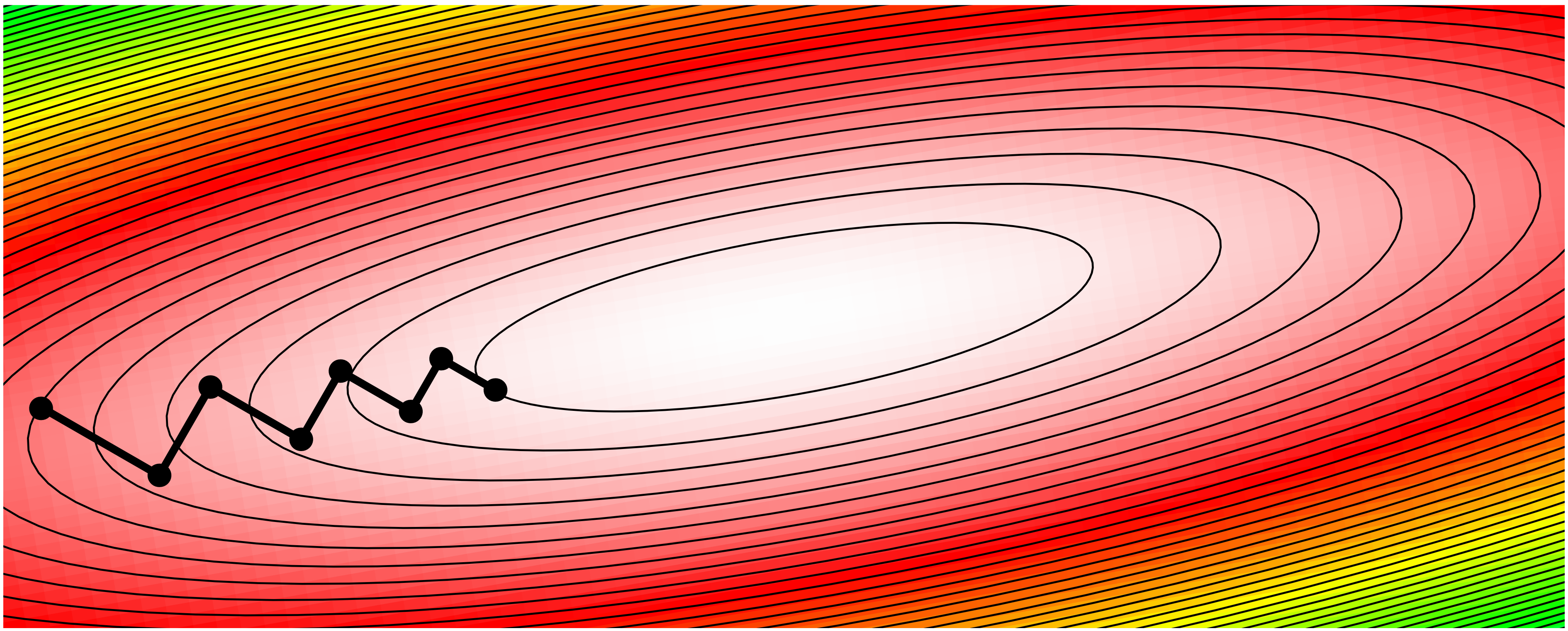

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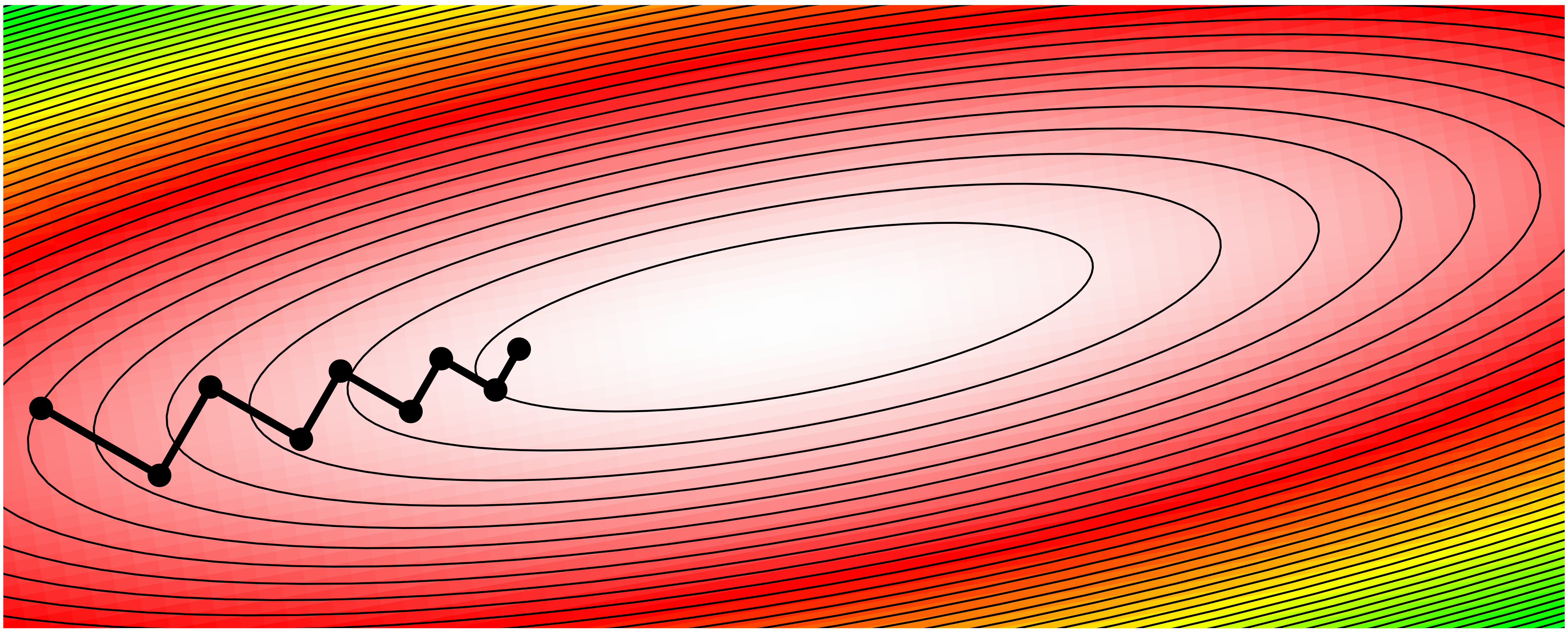

