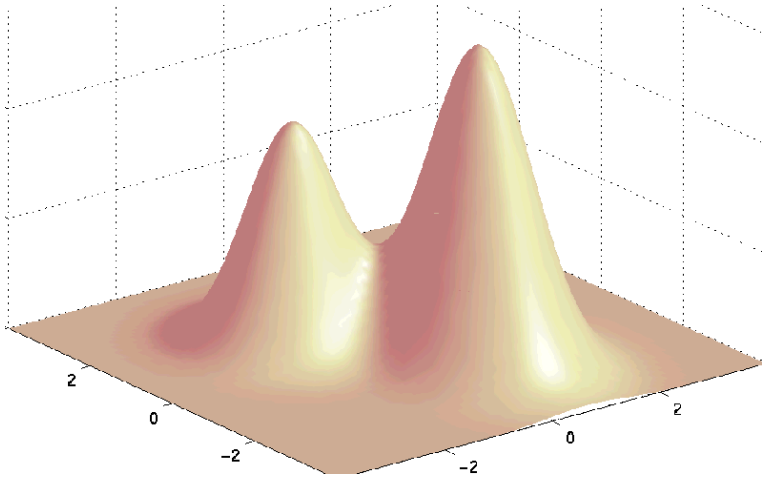
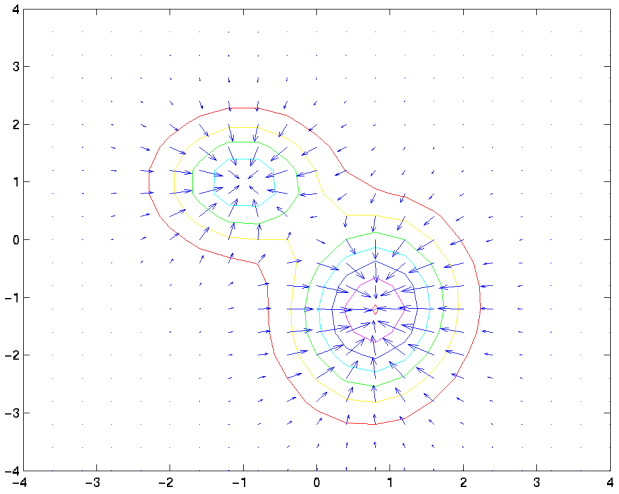
# Advanced Machine Learning

## *Optimisation*



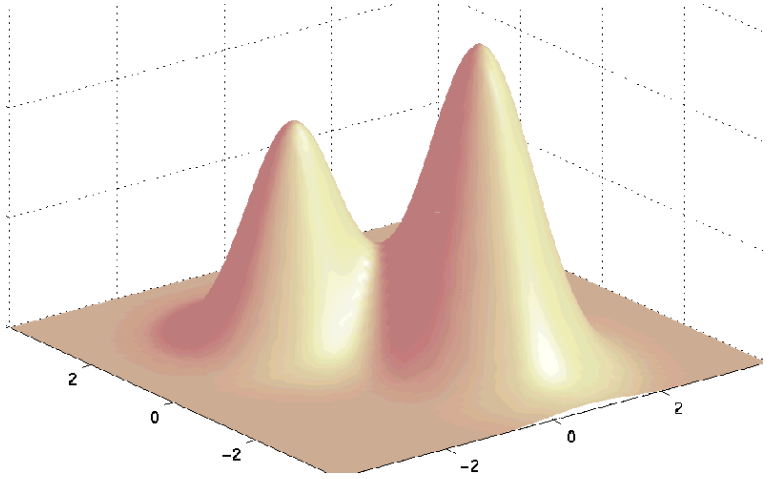




$$z = \mathrm{e}^{-(x+1)^2-(y-1)^2} + 0.6\,\mathrm{e}^{-(x-1)^2-0.5(y+1)^2+0.1(x-3)(y-3)}$$

*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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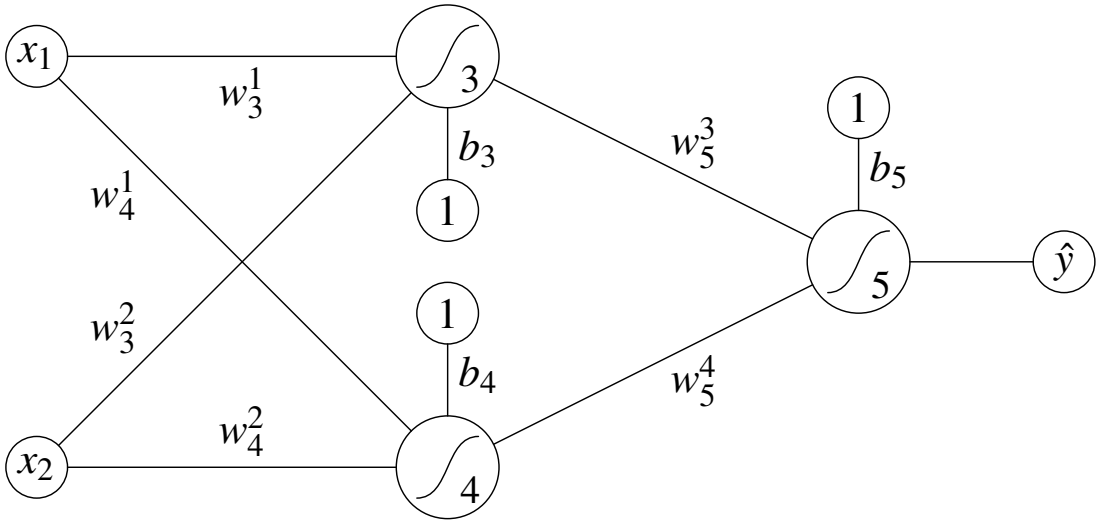
# MLP

- 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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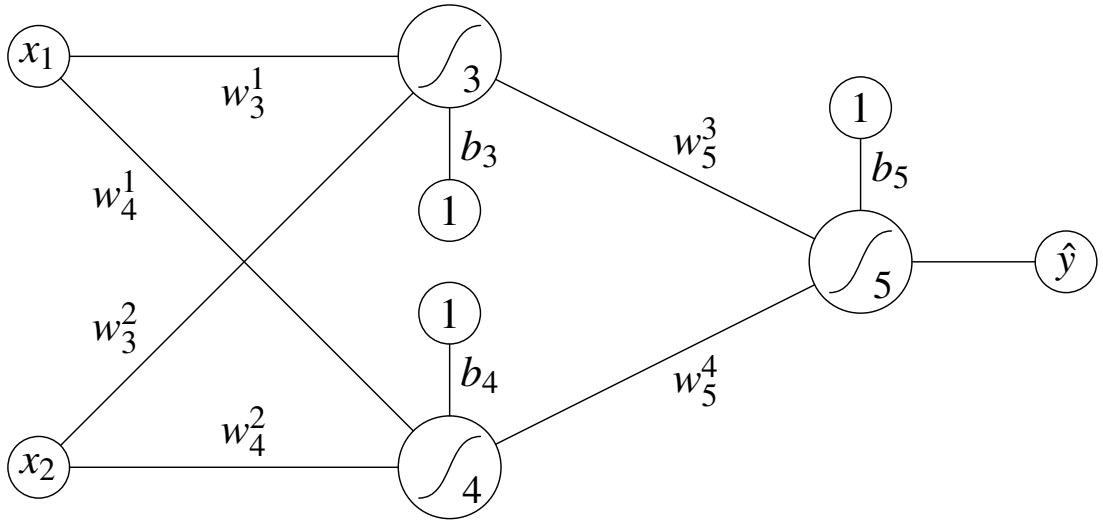


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# Training

- 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

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

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

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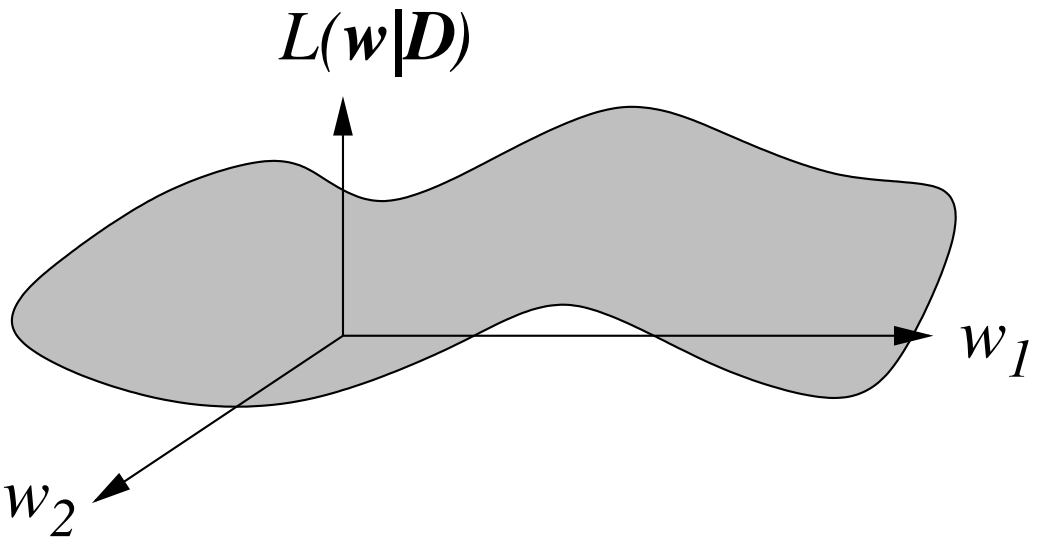
# Computing Gradients

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

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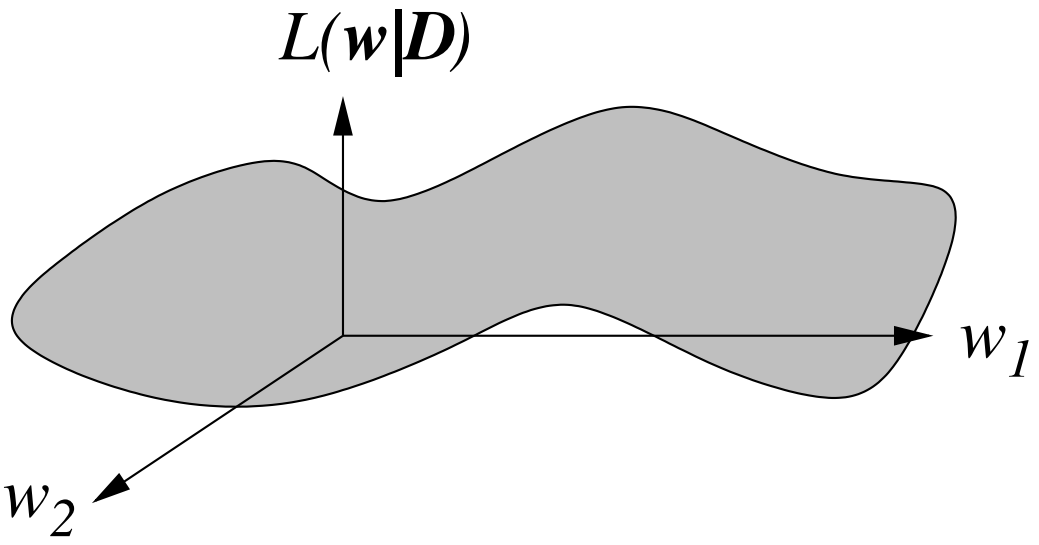


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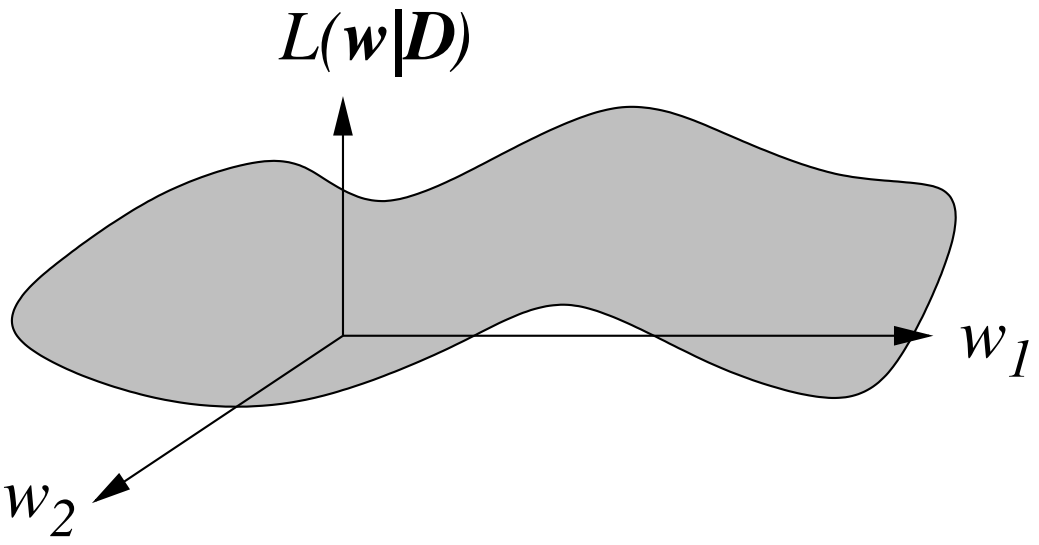


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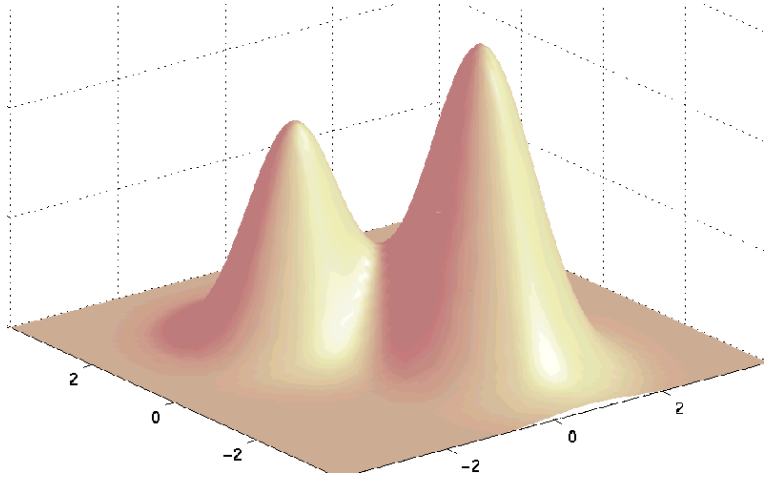

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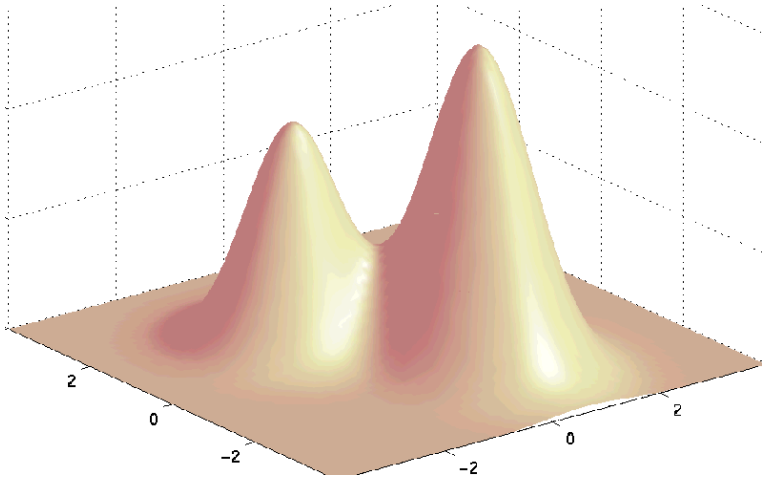
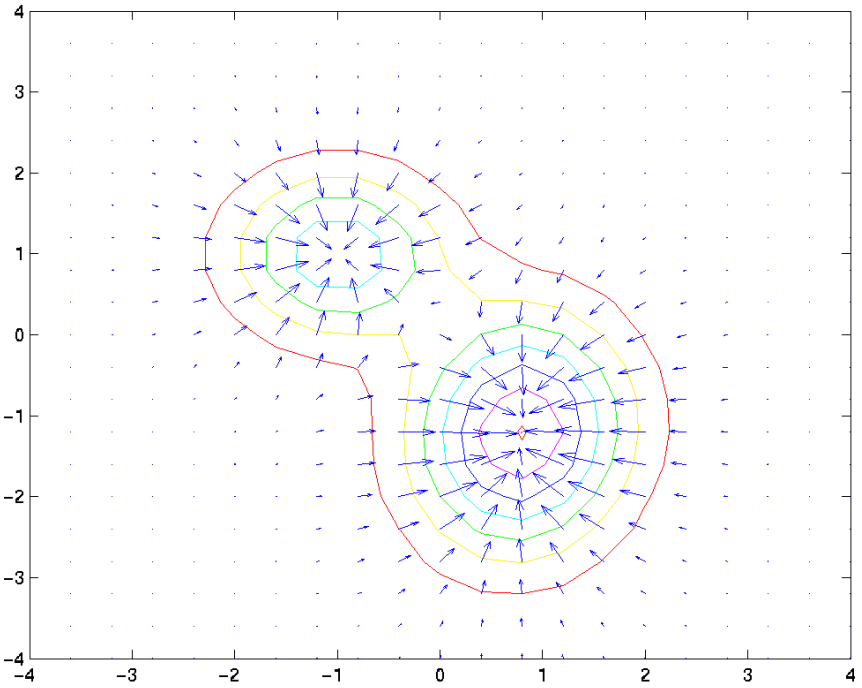
- A maximum or minimum occurs when $\nabla L(\boldsymbol{w}|\mathcal{D}) = \mathbf{0}$
- E.g.

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



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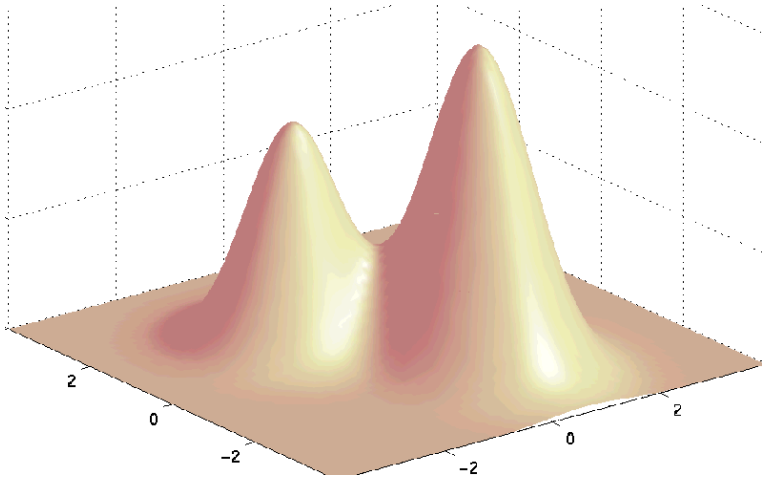


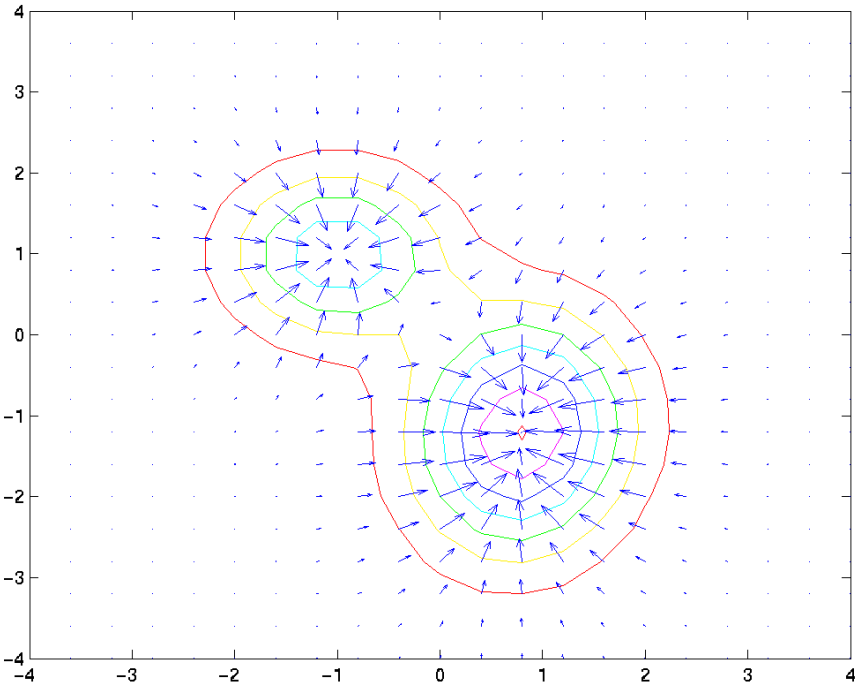

# Gradient Descent

- For a simple function $L(\boldsymbol{w}|\mathcal{D})$ we can solve $\boldsymbol{\nabla} L(\boldsymbol{w}|\mathcal{D}) = \mathbf{0}$ 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: $\boldsymbol{w} \rightarrow \boldsymbol{w}' = \boldsymbol{w} + r\boldsymbol{\nabla} L(\boldsymbol{w}|\mathcal{D})$
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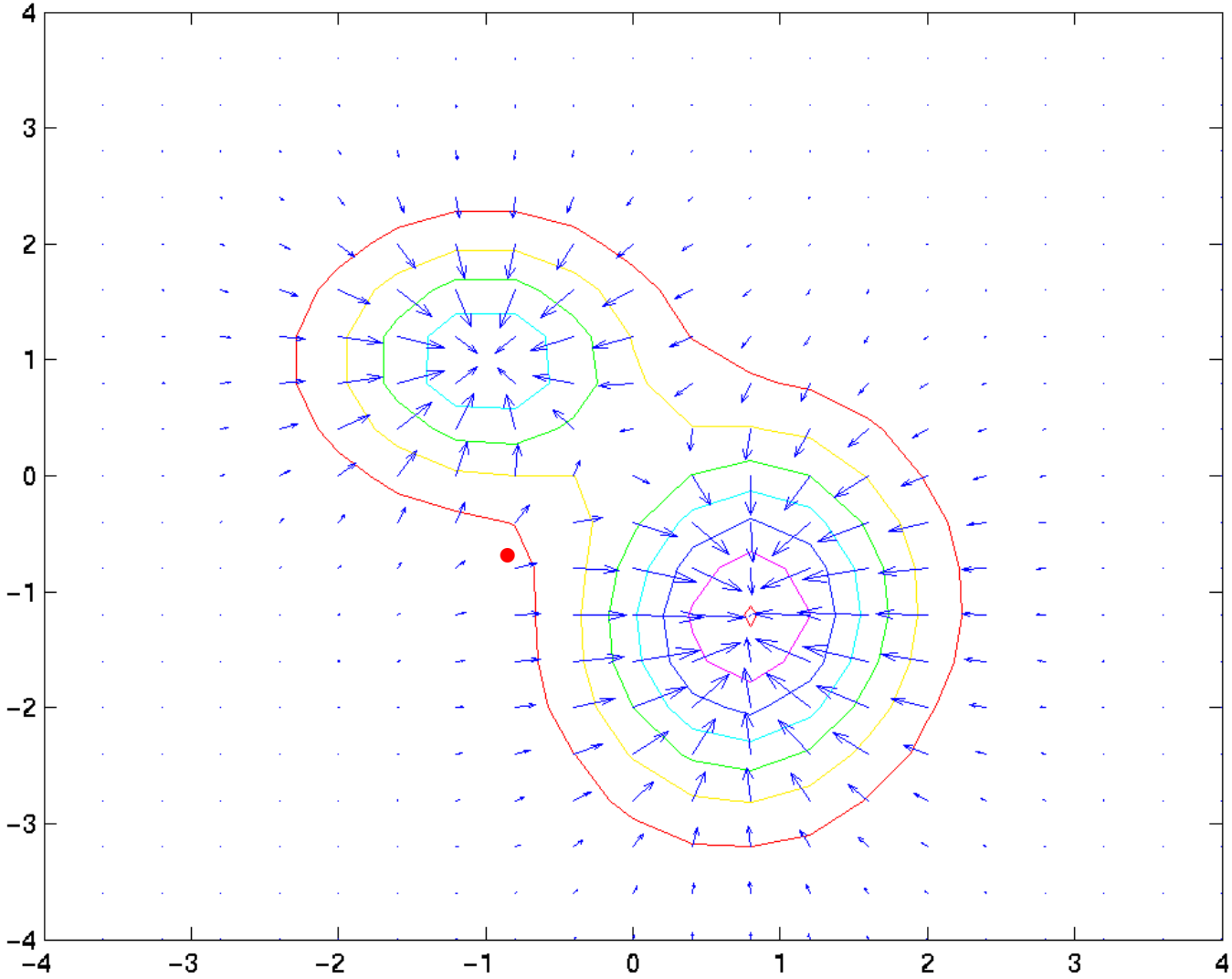
# Hill-Climbing