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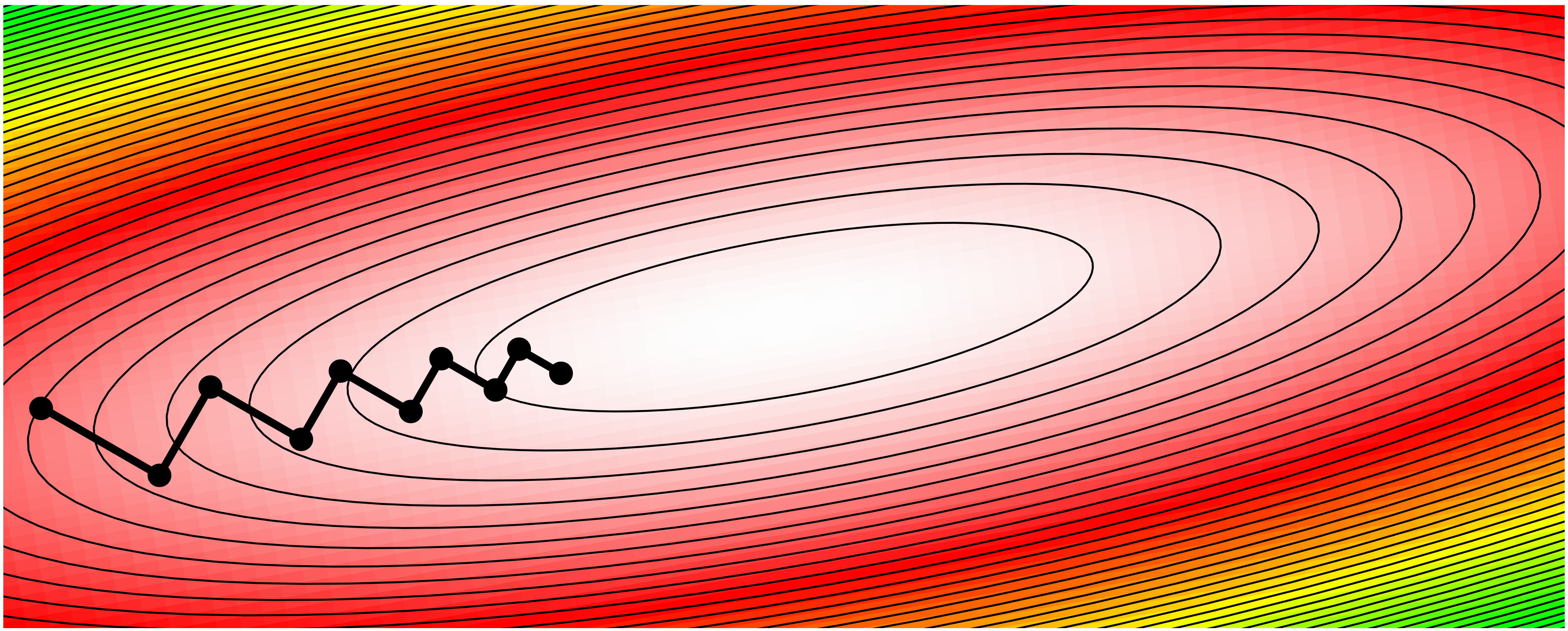

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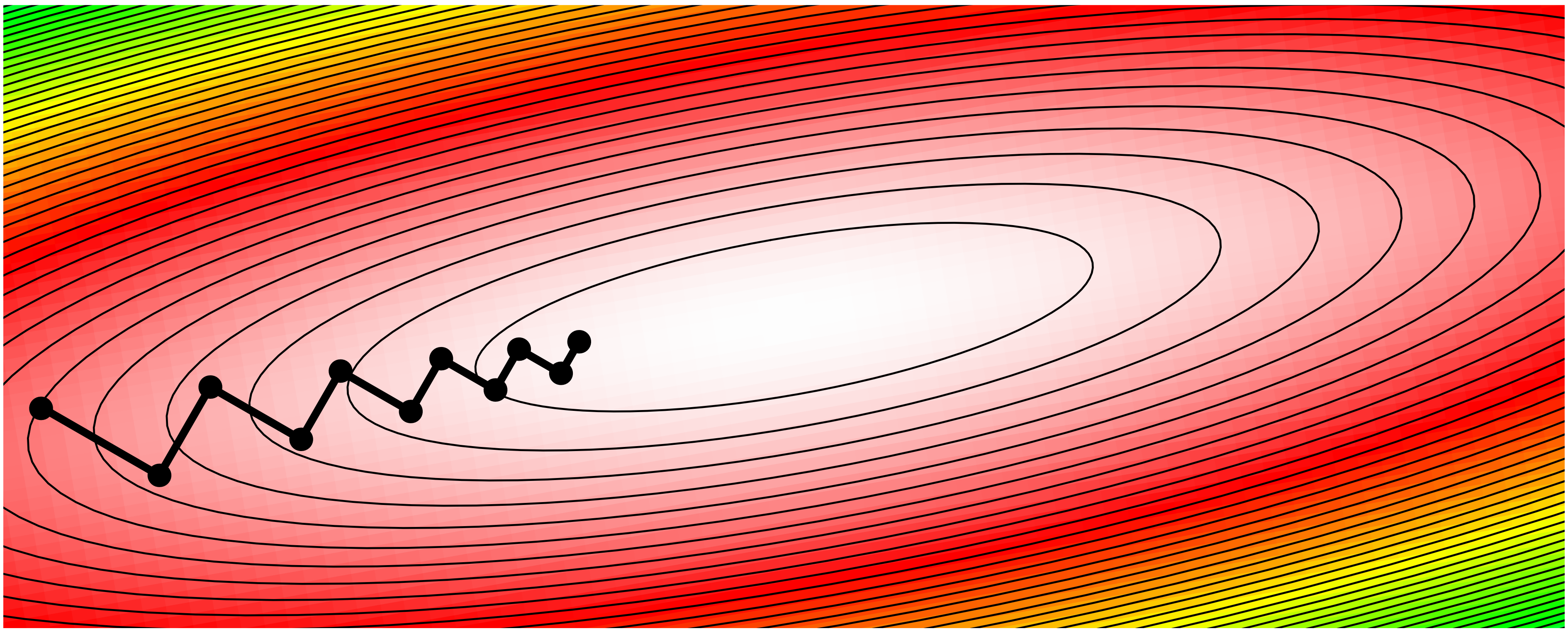
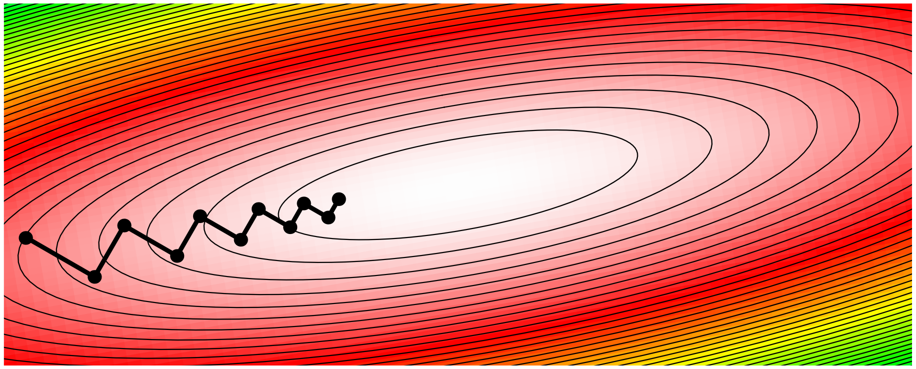


Zig-Zag

- Note that in high dimensions gradient descent tends to zigzag



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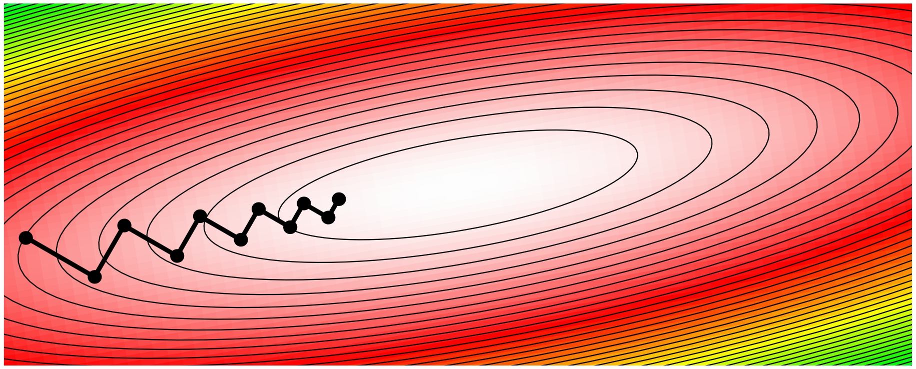