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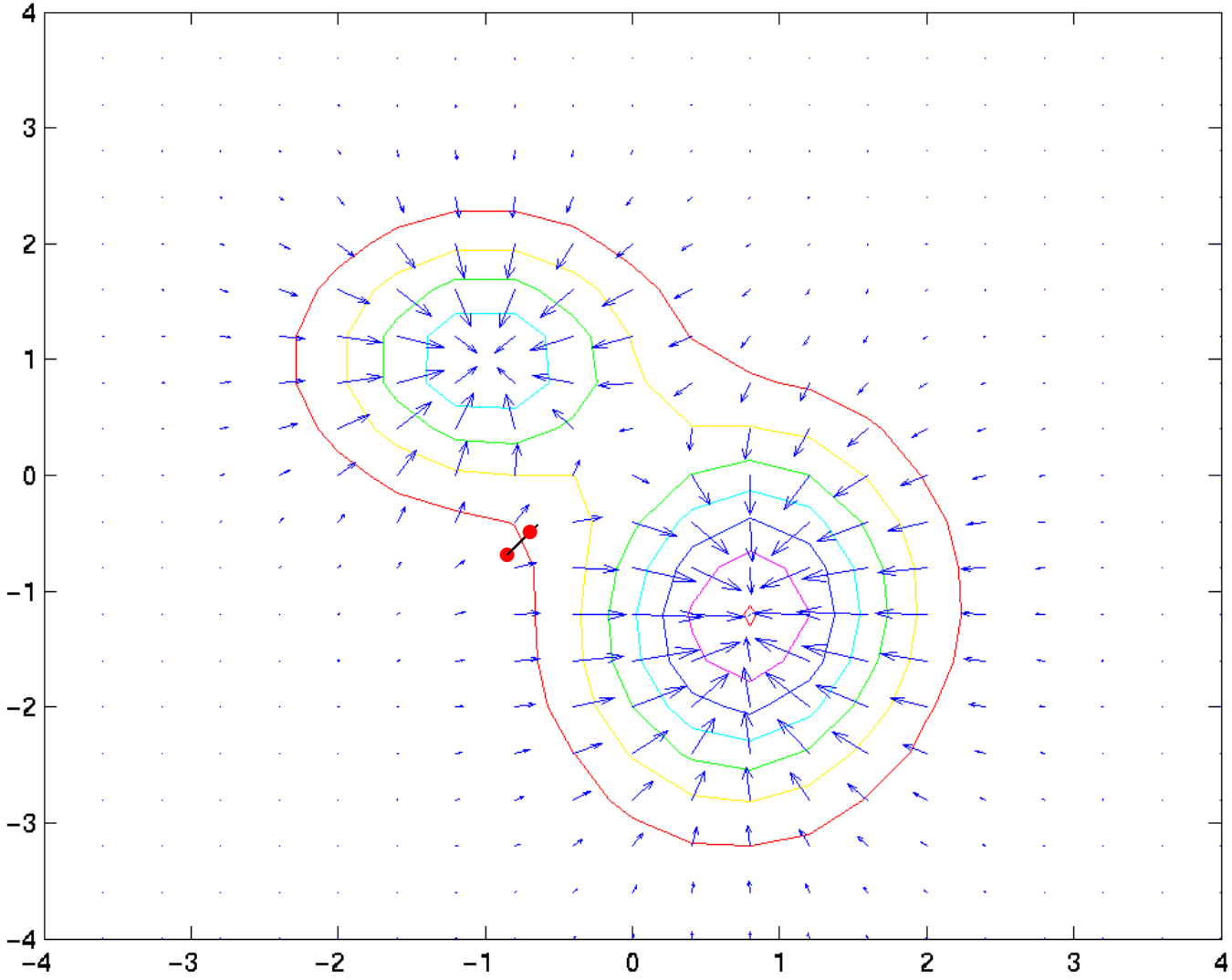

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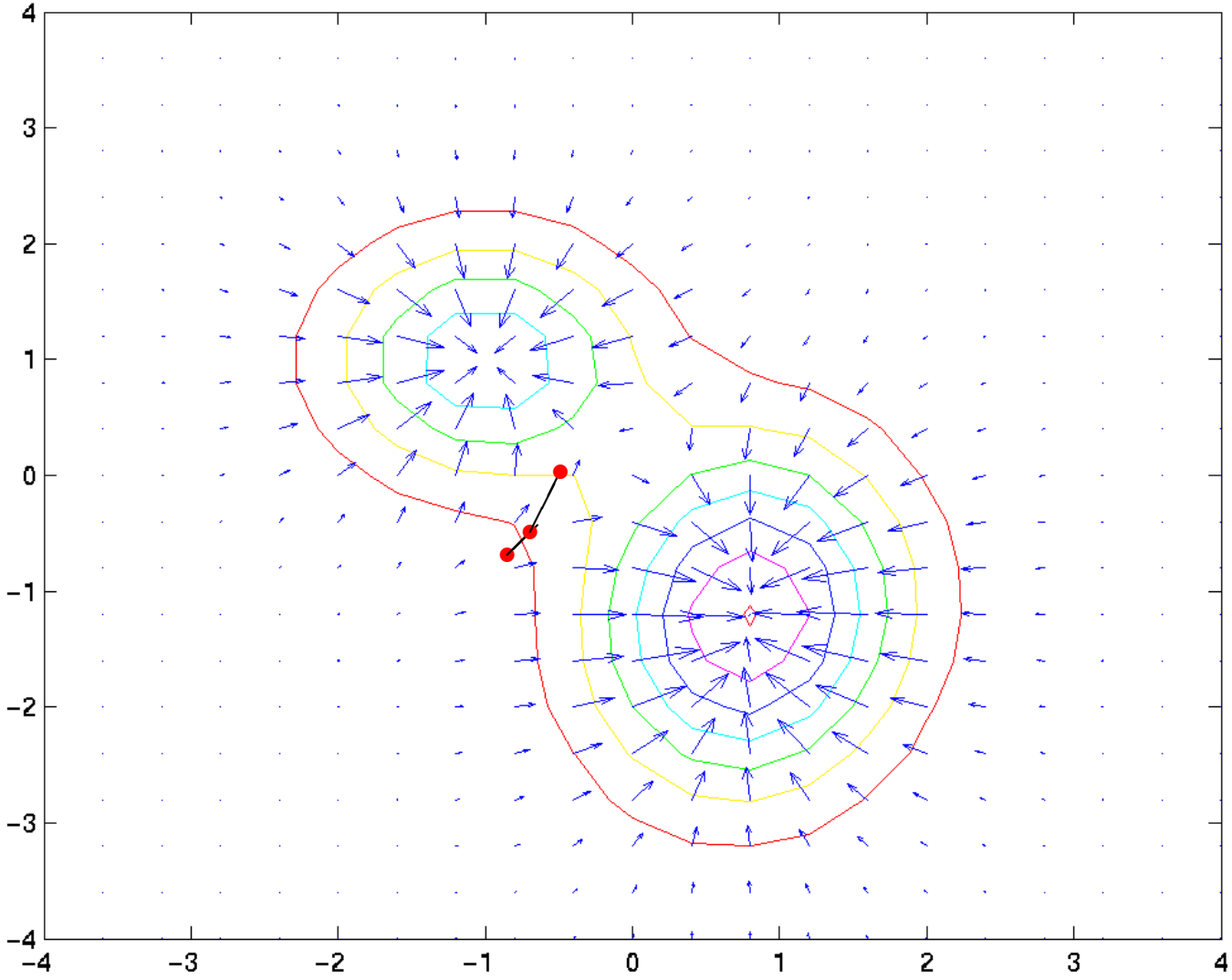

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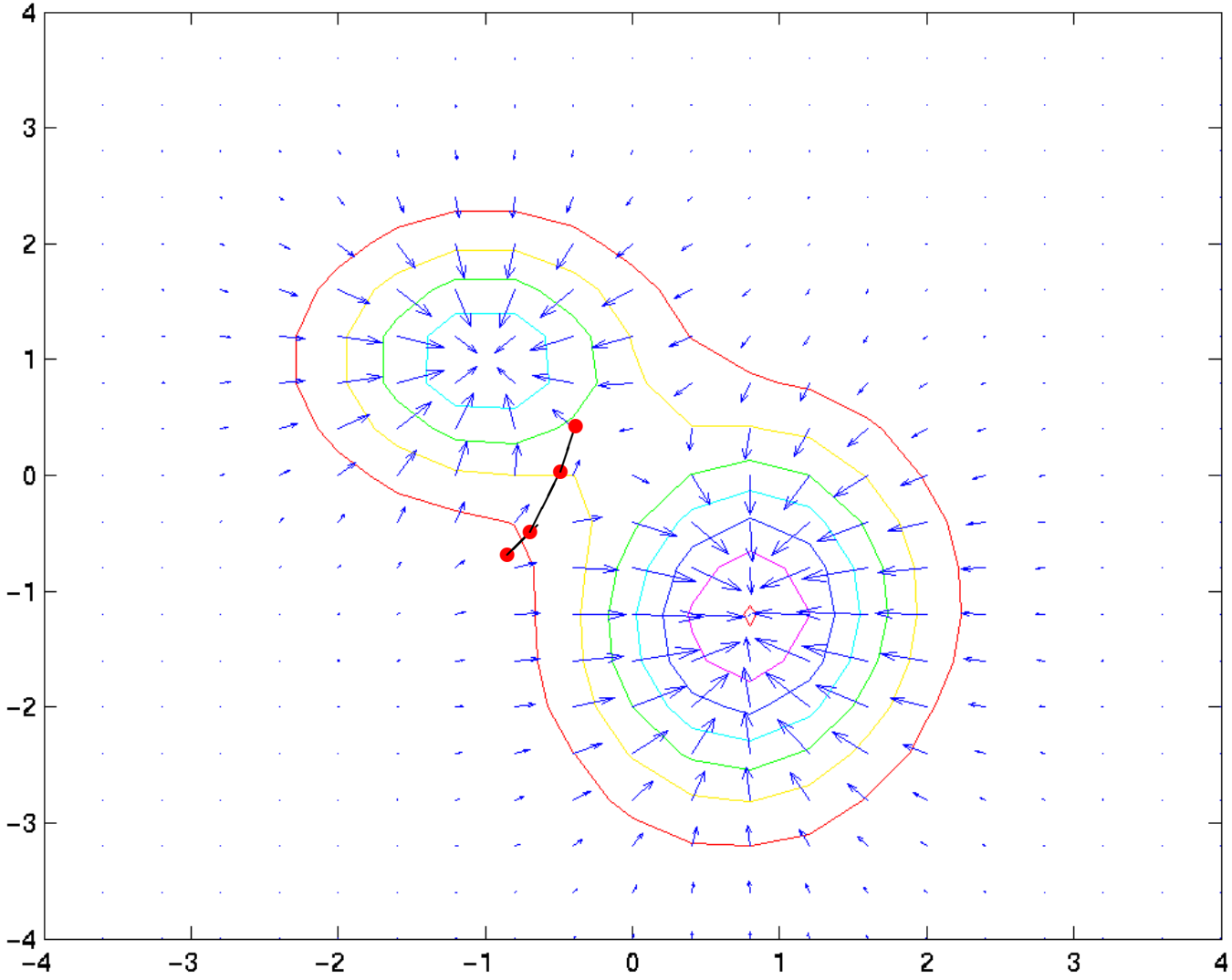

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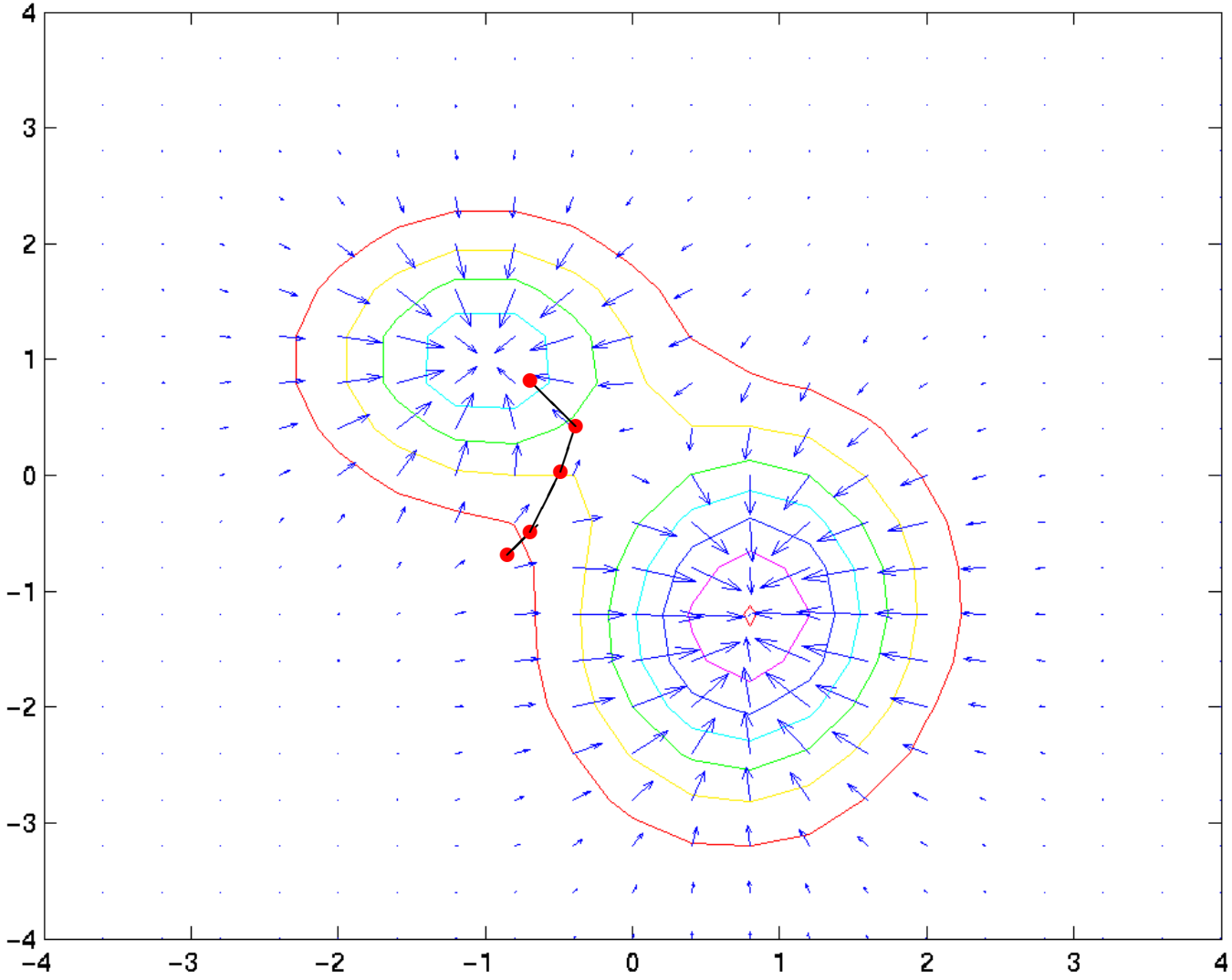

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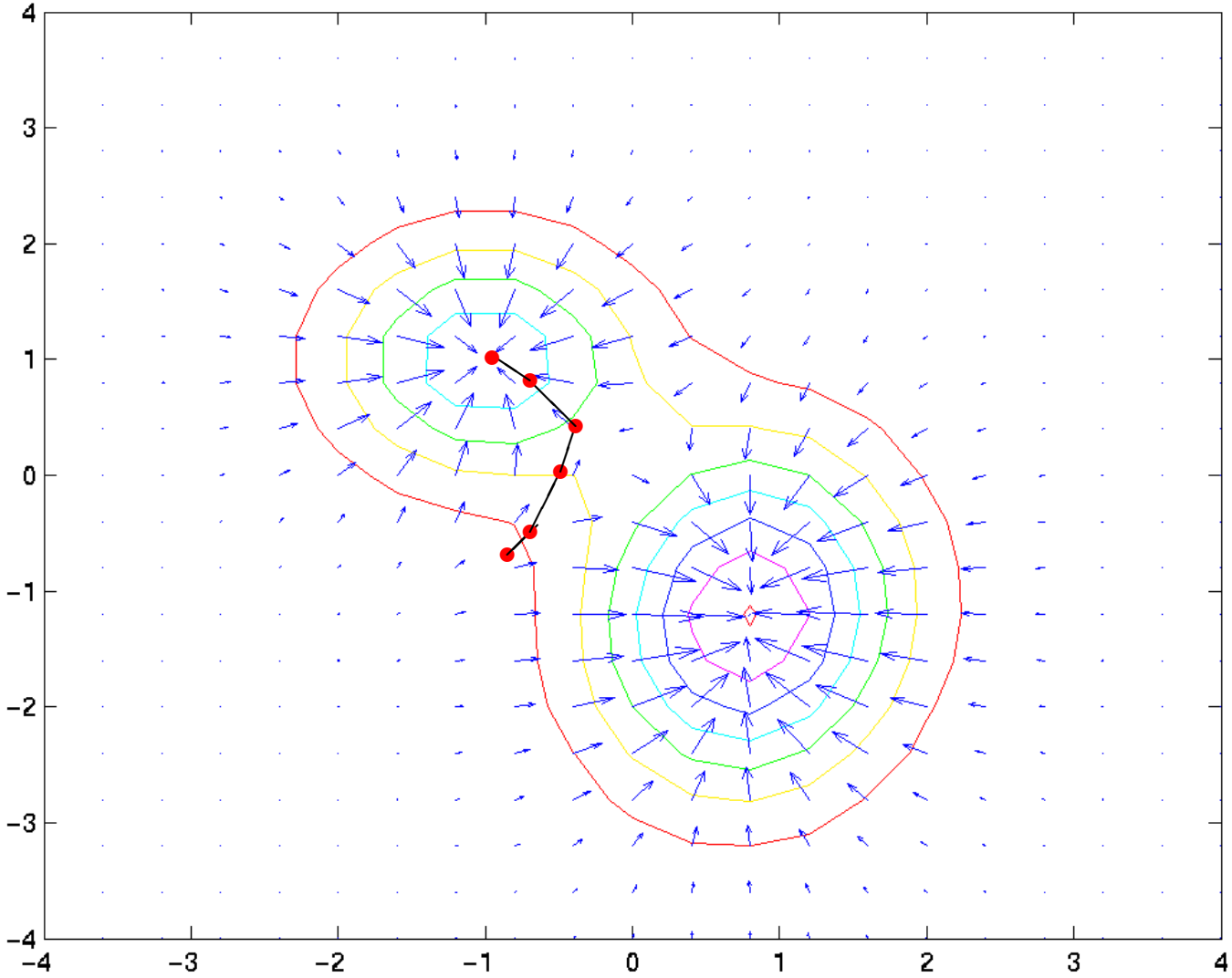
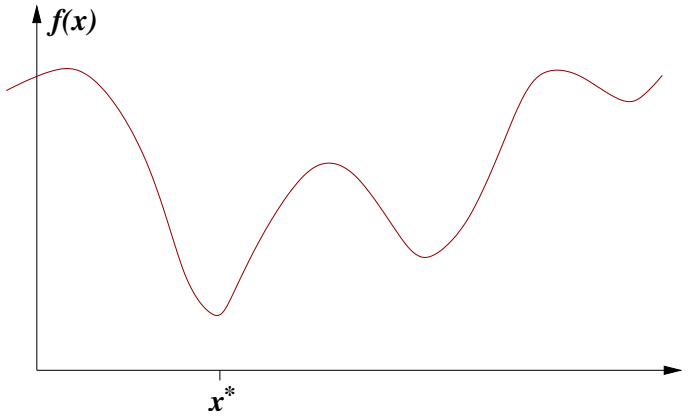


# What Goes Right

- 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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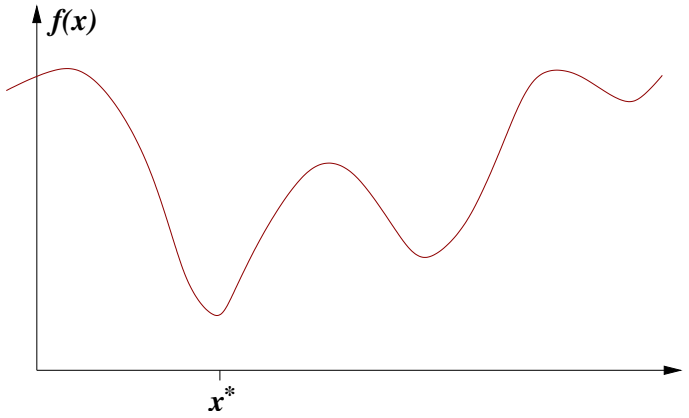


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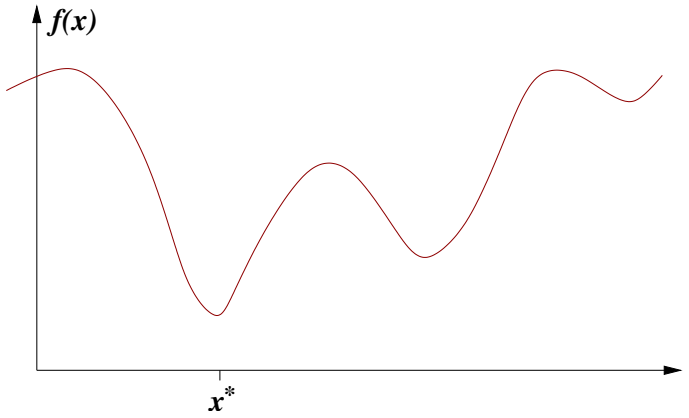


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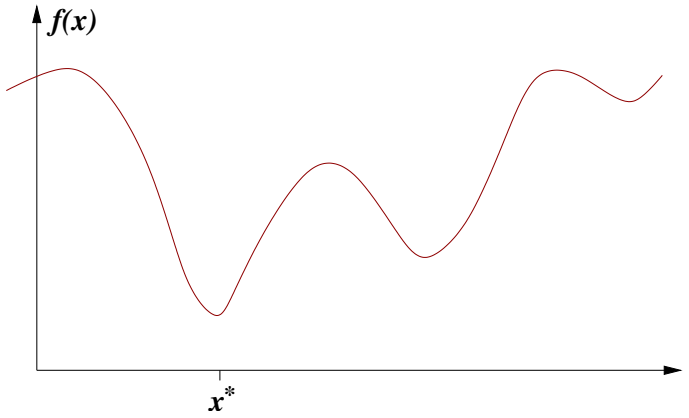


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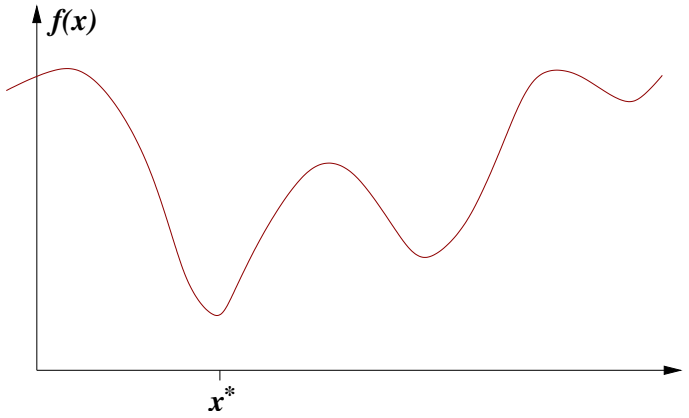


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# Newton's Method

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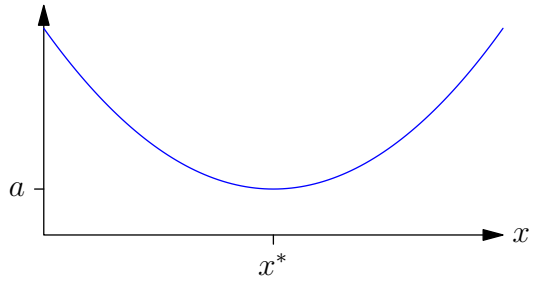
$$f(x) = a + \frac{b}{2}\left(x - x^*\right)^2$$




- then

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

- so

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

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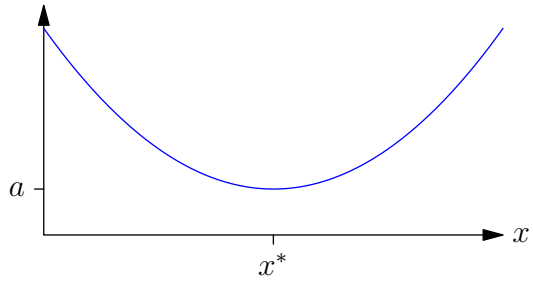


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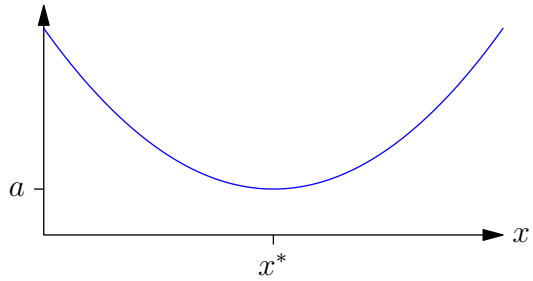


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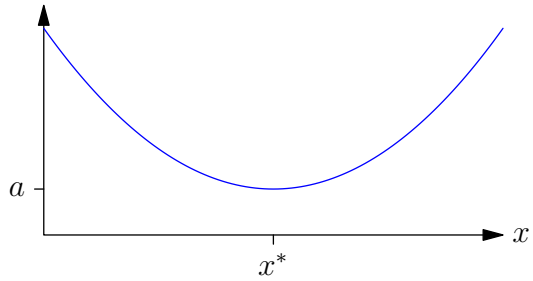


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- This is Newton's methods
- For non-quadratic functions Newtons method converges **quadratically** provided we are sufficiently close to a minimum
- If we are at a distance $x - x^* = \epsilon$ from the minima then after one cycle we will be a distance $\epsilon^2$ after two cycles we will be at a distance $\epsilon^4$, etc.
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# 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

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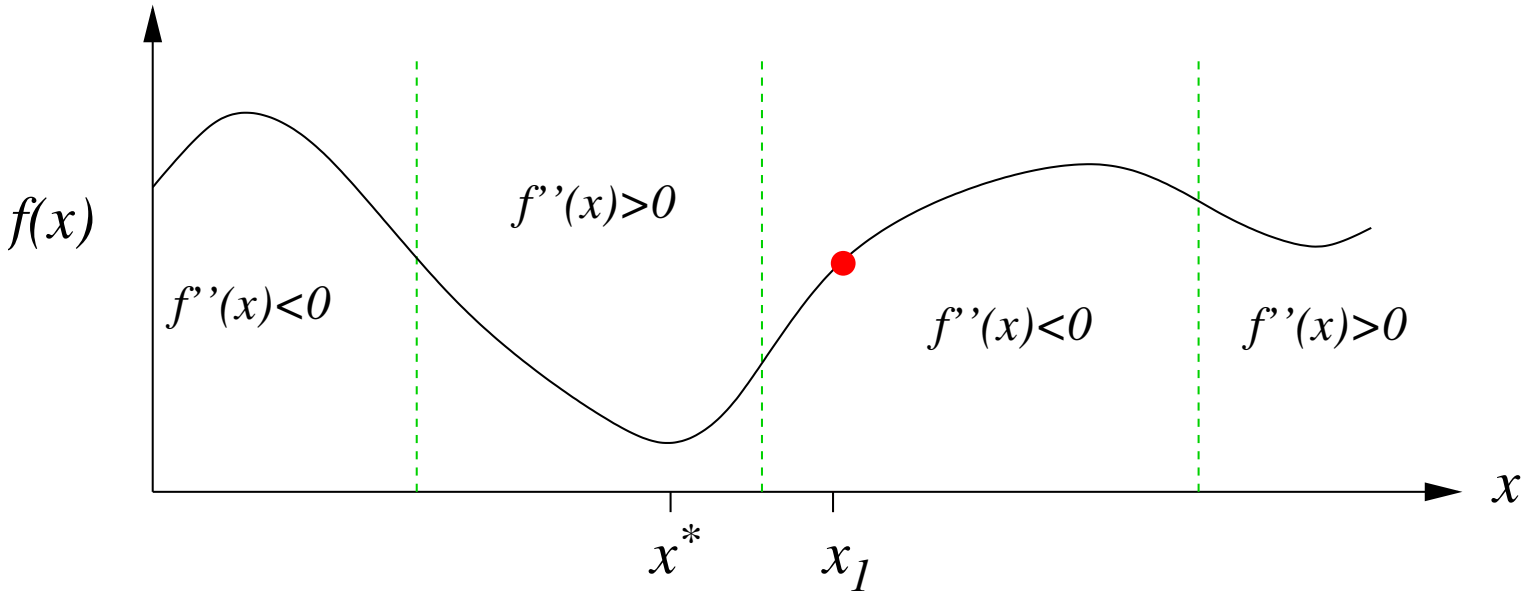

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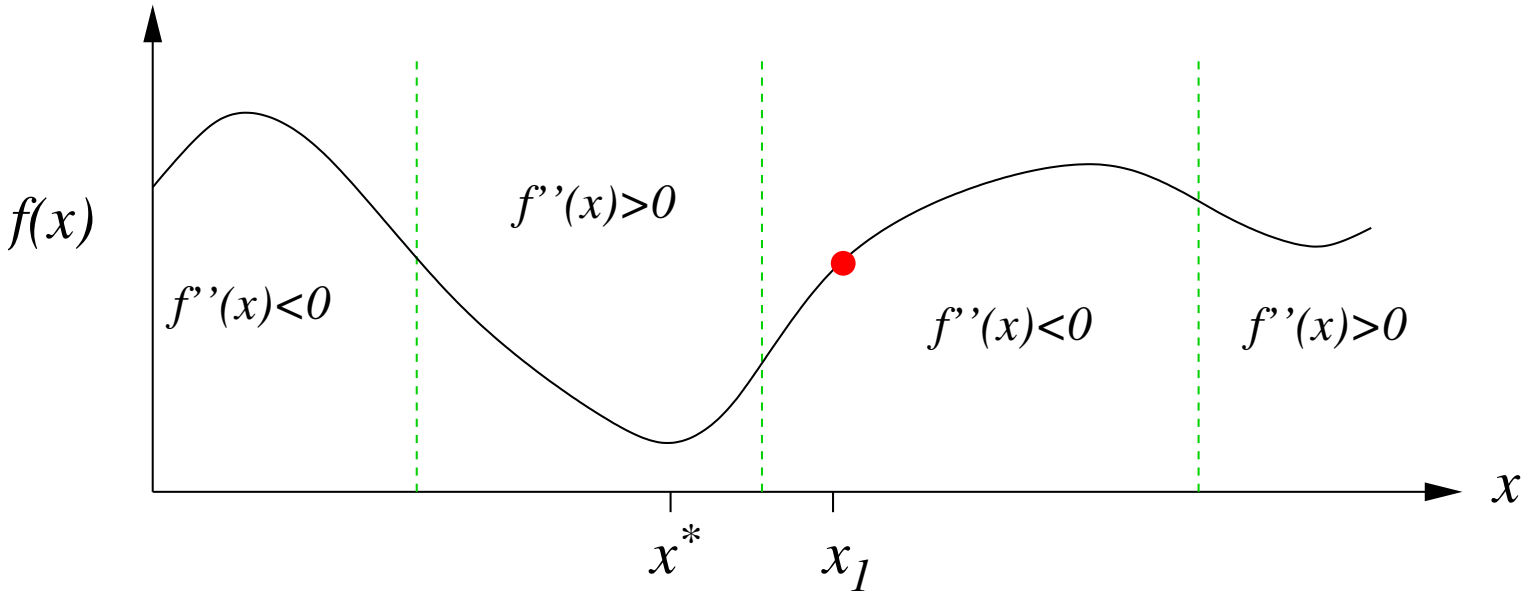

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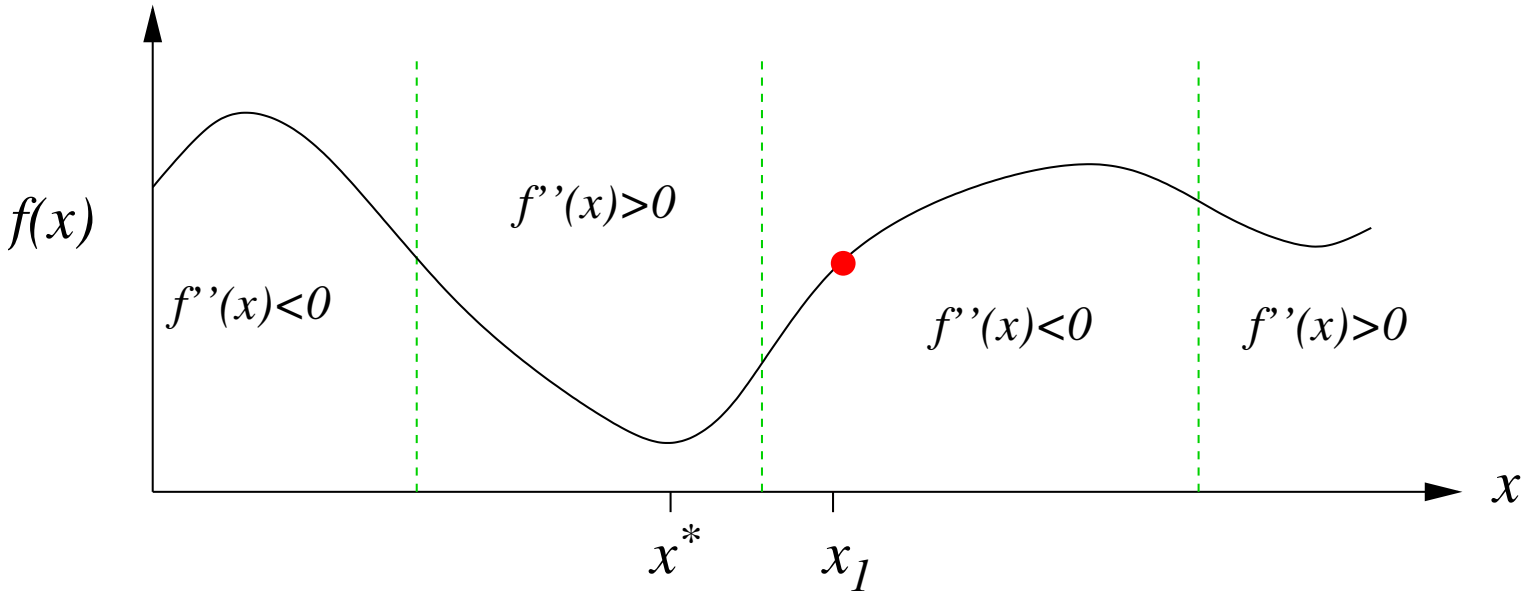

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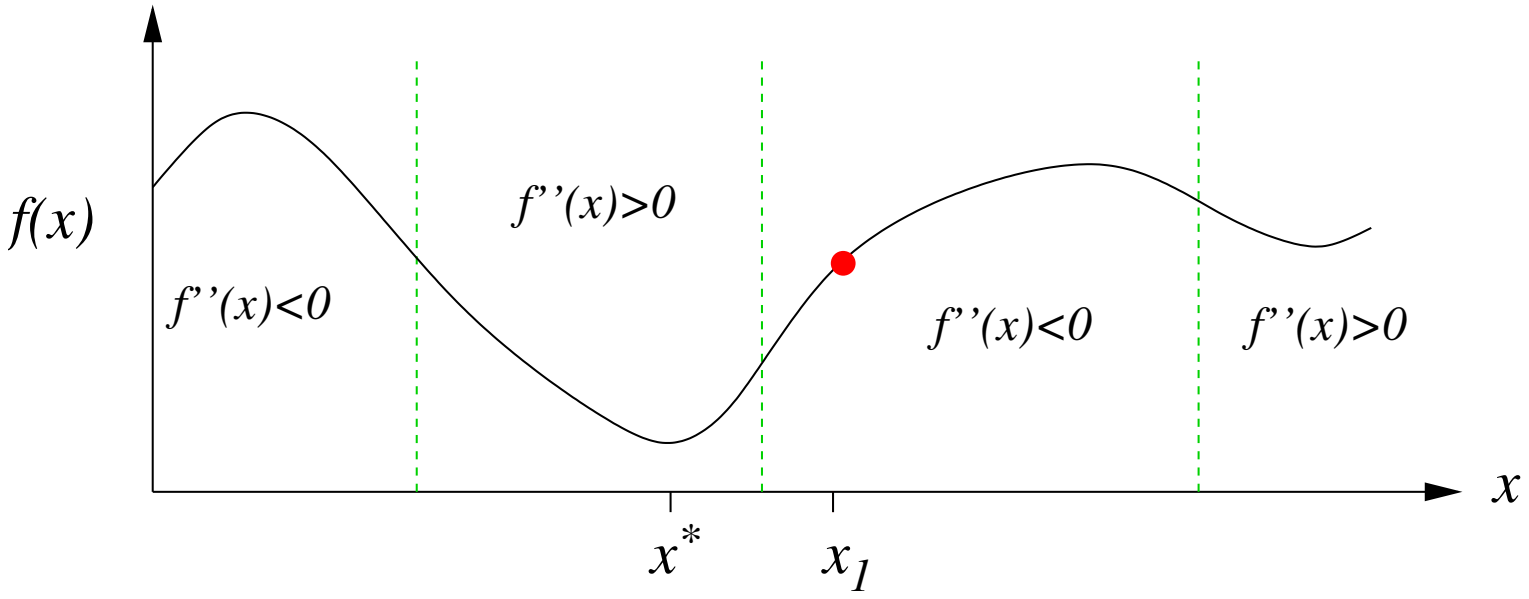

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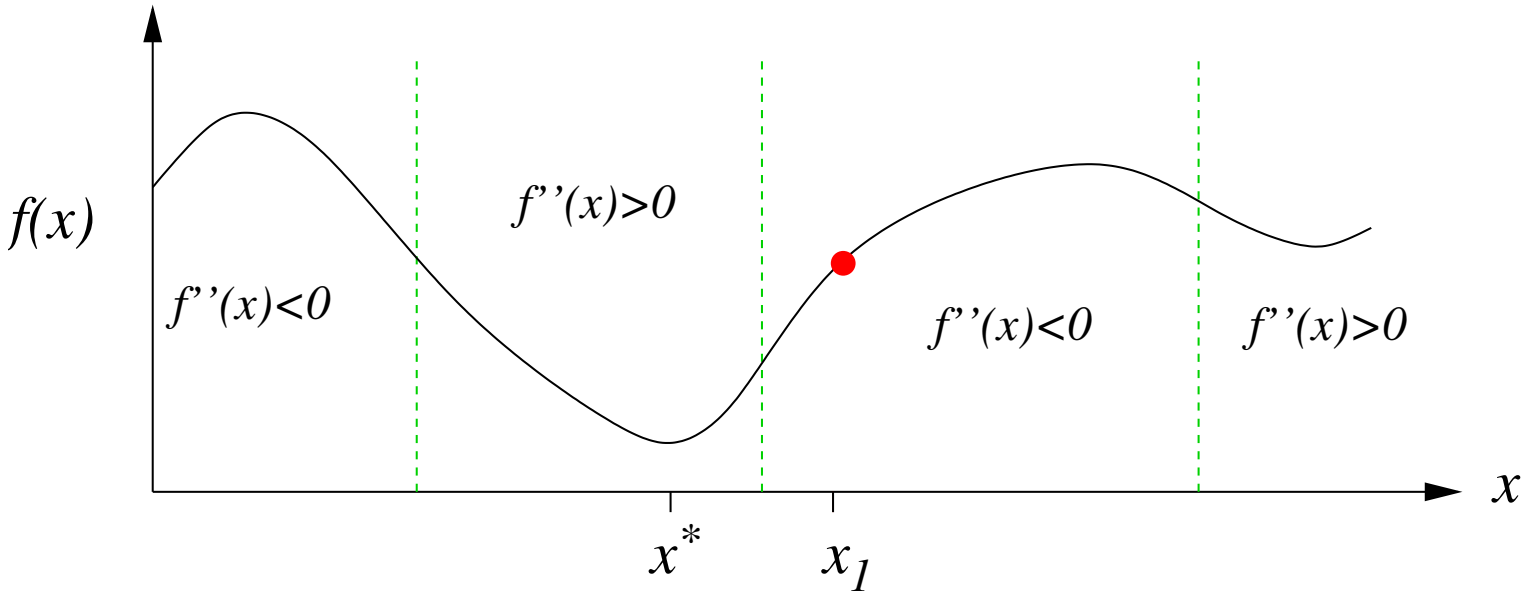
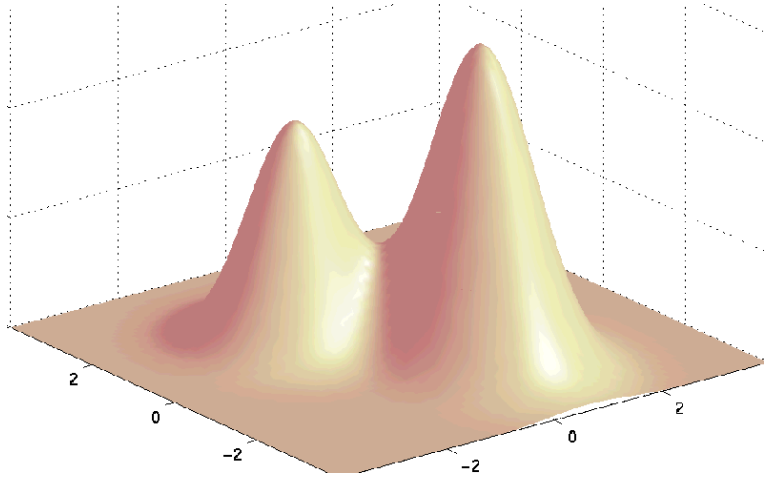