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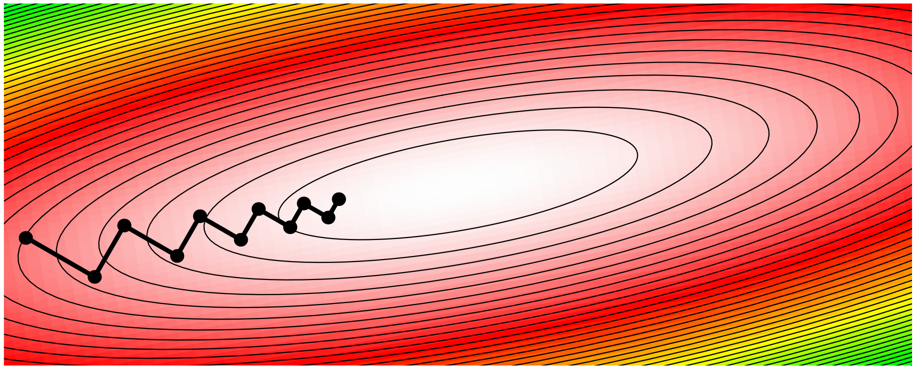

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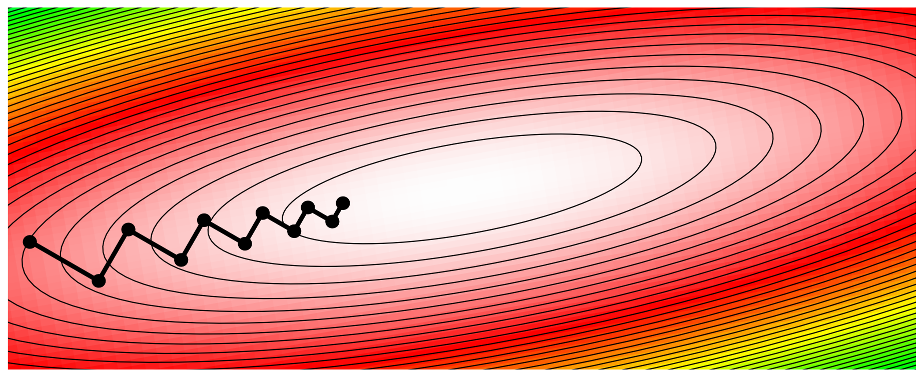

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  - ⋆ Uses gradient, but does not go along it
  - ⋆ For a quadratic minimum in d dimensions it reaches the minimum in d steps

- E.g. Levenberg-Marquardt
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Trust Region

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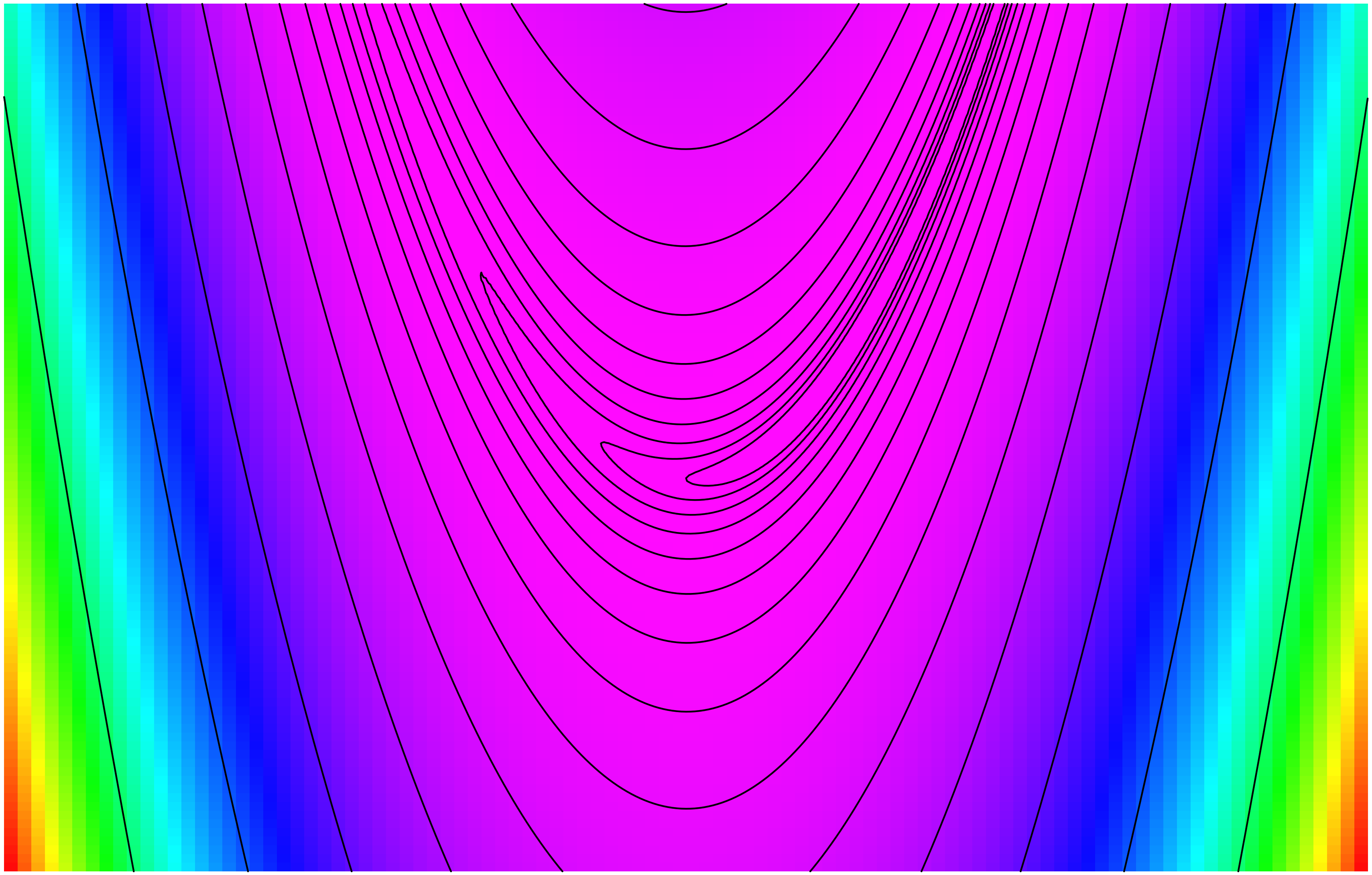