# Outline

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



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- Gradient descent

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

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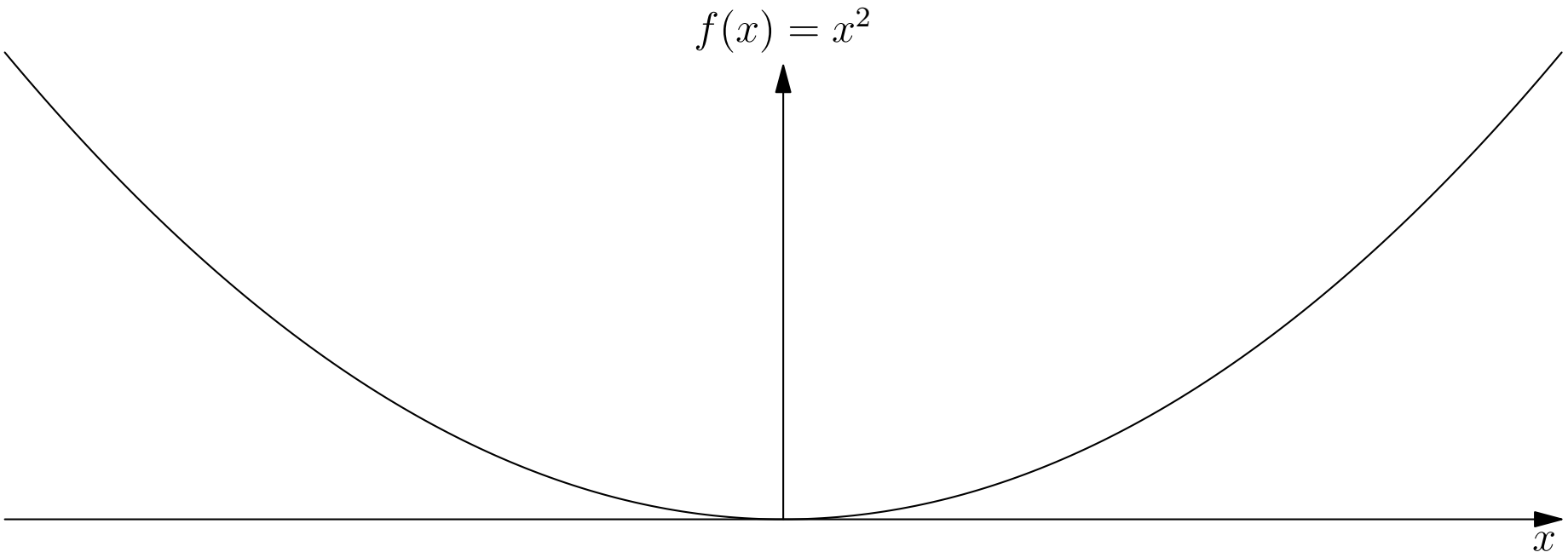

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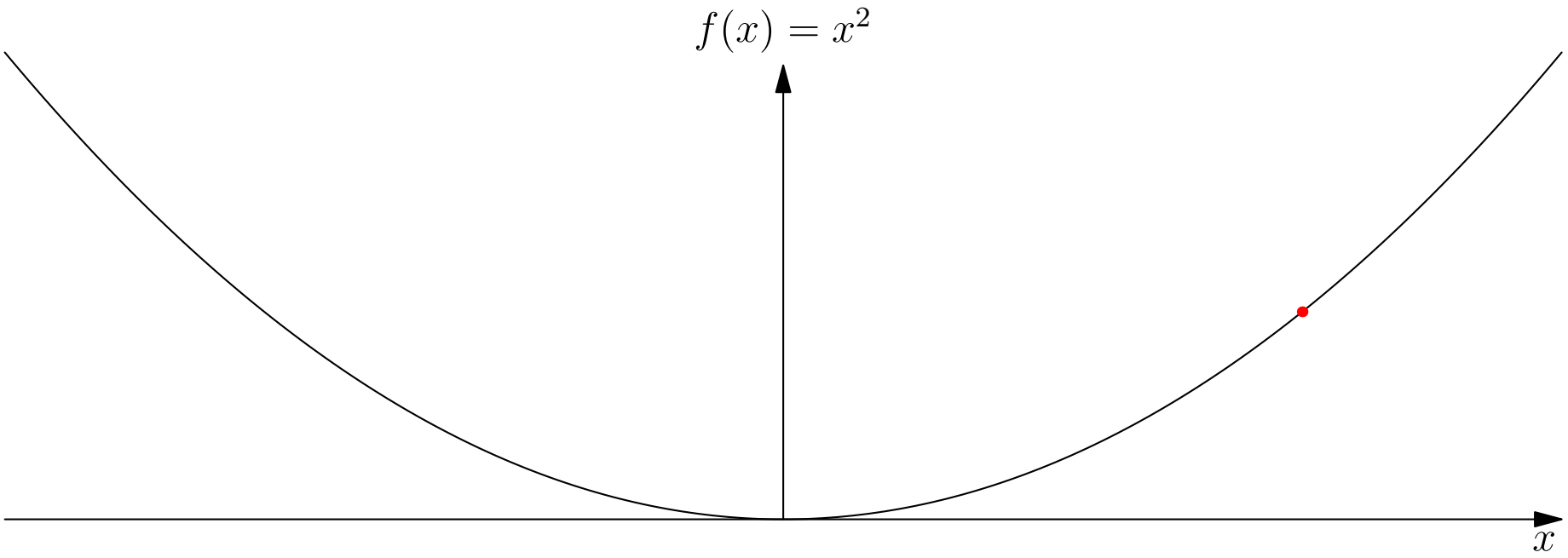


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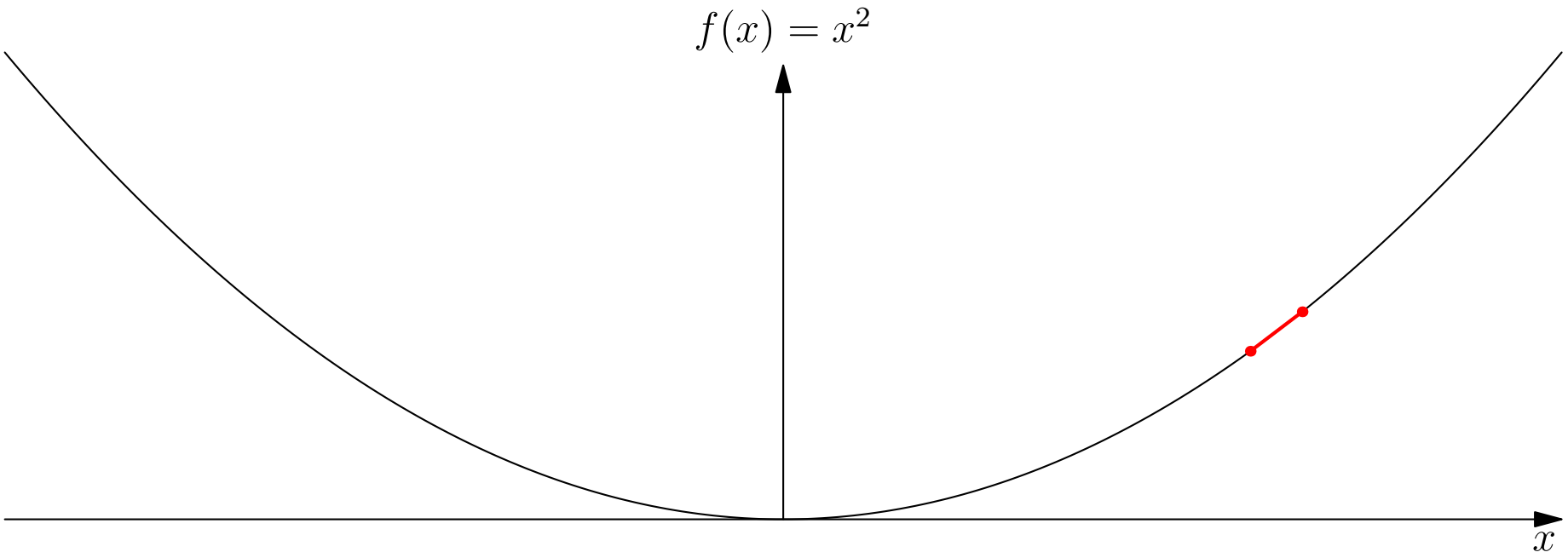


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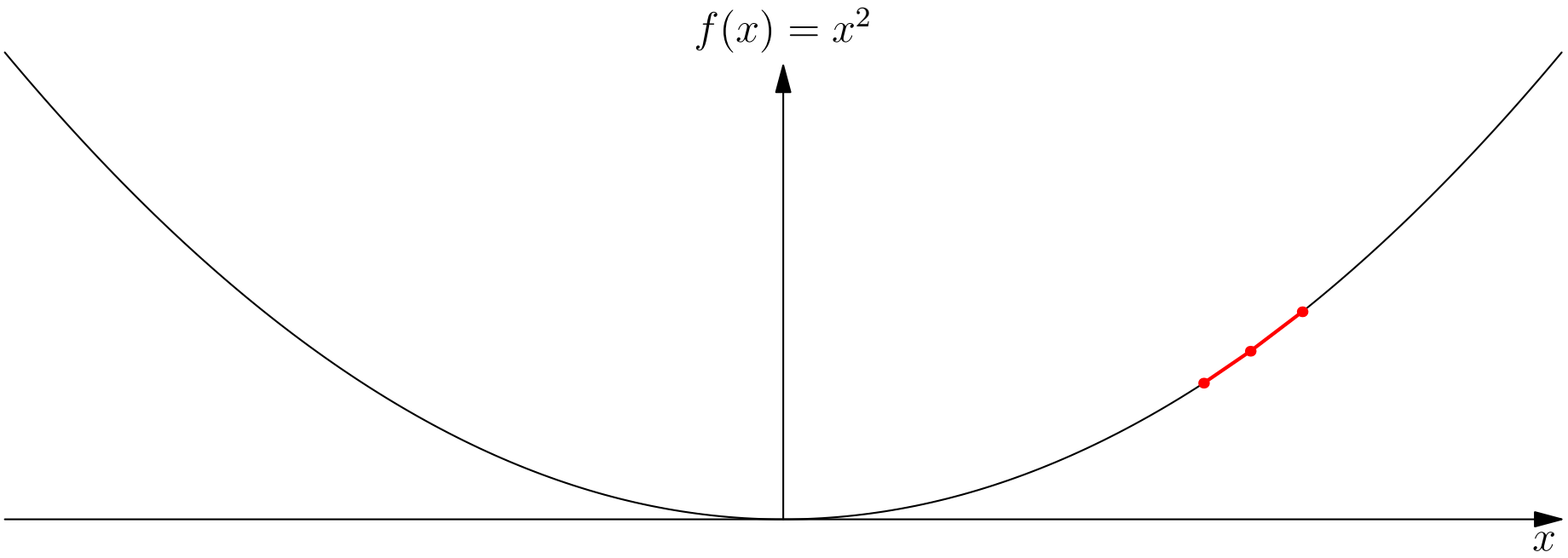


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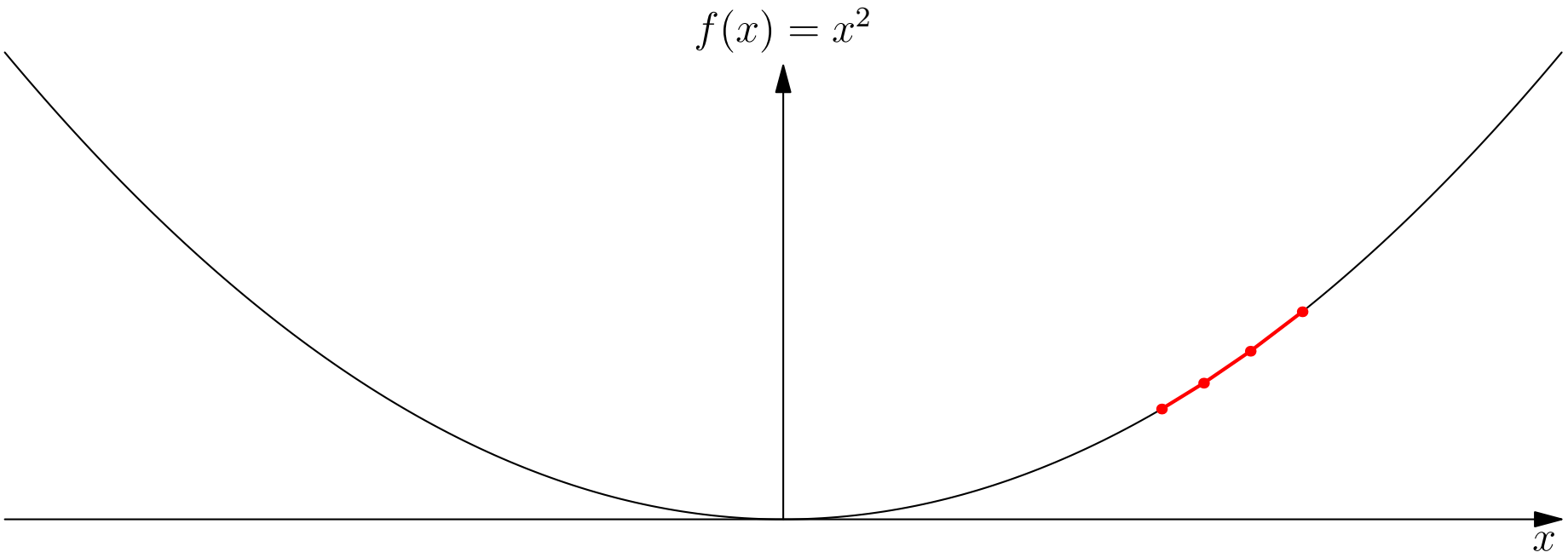


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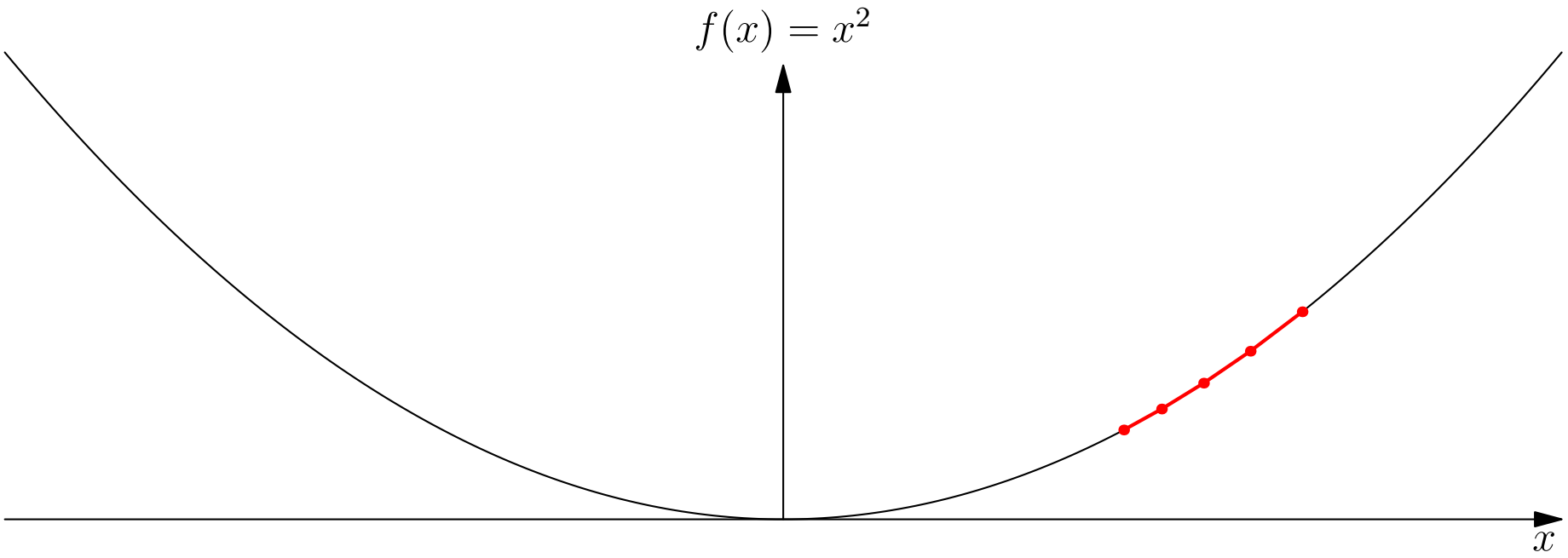


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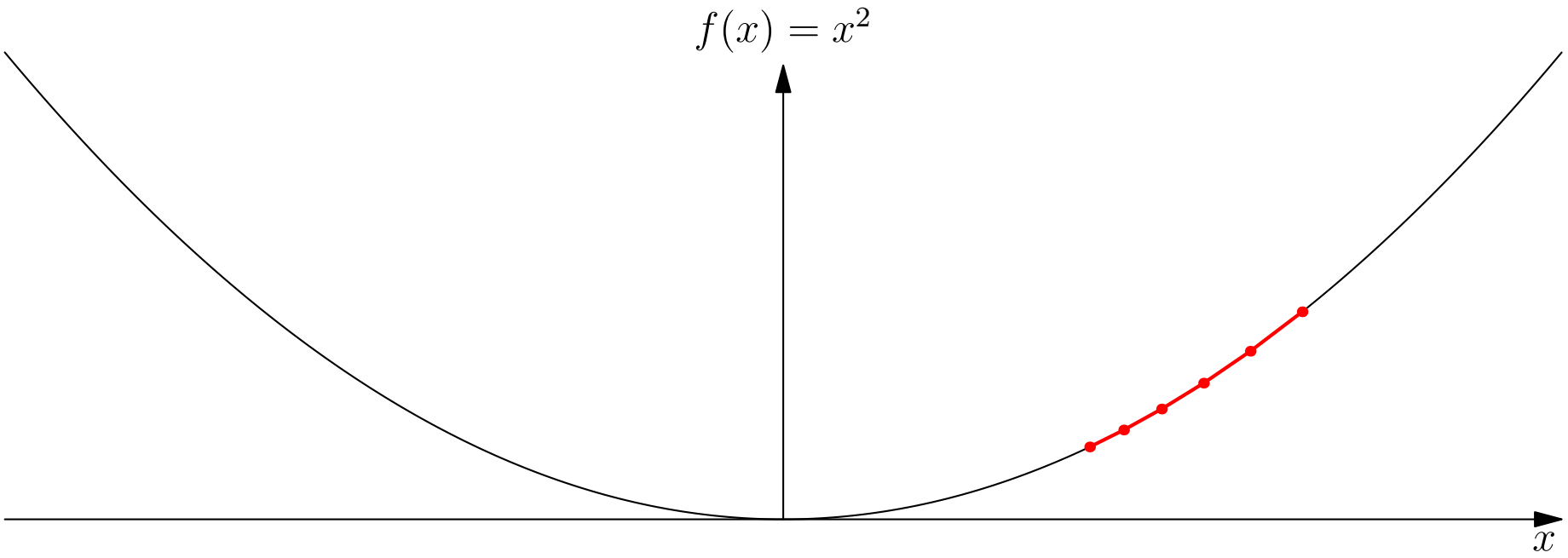


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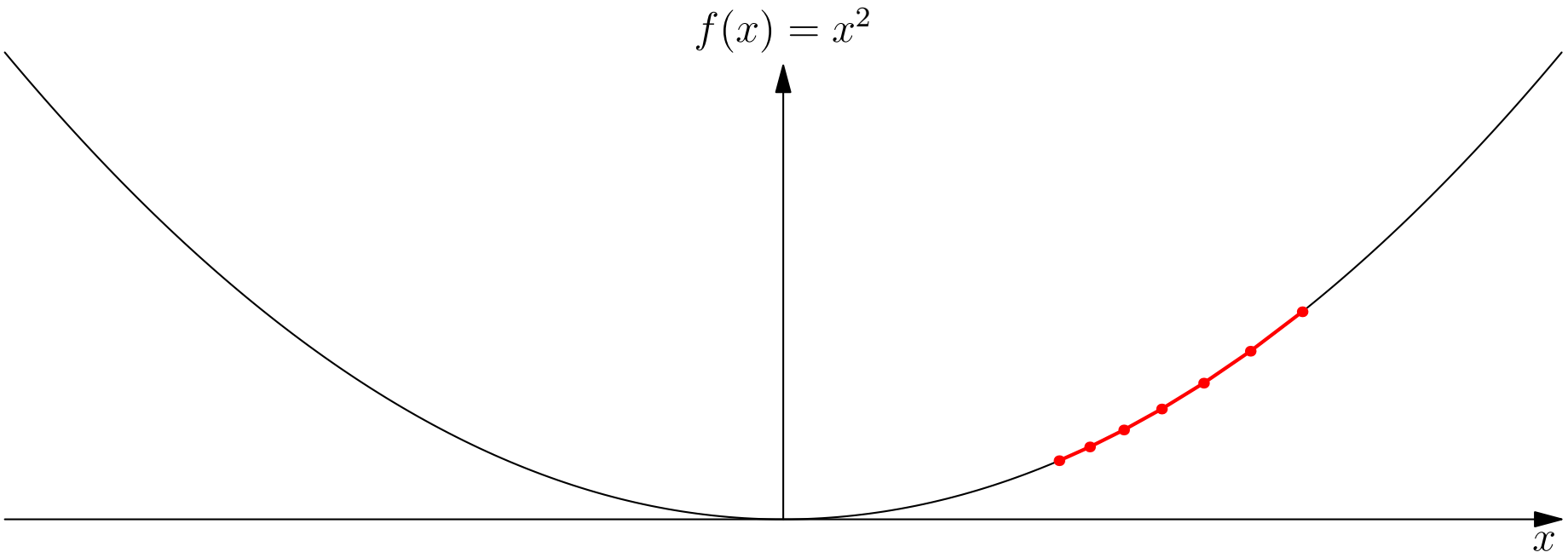


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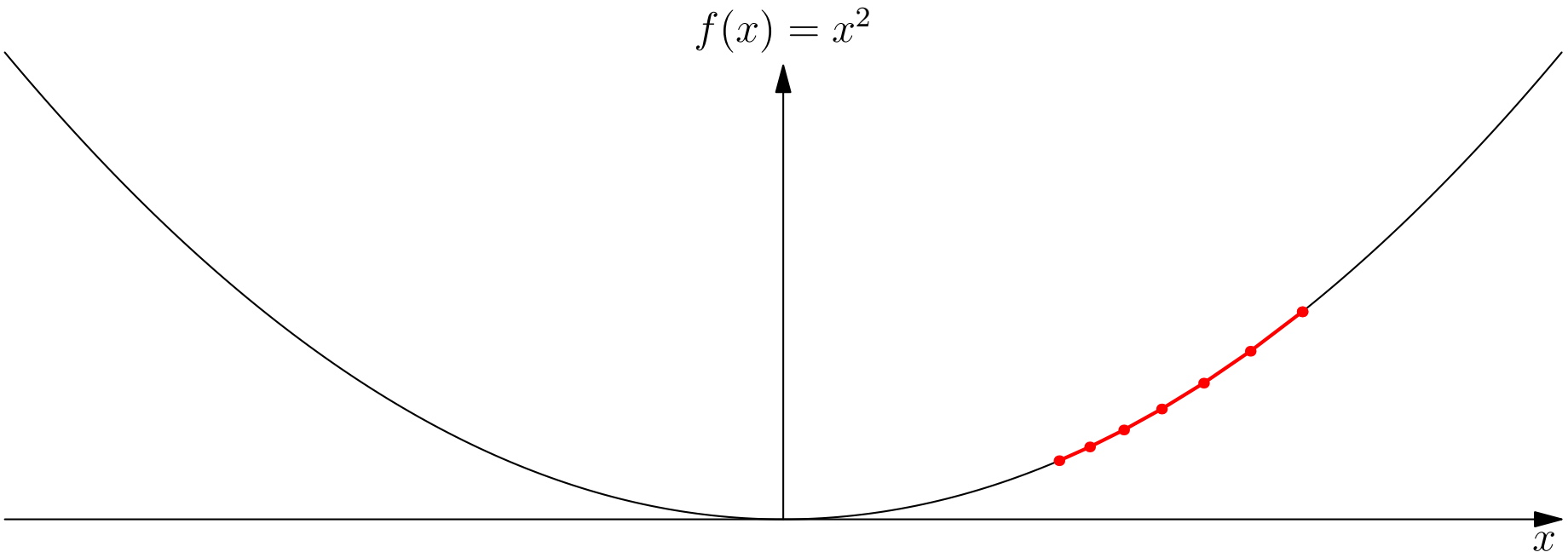


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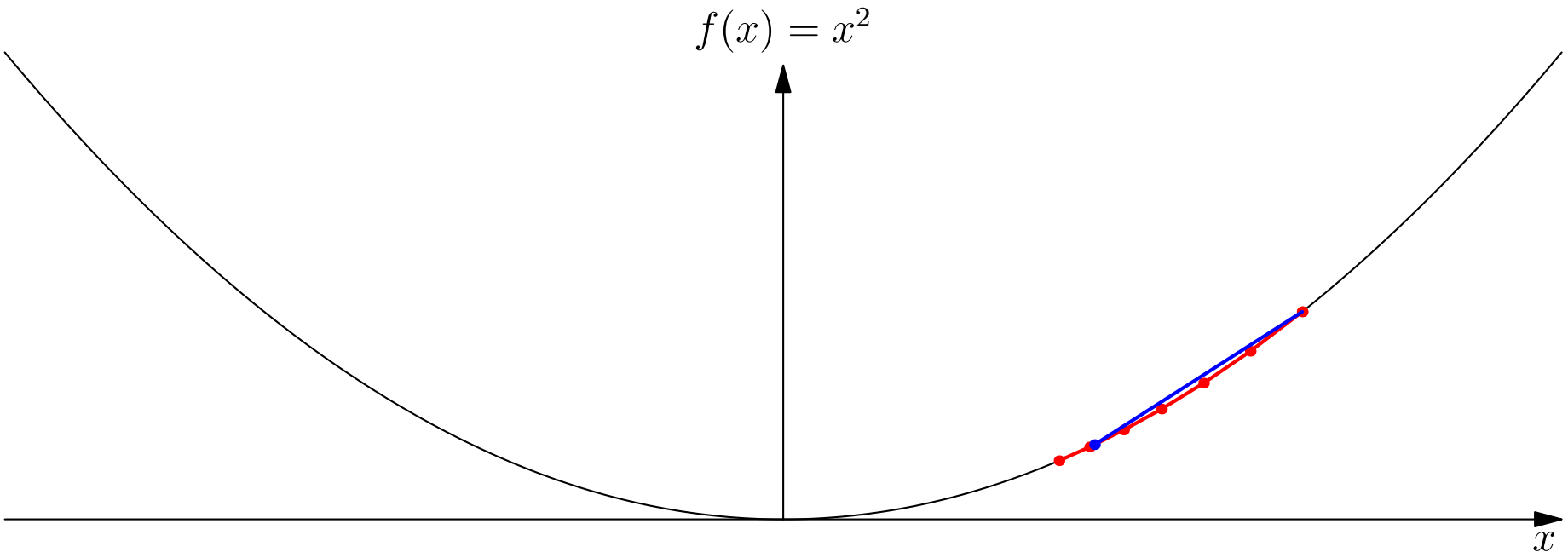


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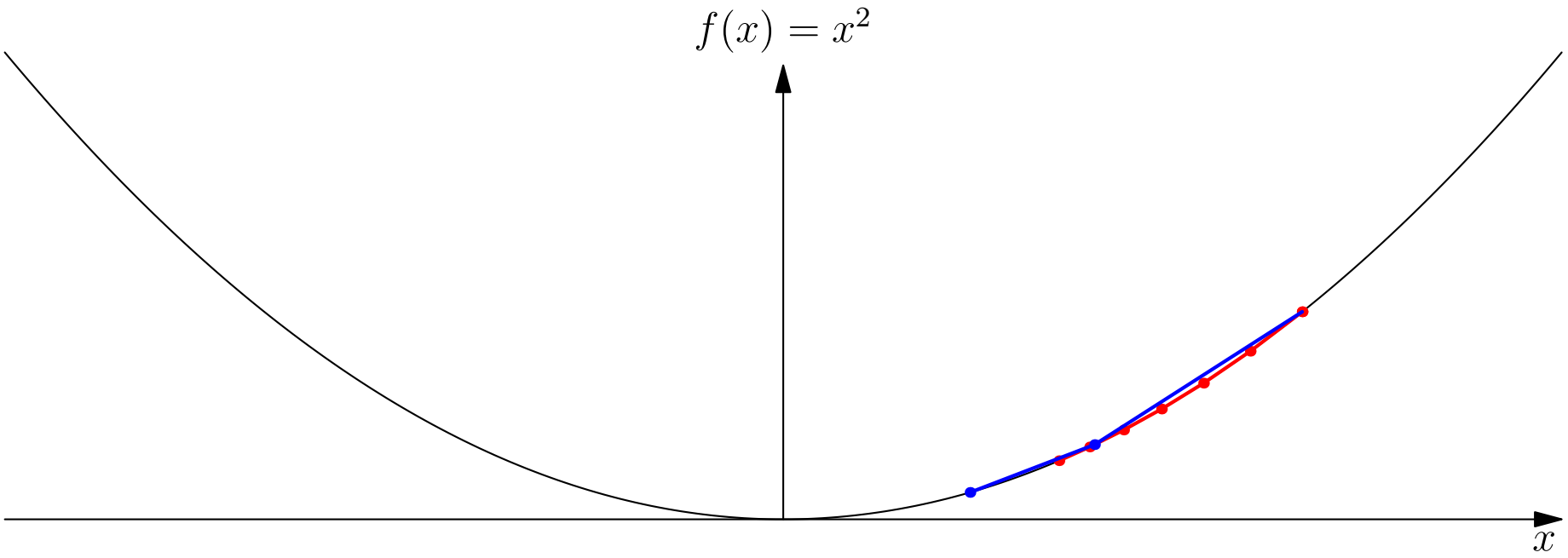


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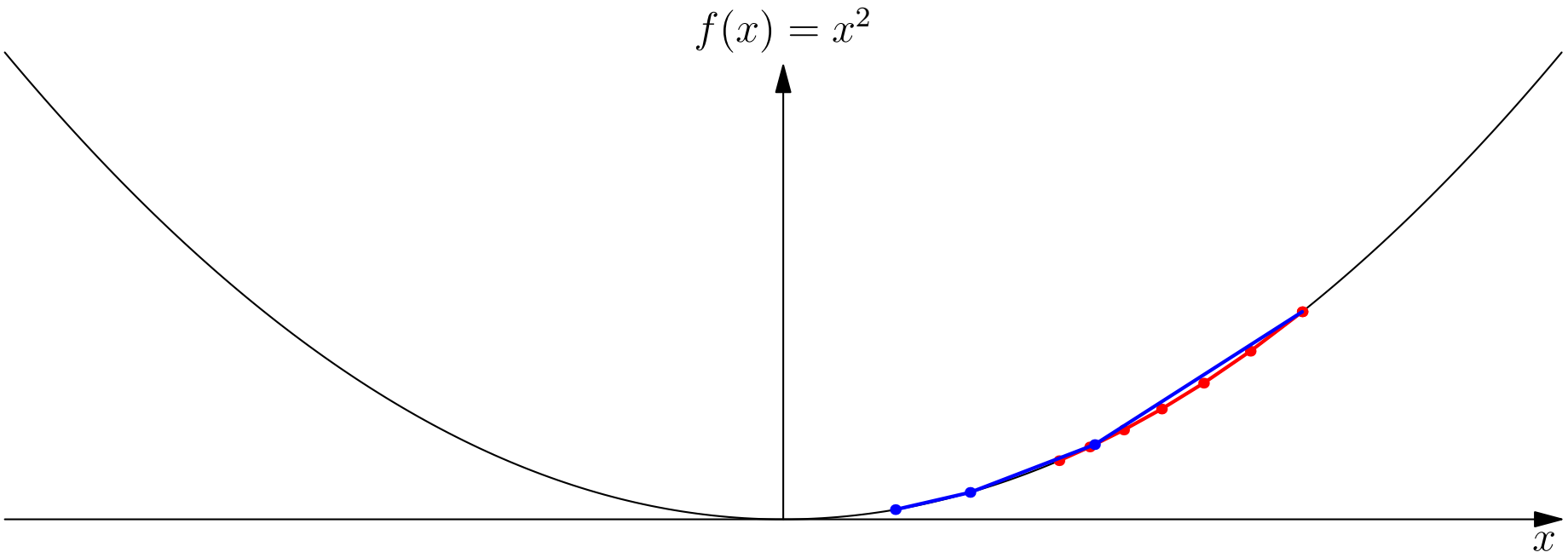


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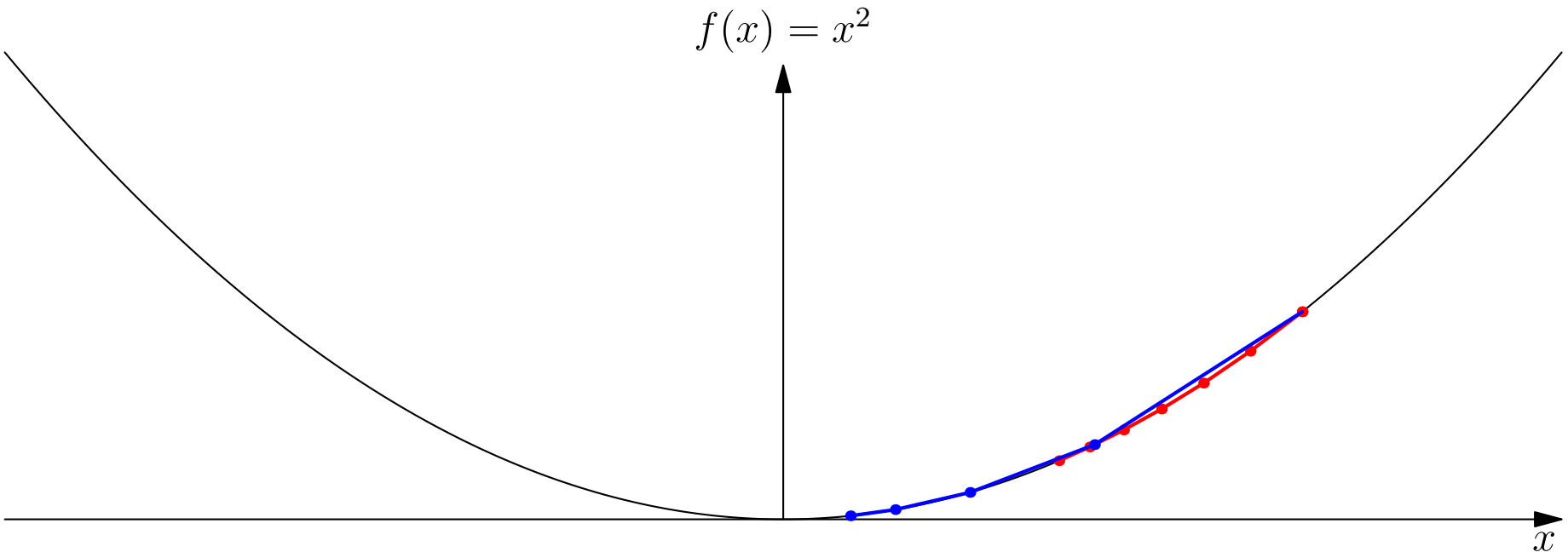


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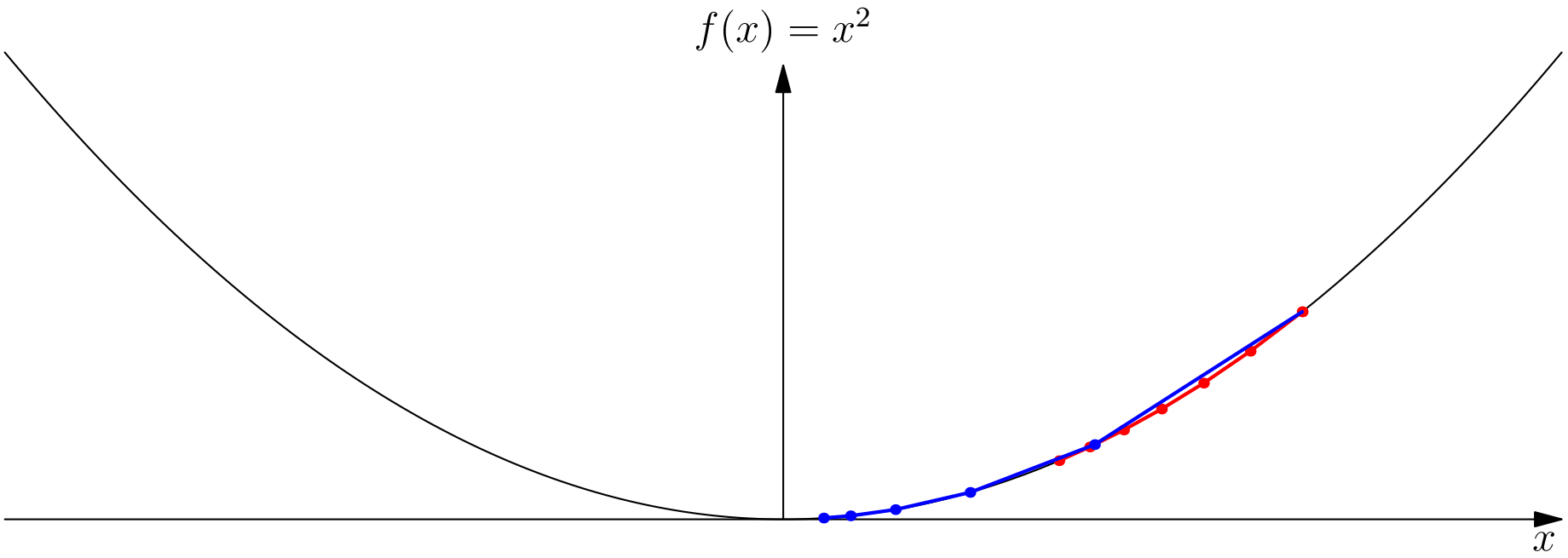


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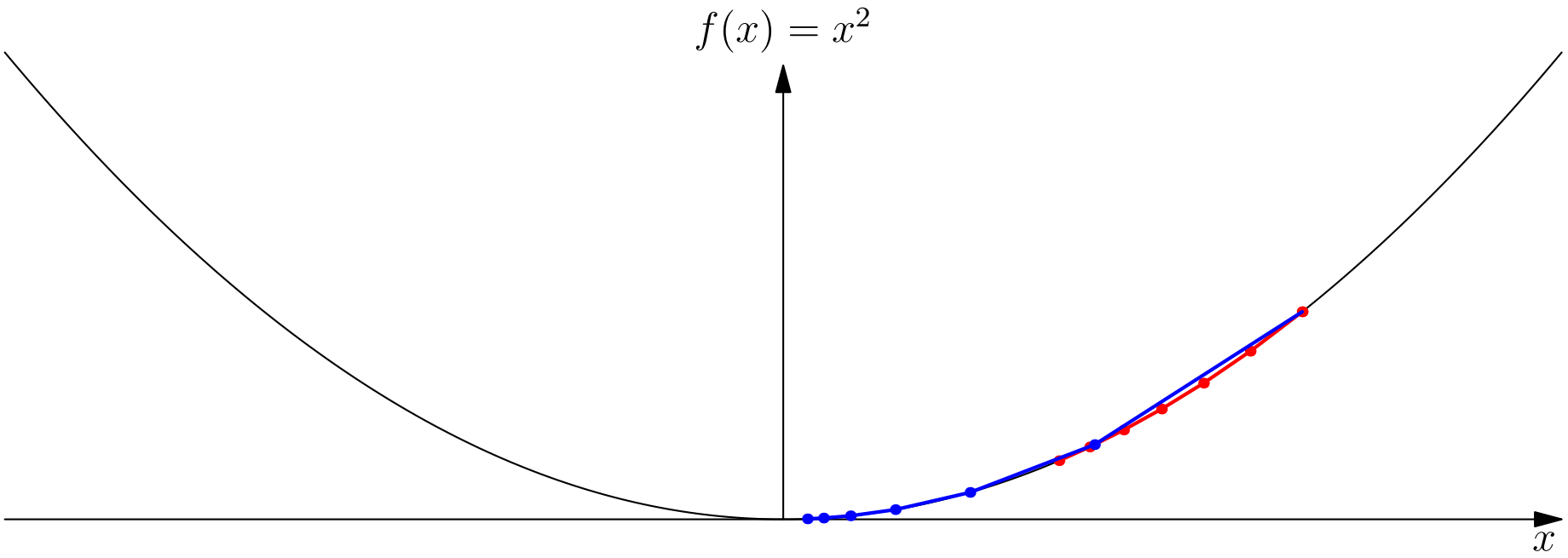


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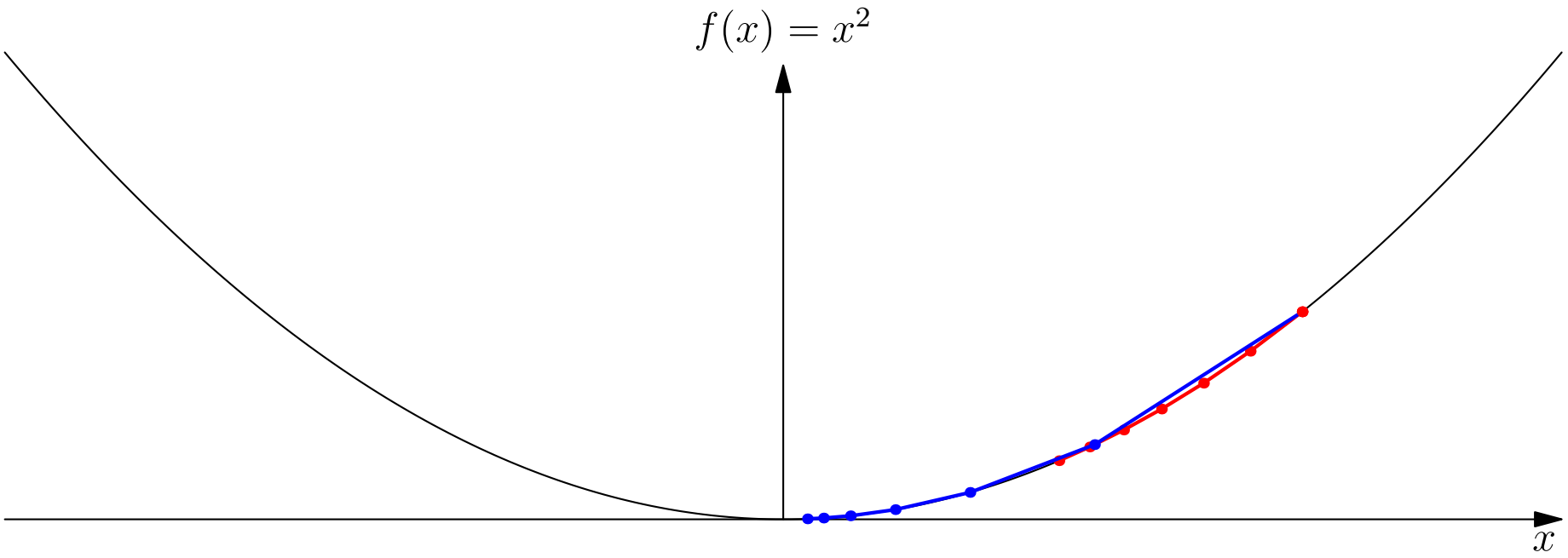


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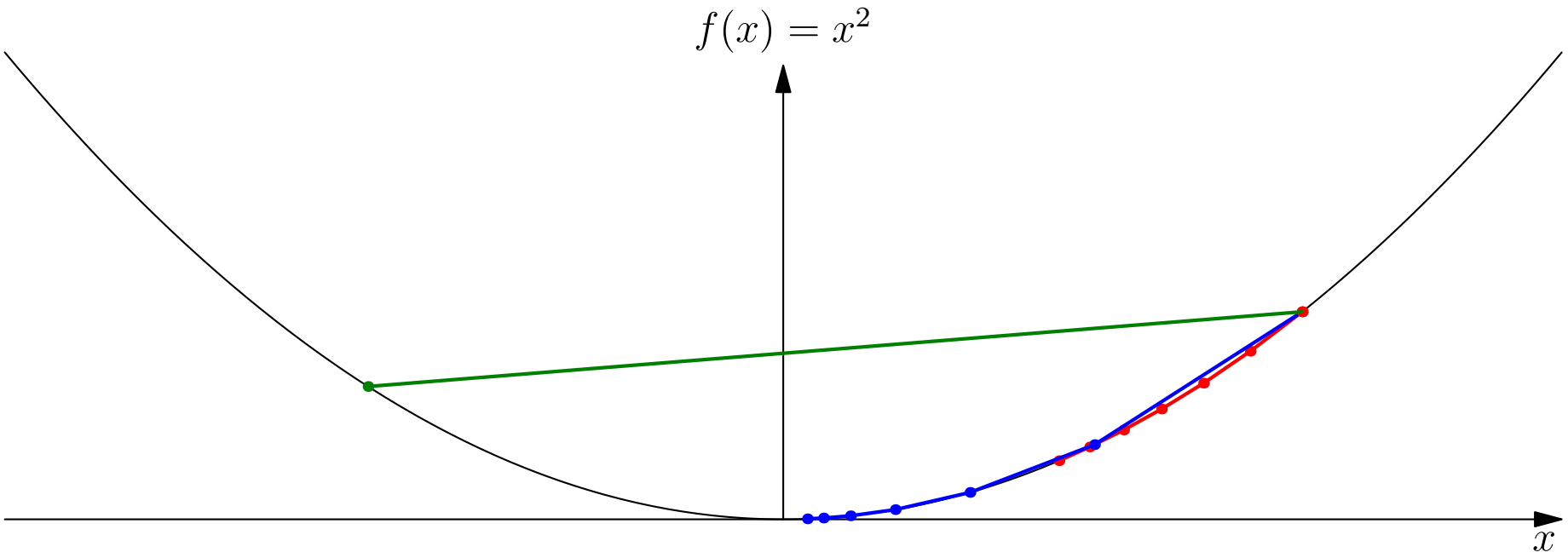