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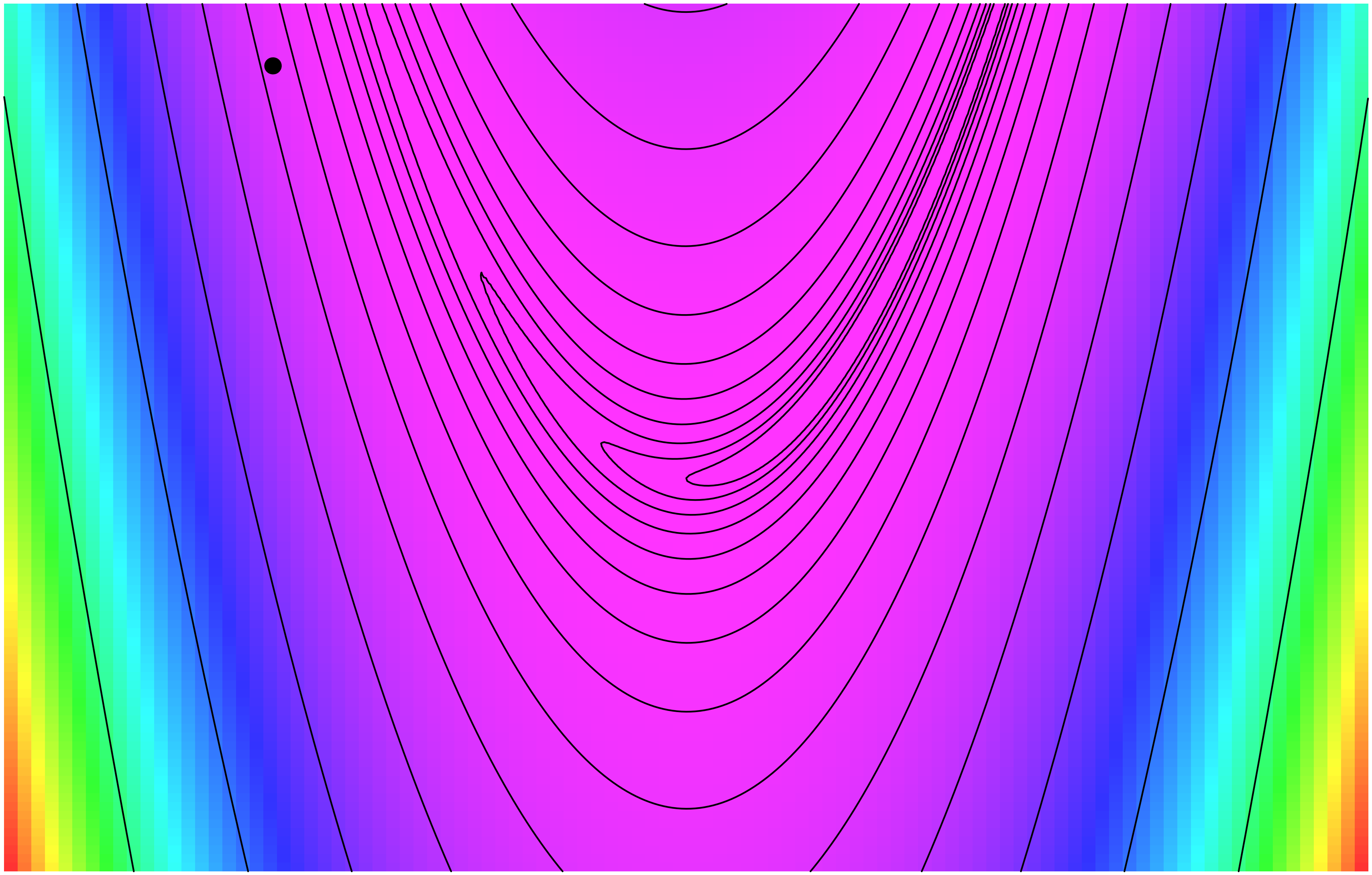