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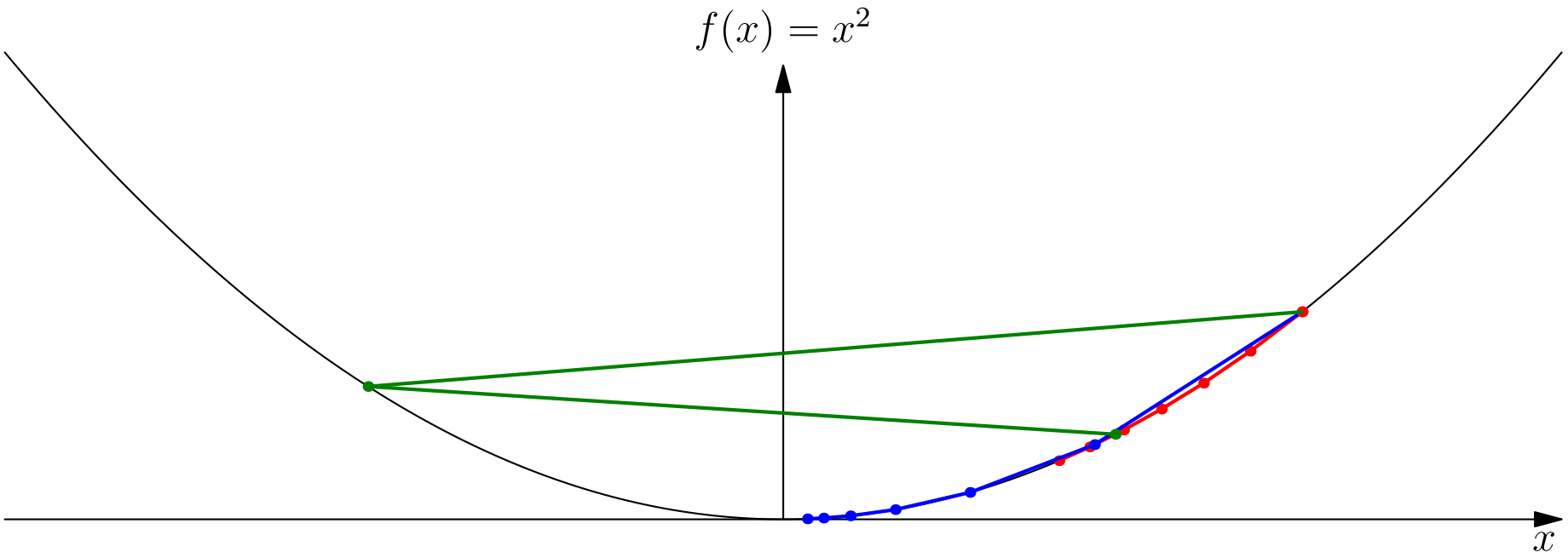


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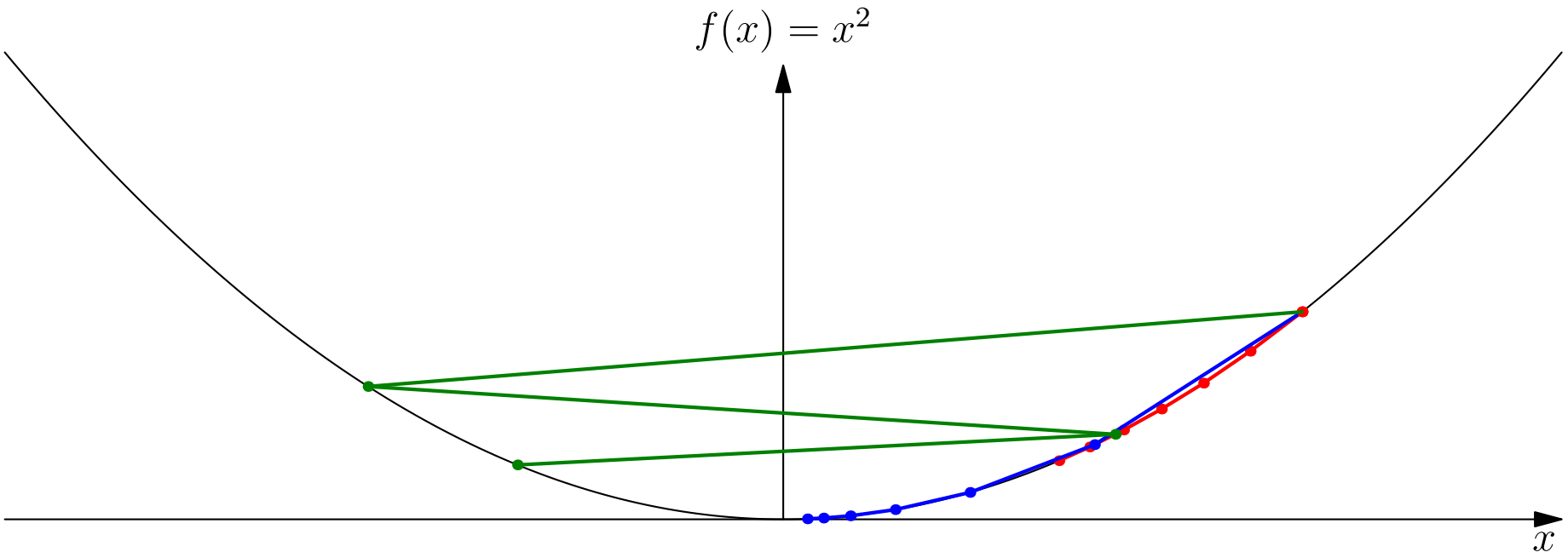


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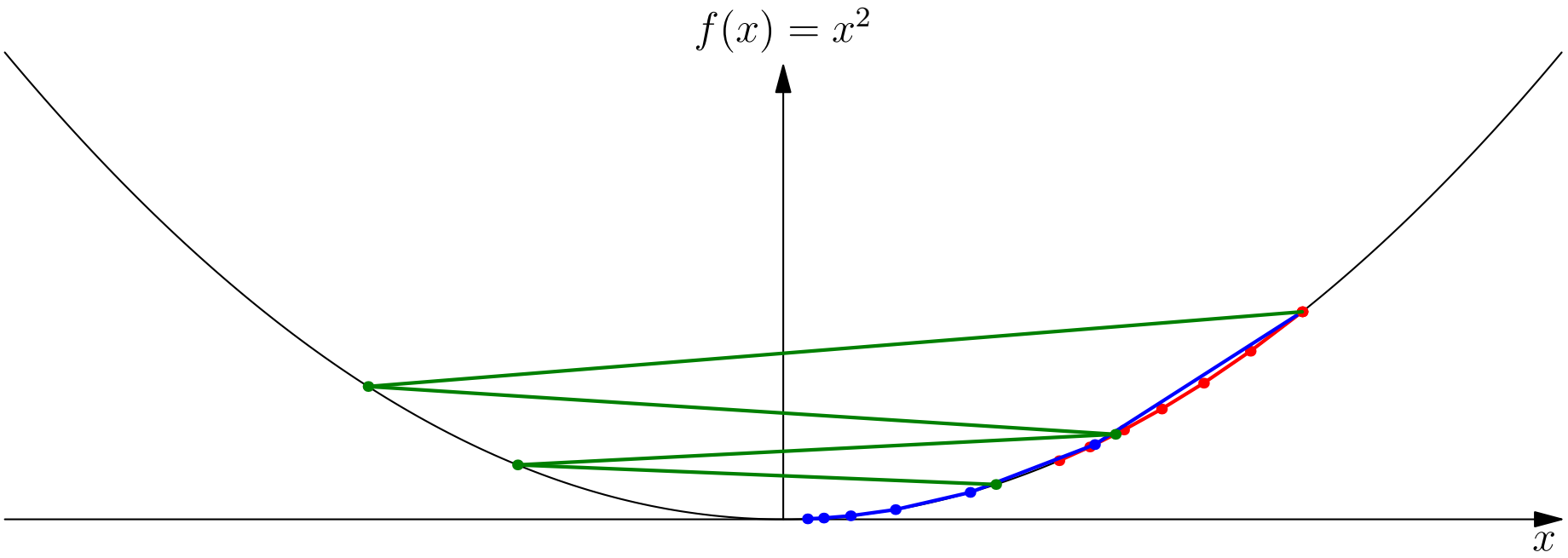


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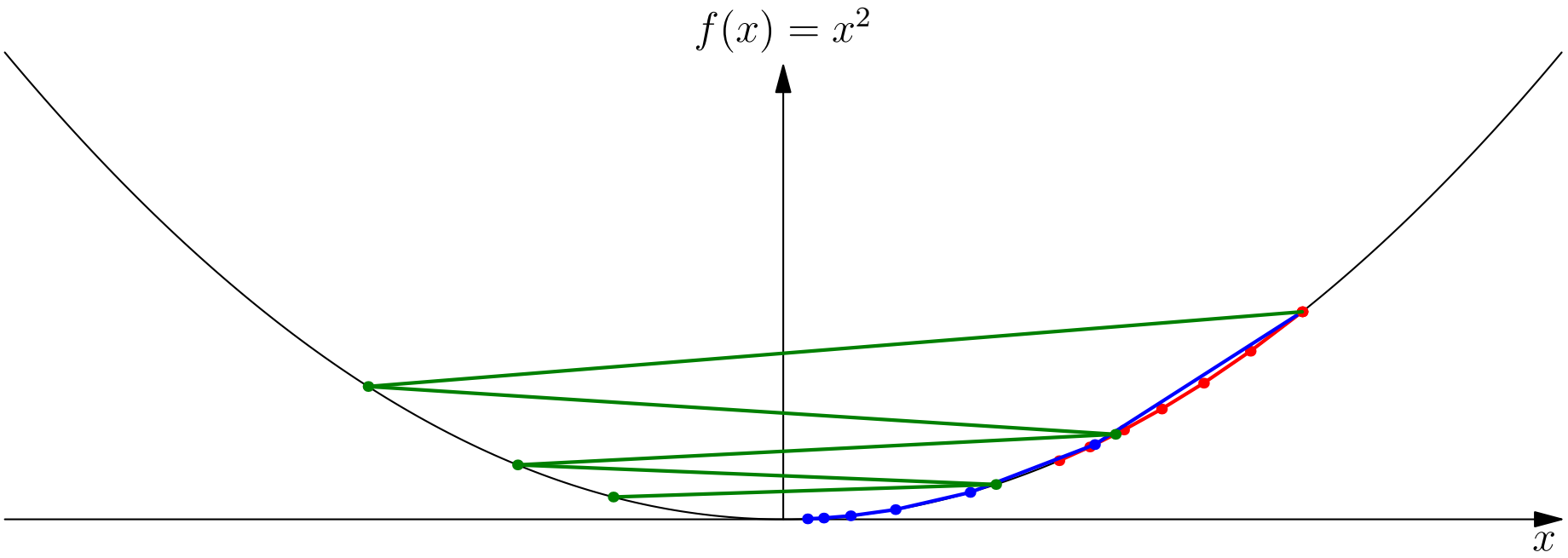


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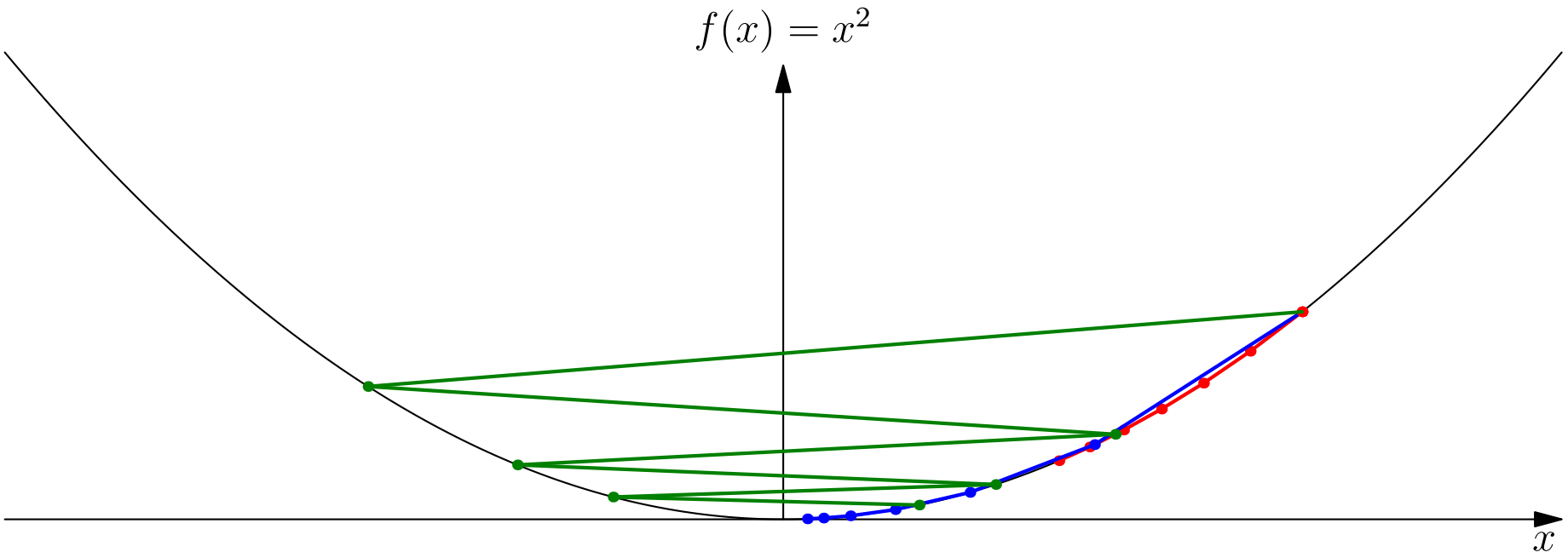


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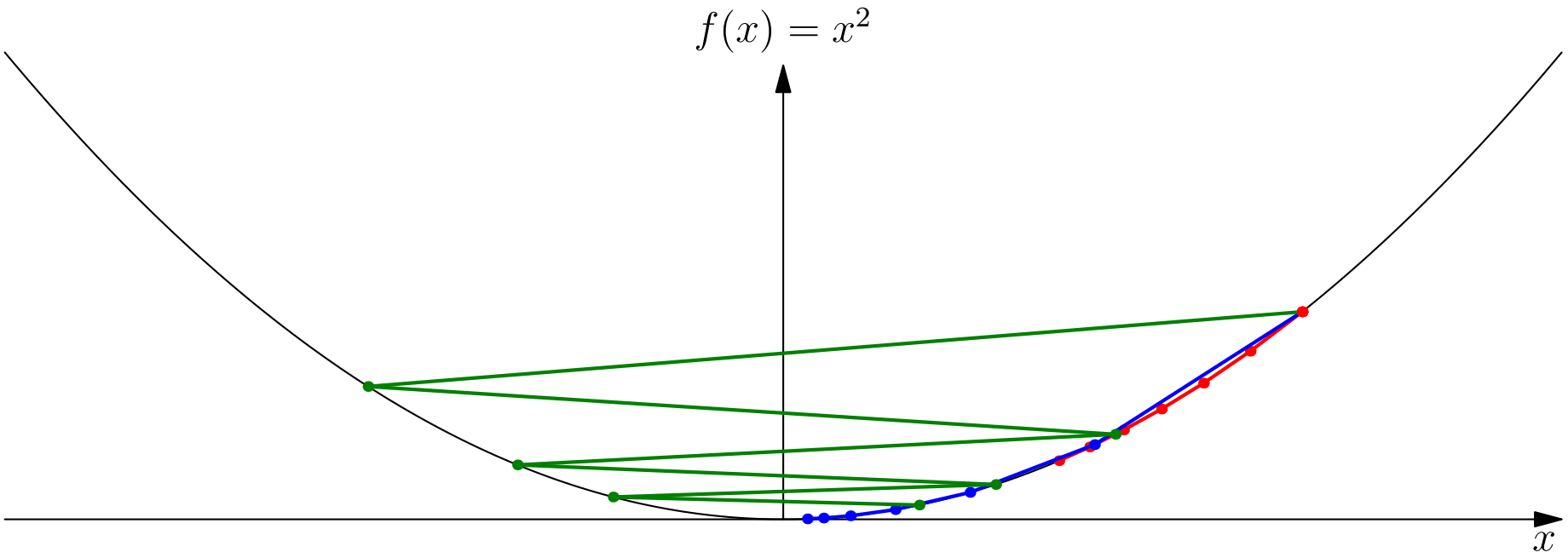

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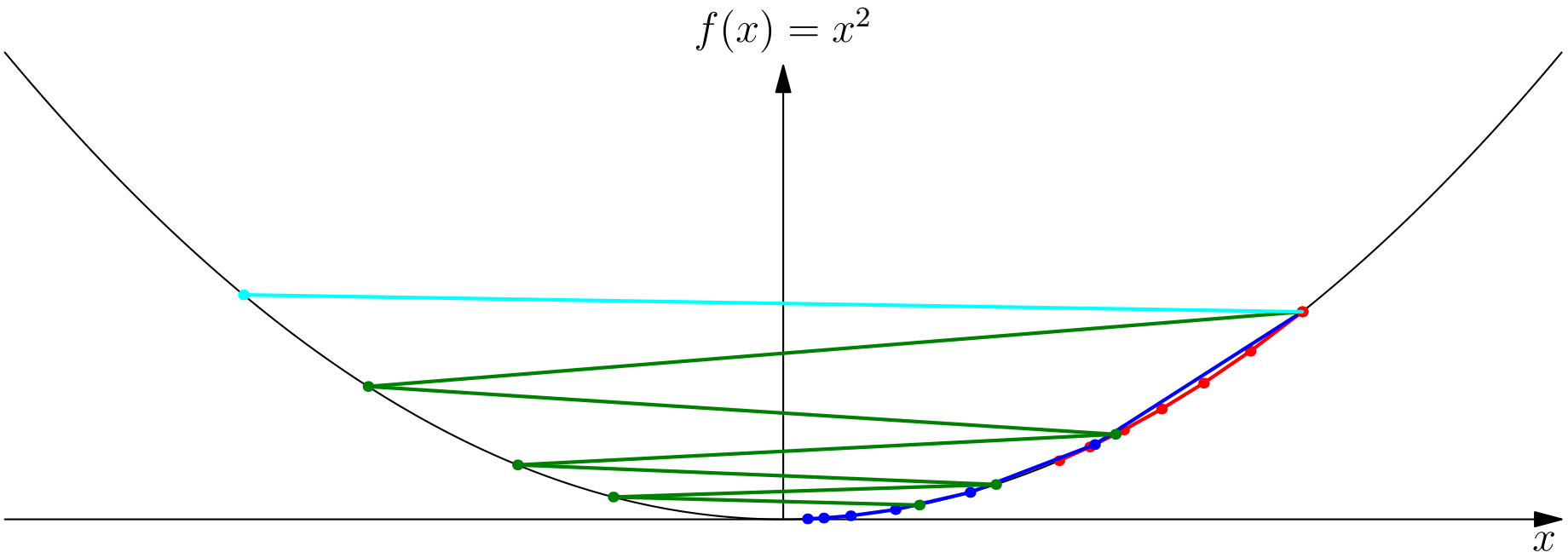

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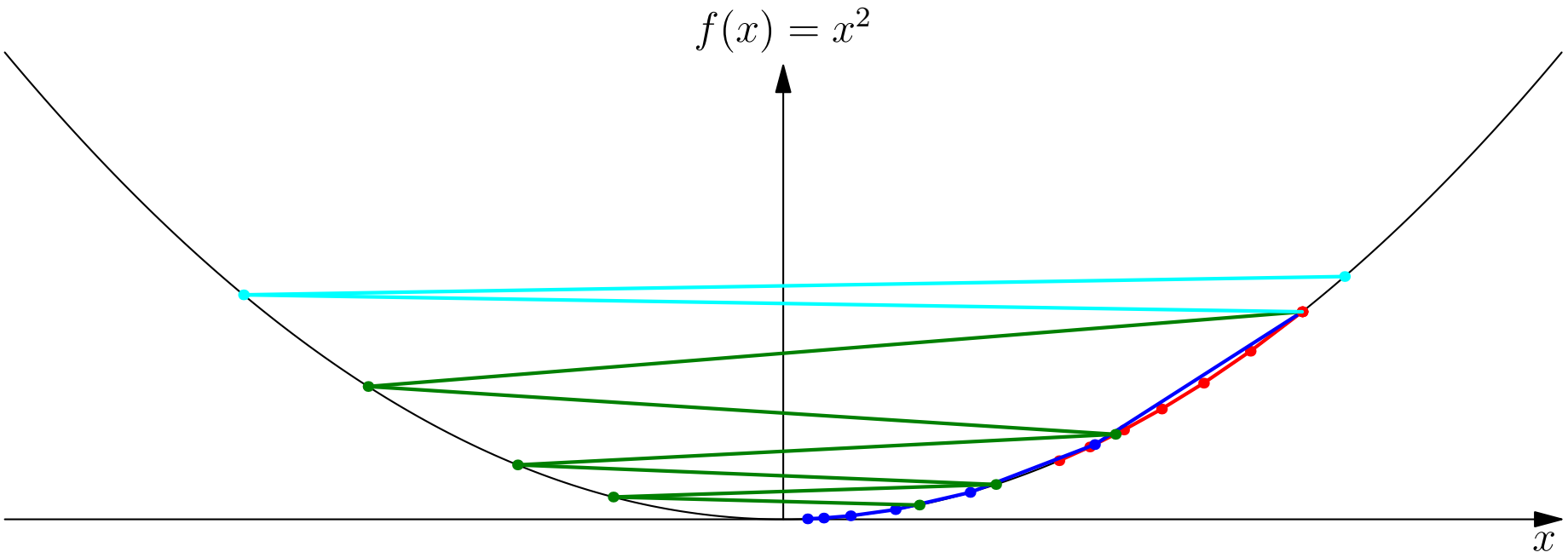

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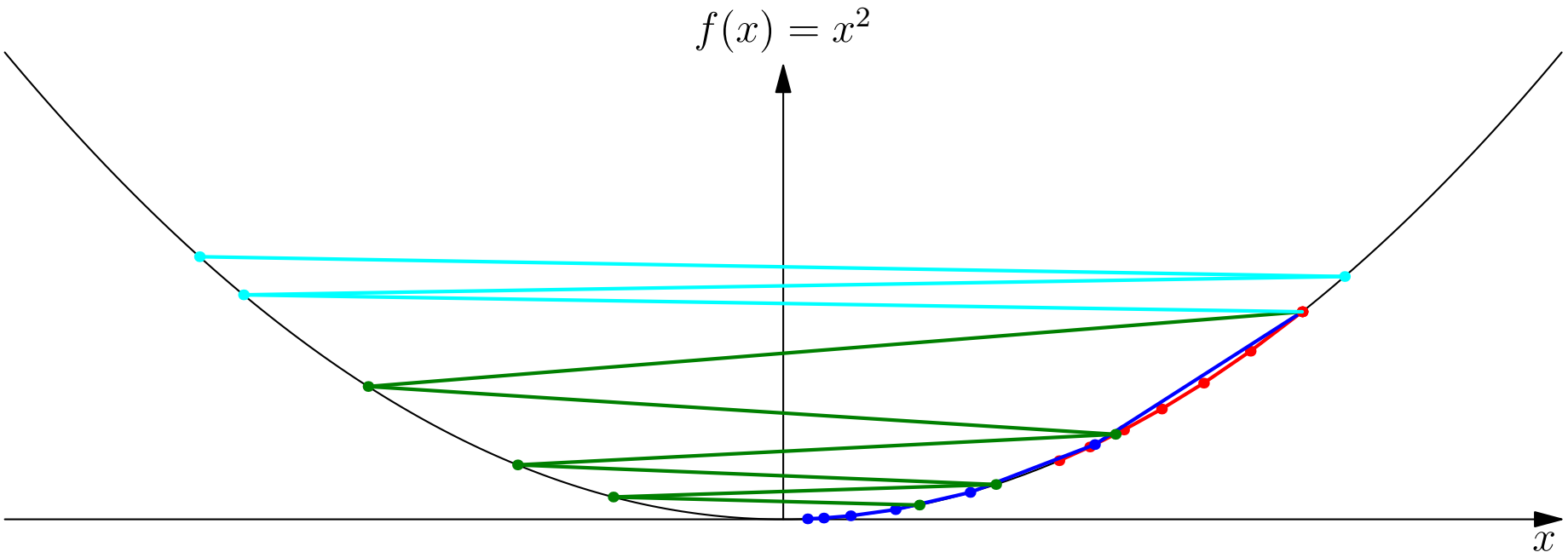

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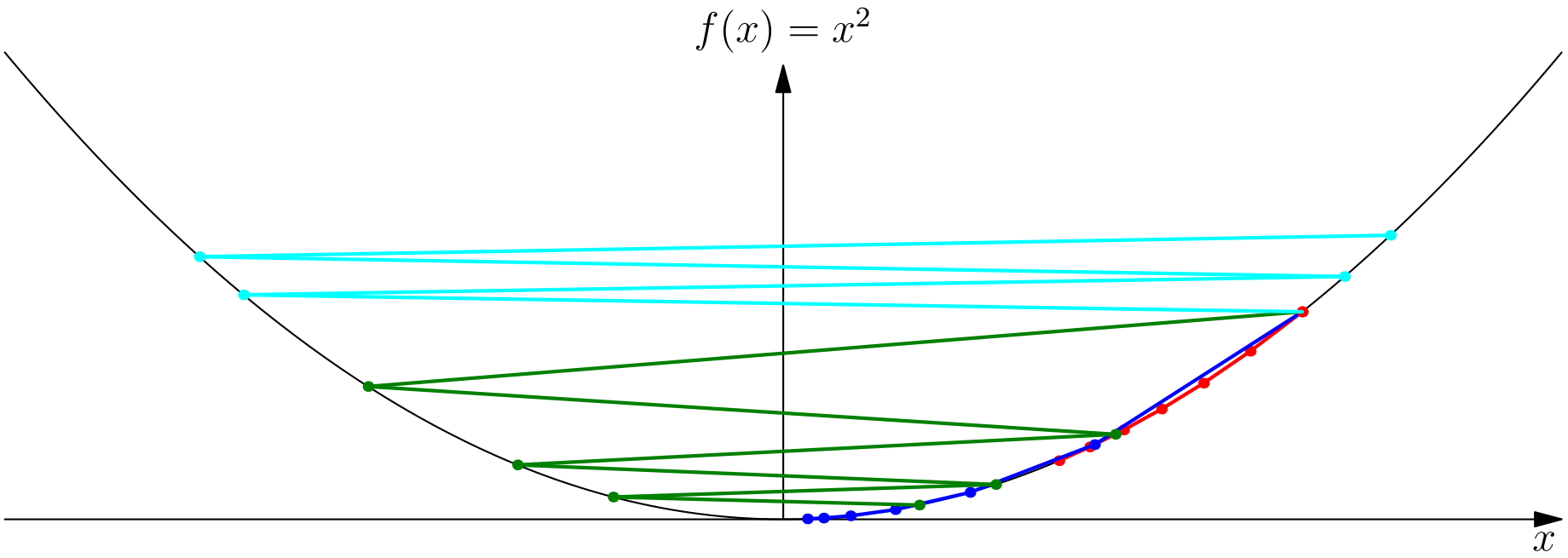


r $= 0.05$ r $= 0.2$ r $= 0.9$ r $= 1.02$

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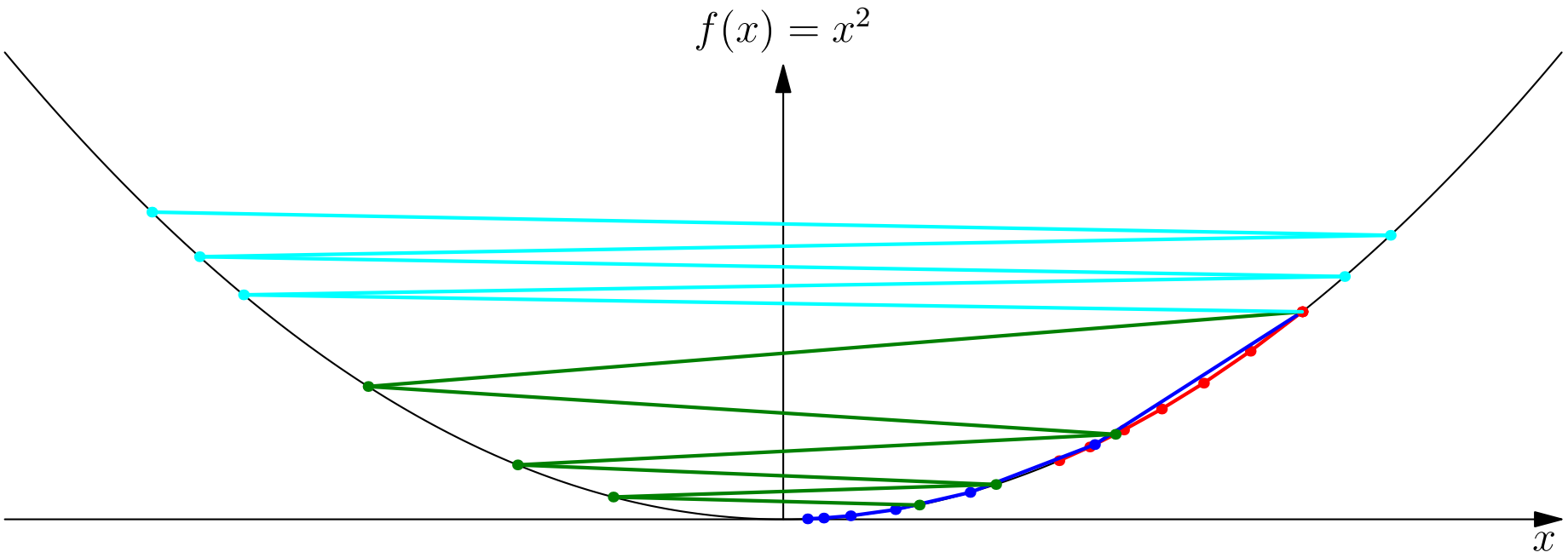


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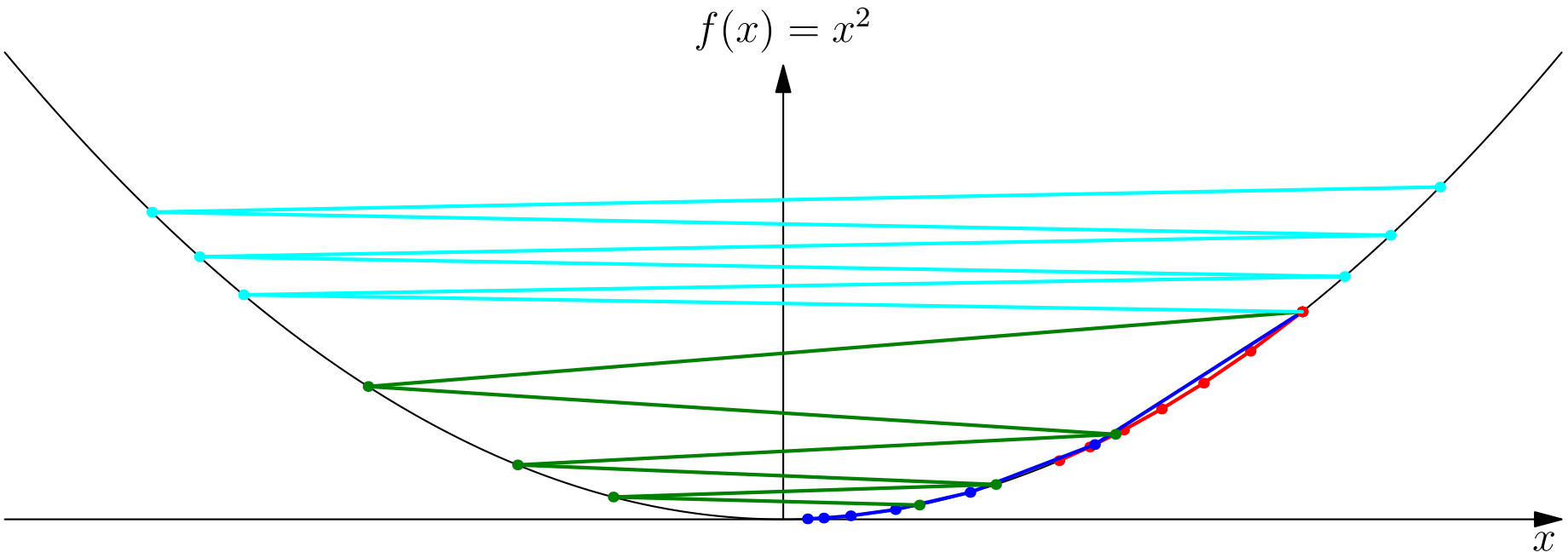

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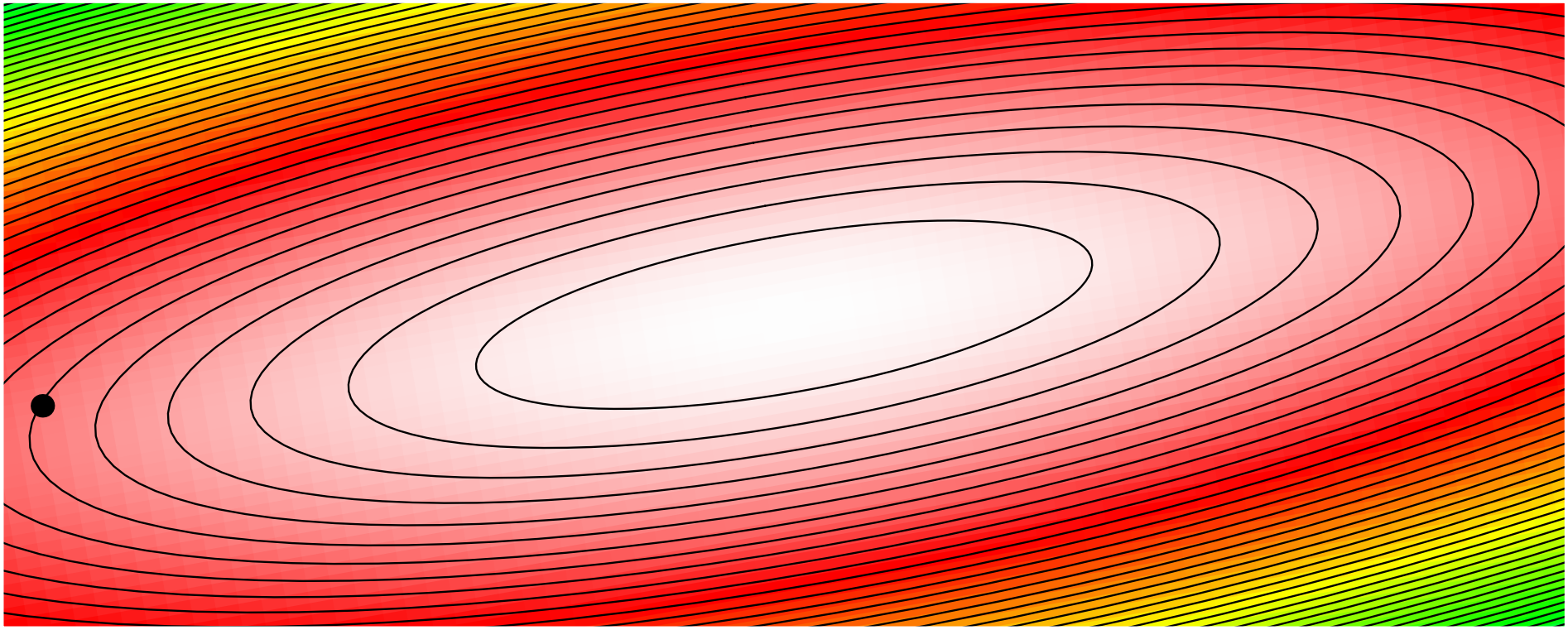

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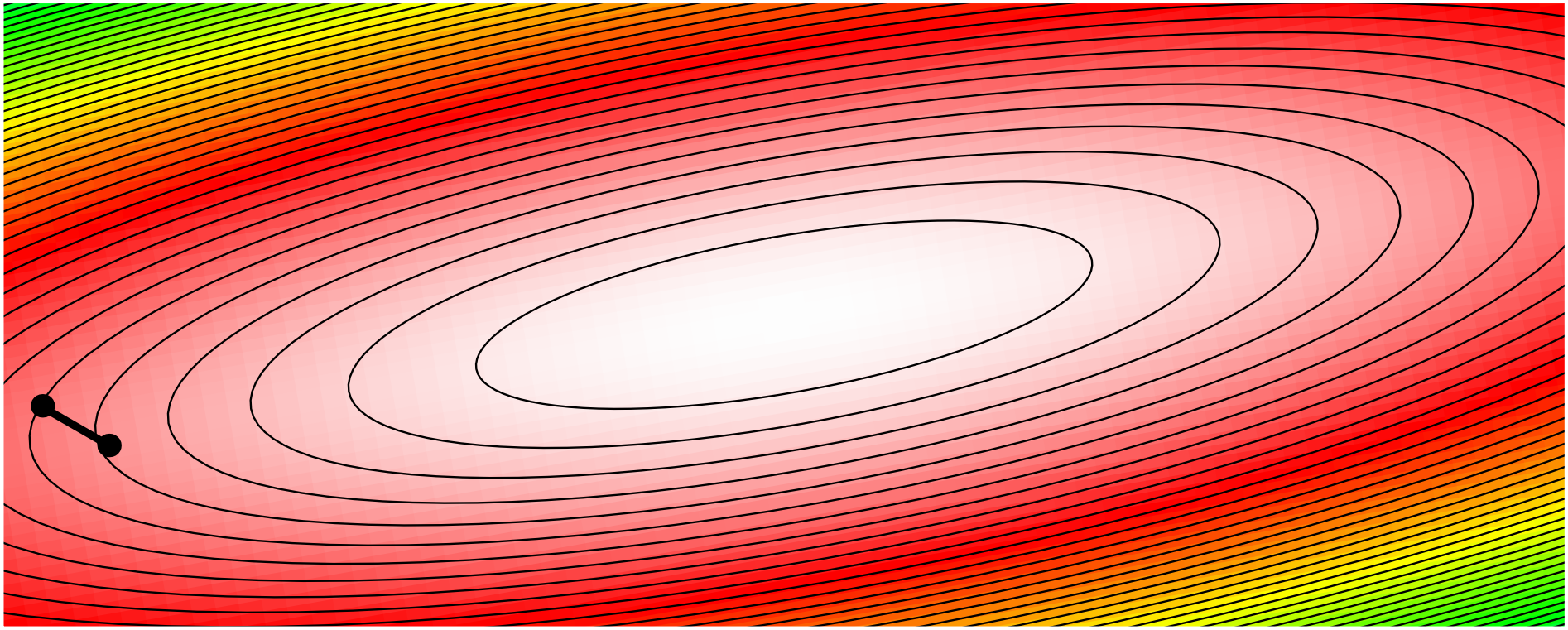

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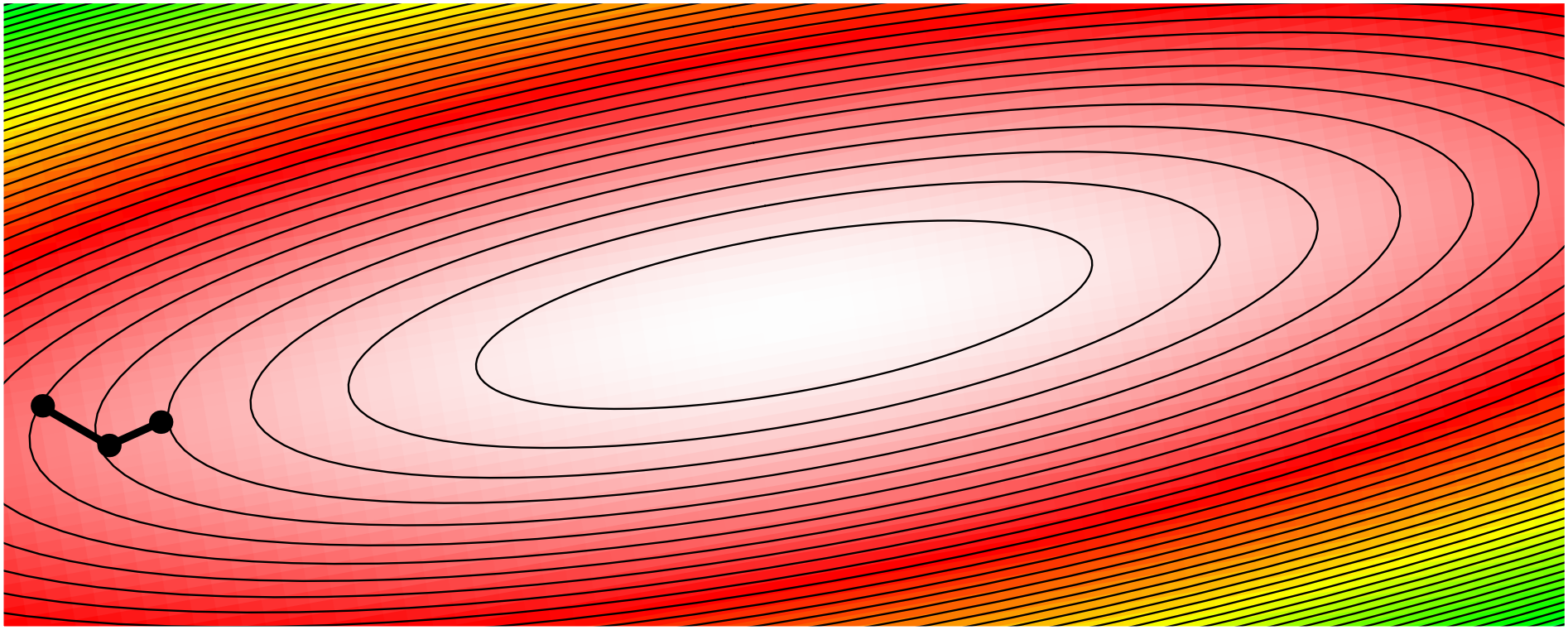

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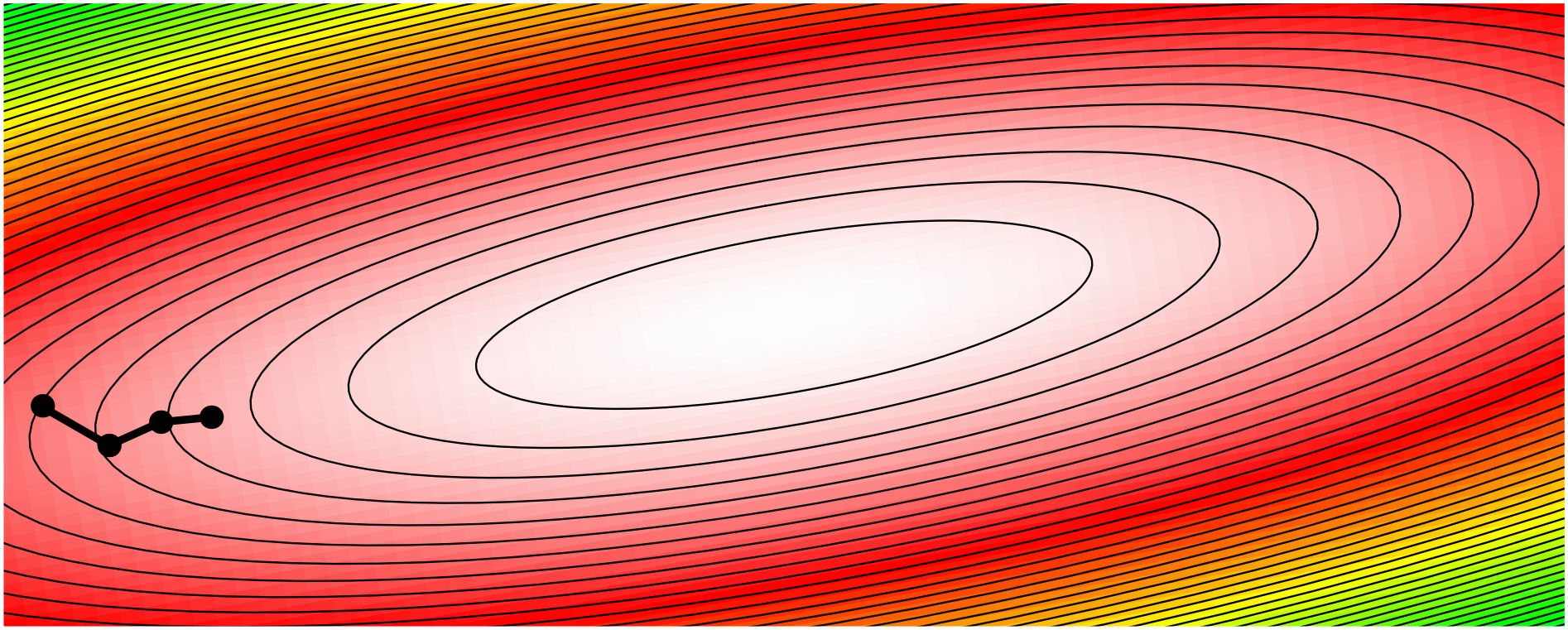