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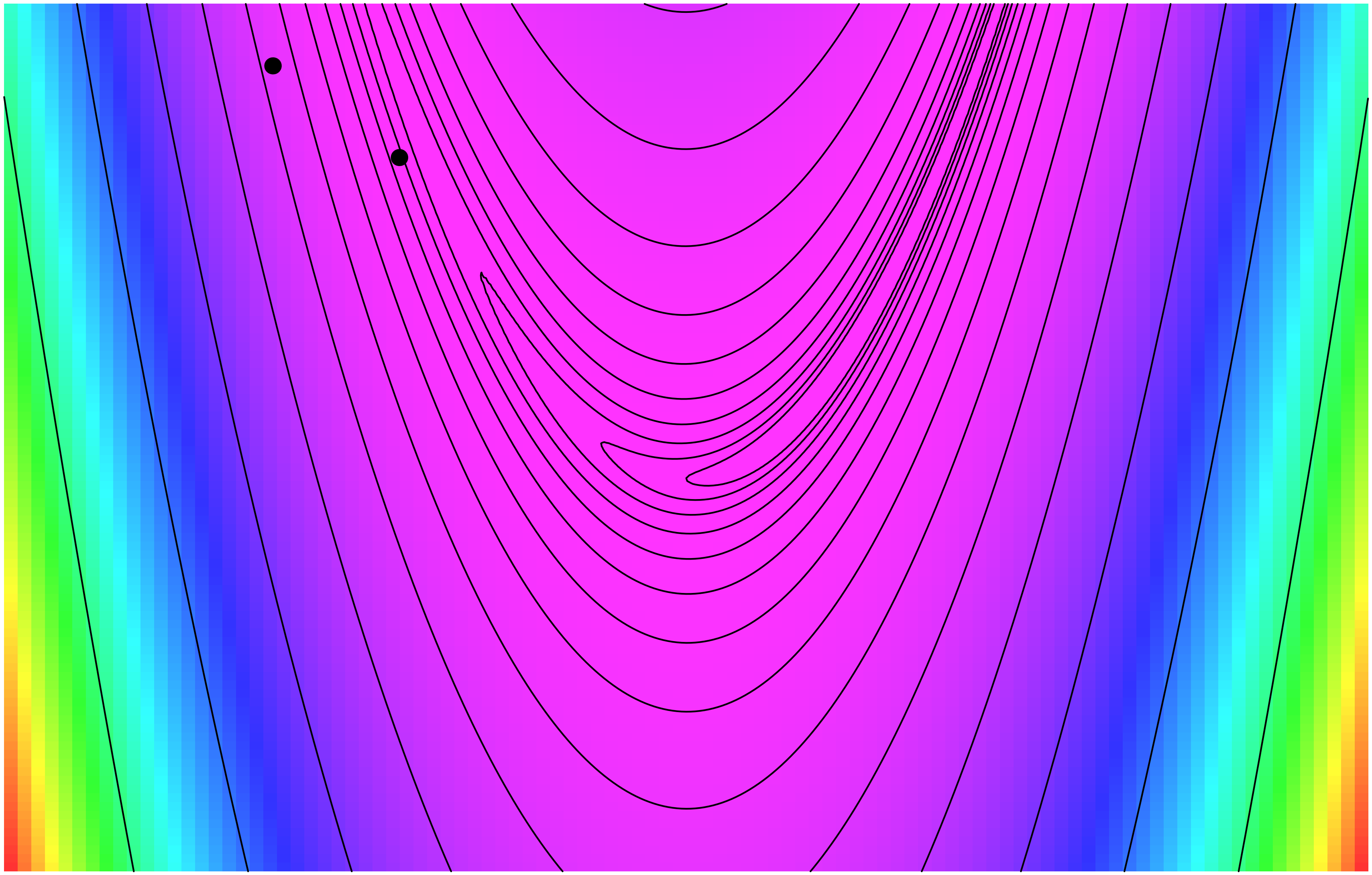

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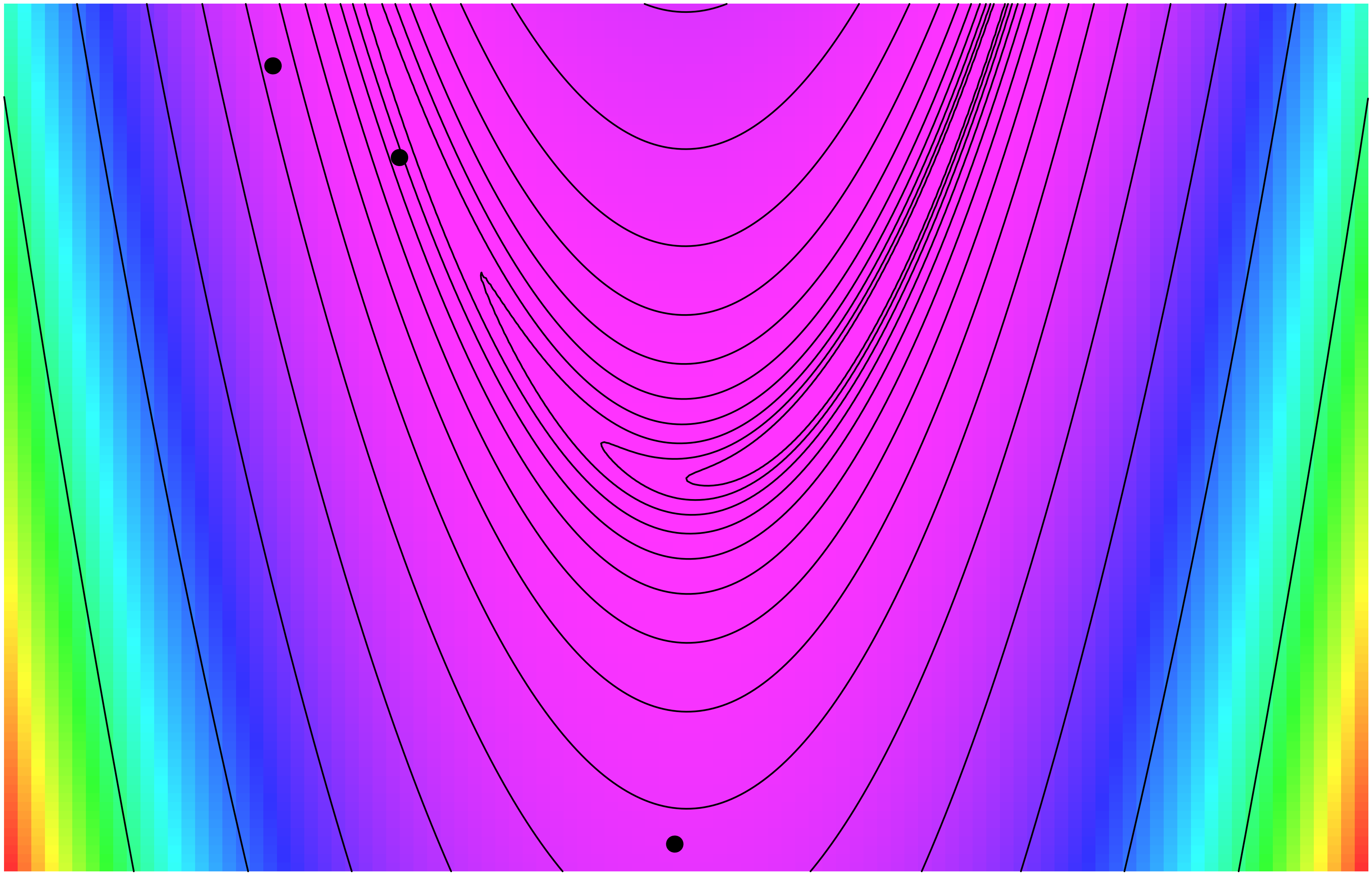

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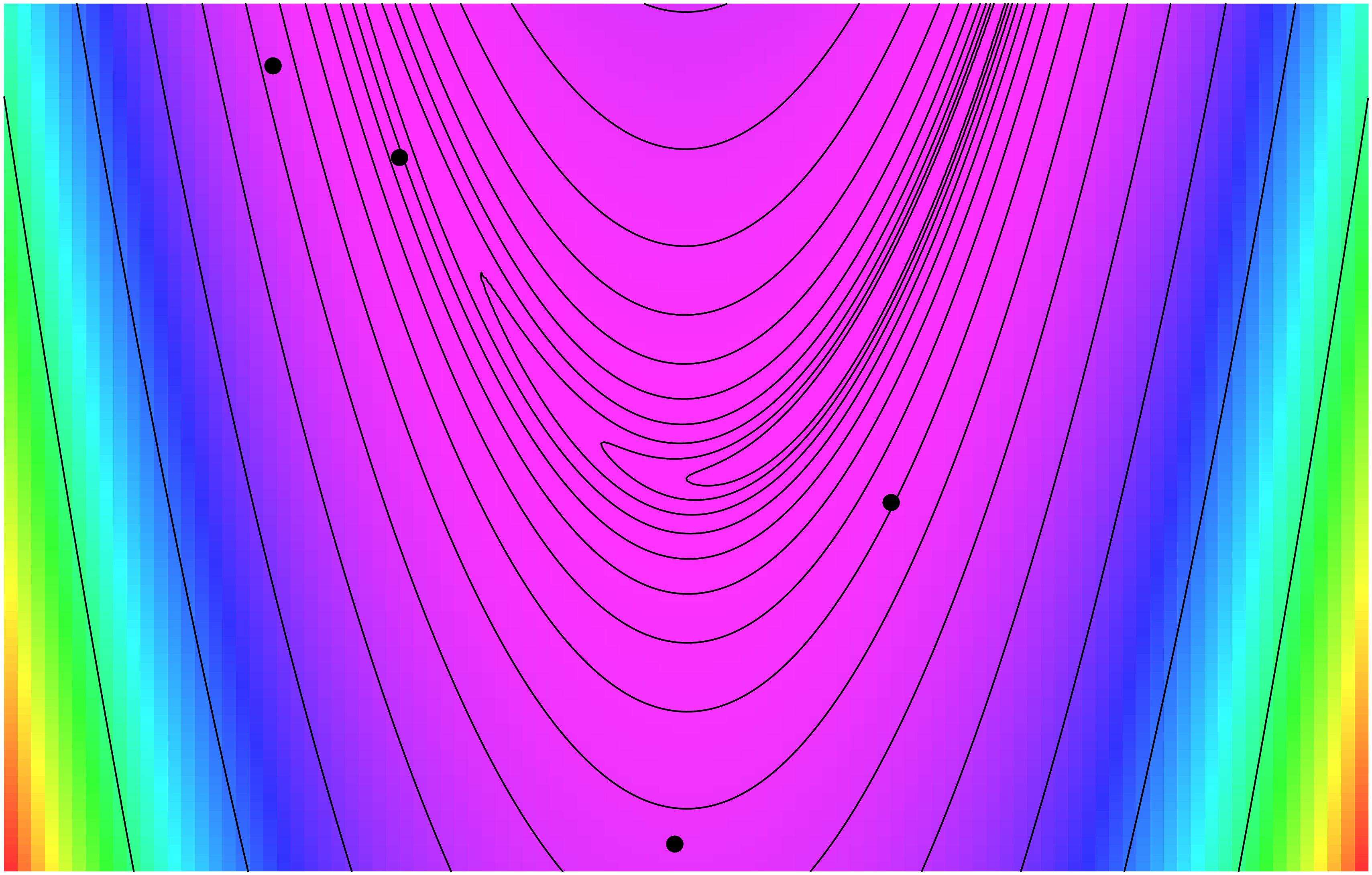

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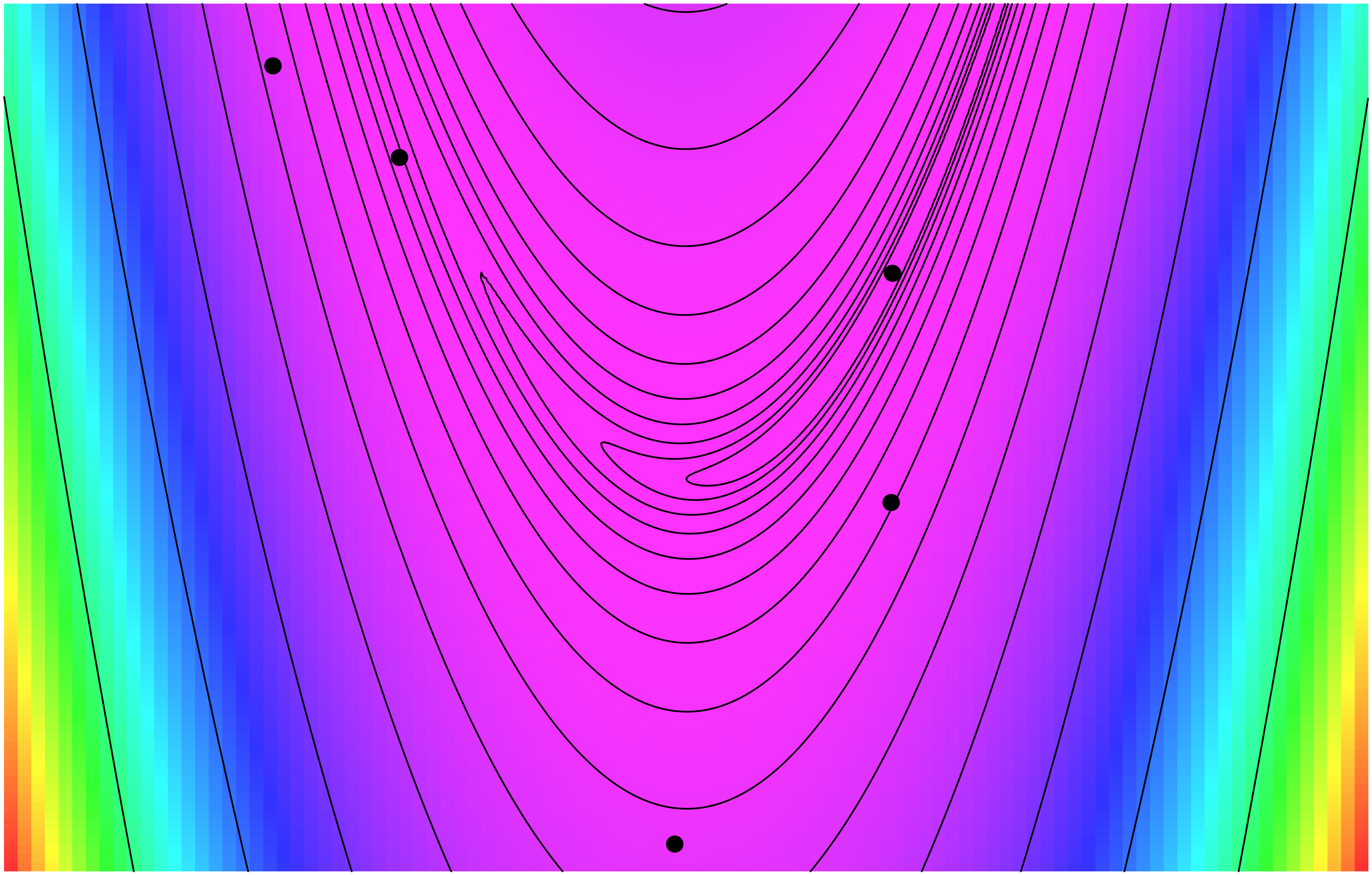

Summary

- There are some **non-gradient methods** (Nelder Mead, evolutionary strategies, Powell's method), but in very high dimensions these are not very competitive
- There are **gradient methods** (first order methods) that suffer from the problem of having to choose a single step size with conflicting requirements in different directions
- **Newton's method** (a second order method) requires computing the Hessian matrix, gives very fast convergent, but can take you in the wrong direction if you are not sufficiently close to a minimum
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