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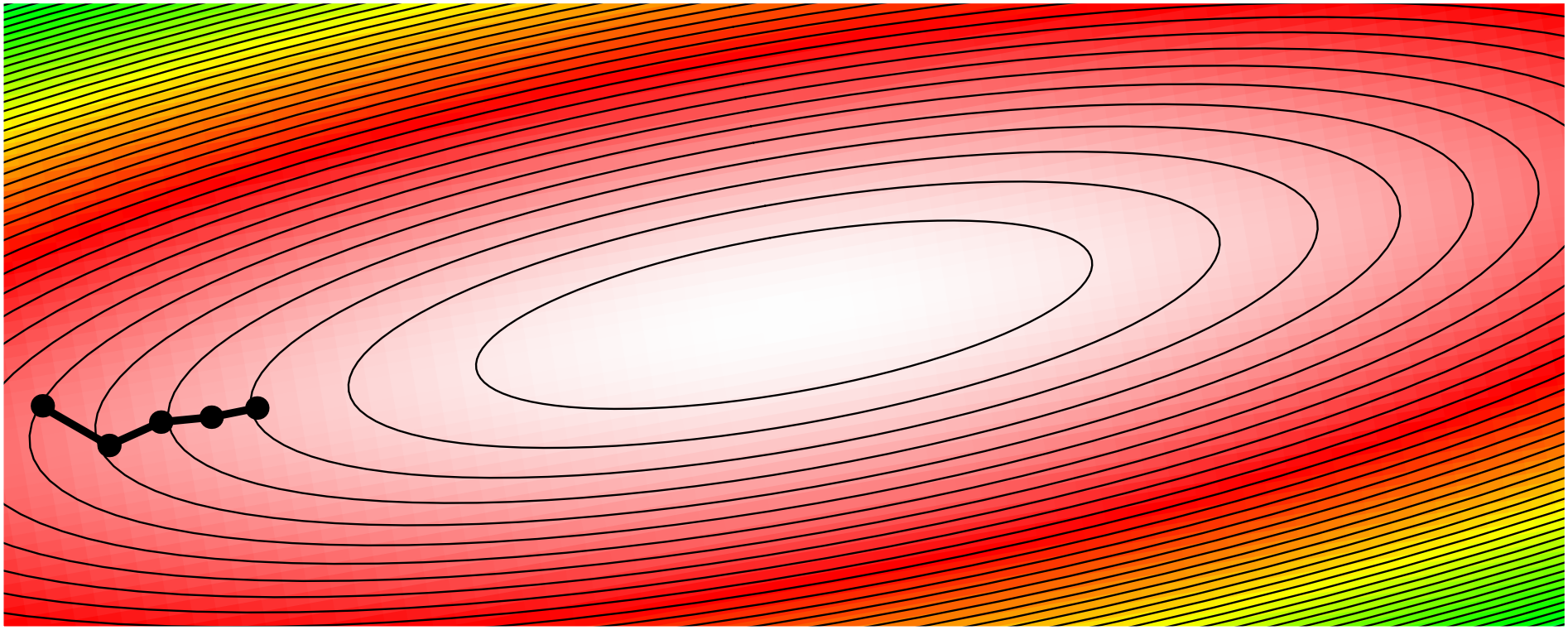

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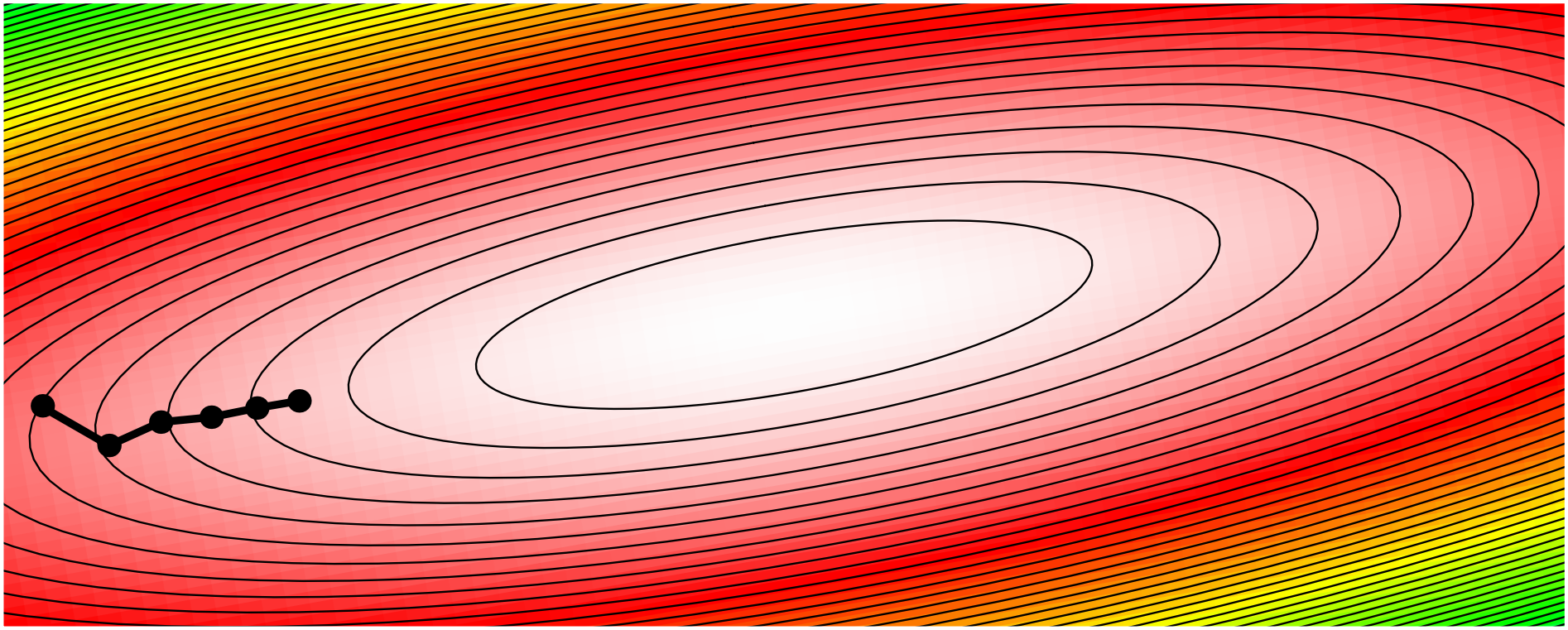

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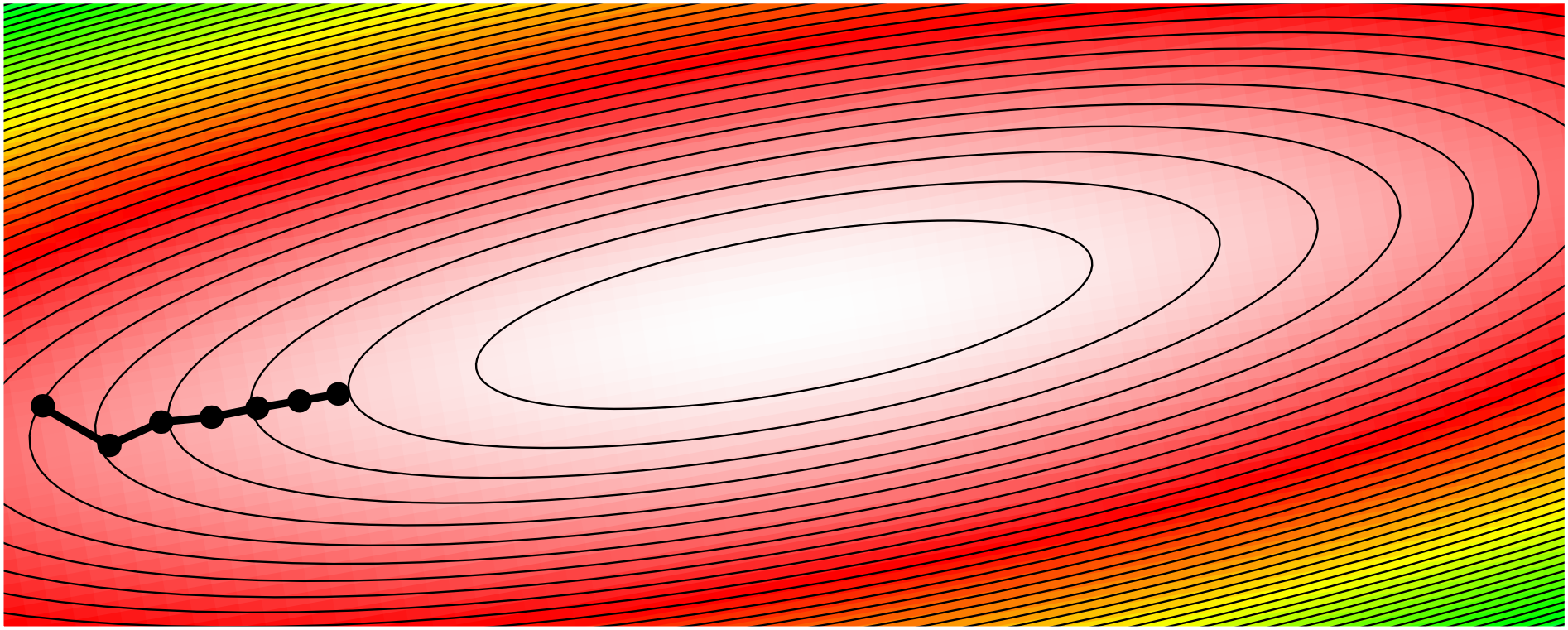

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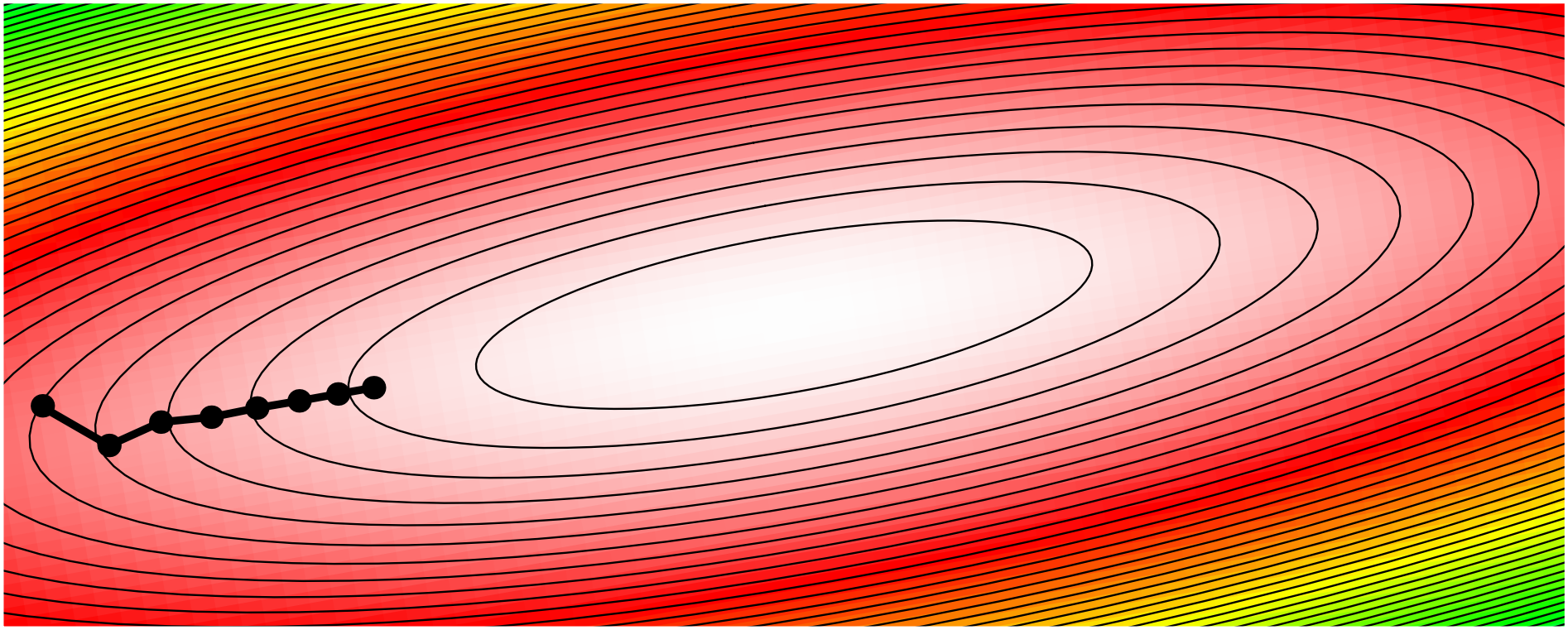

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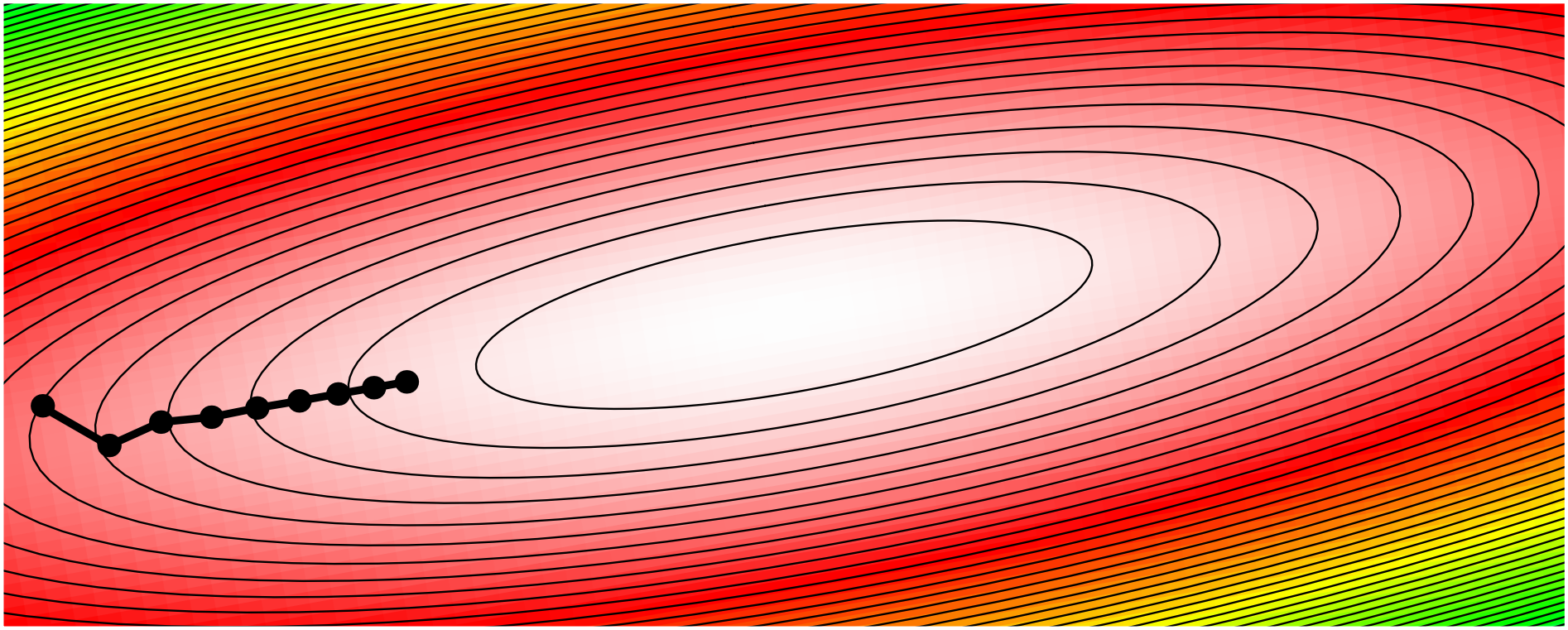

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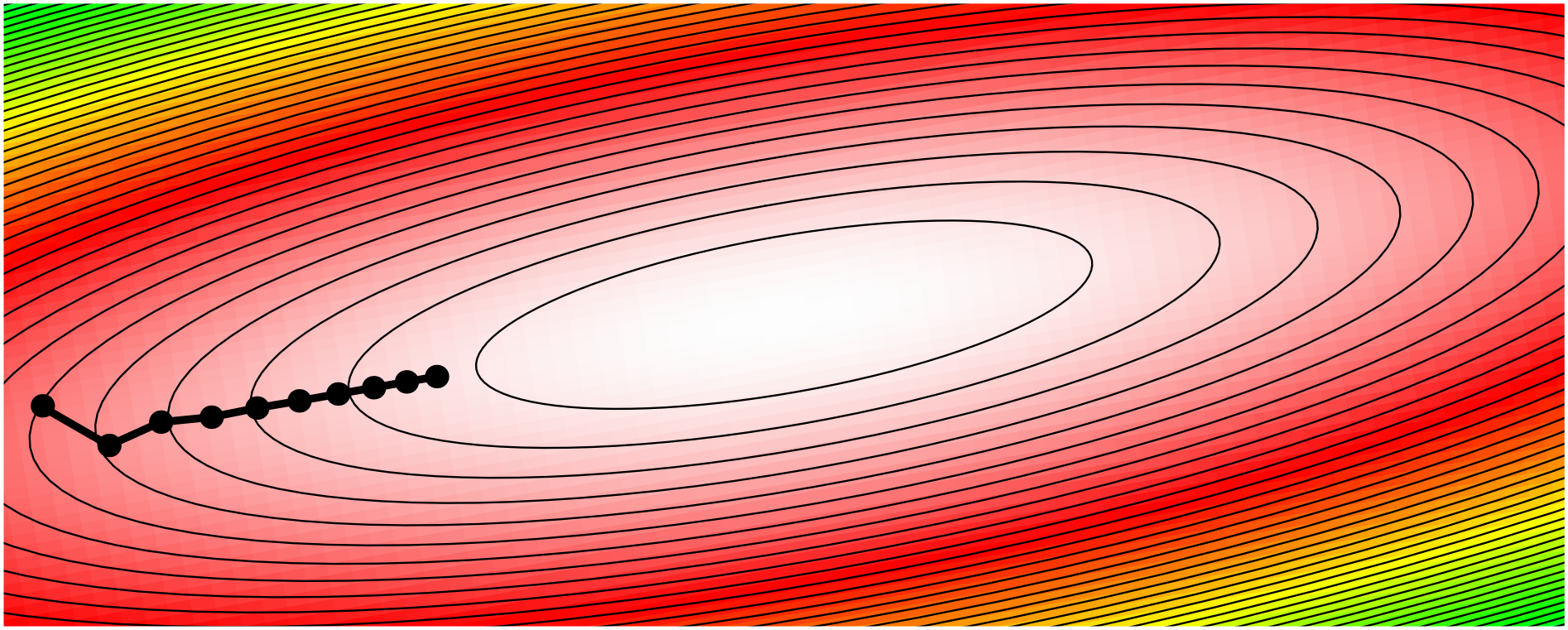

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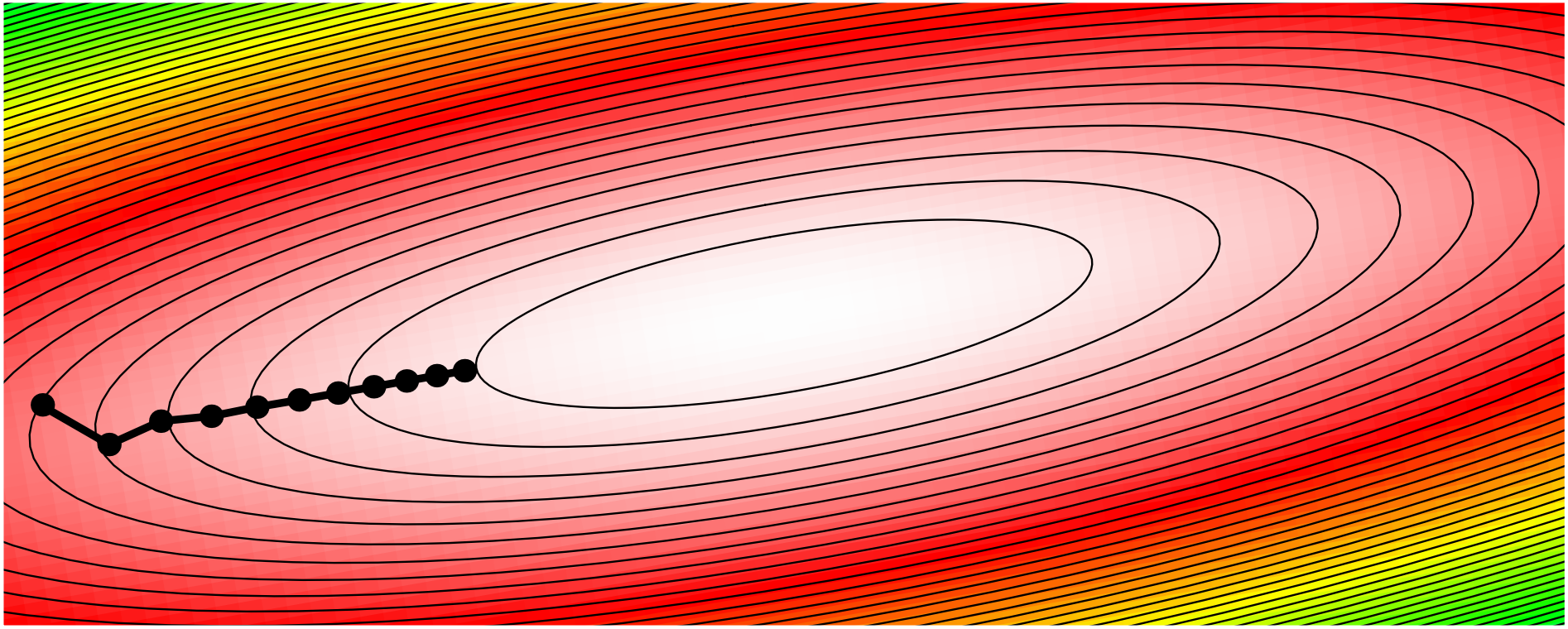

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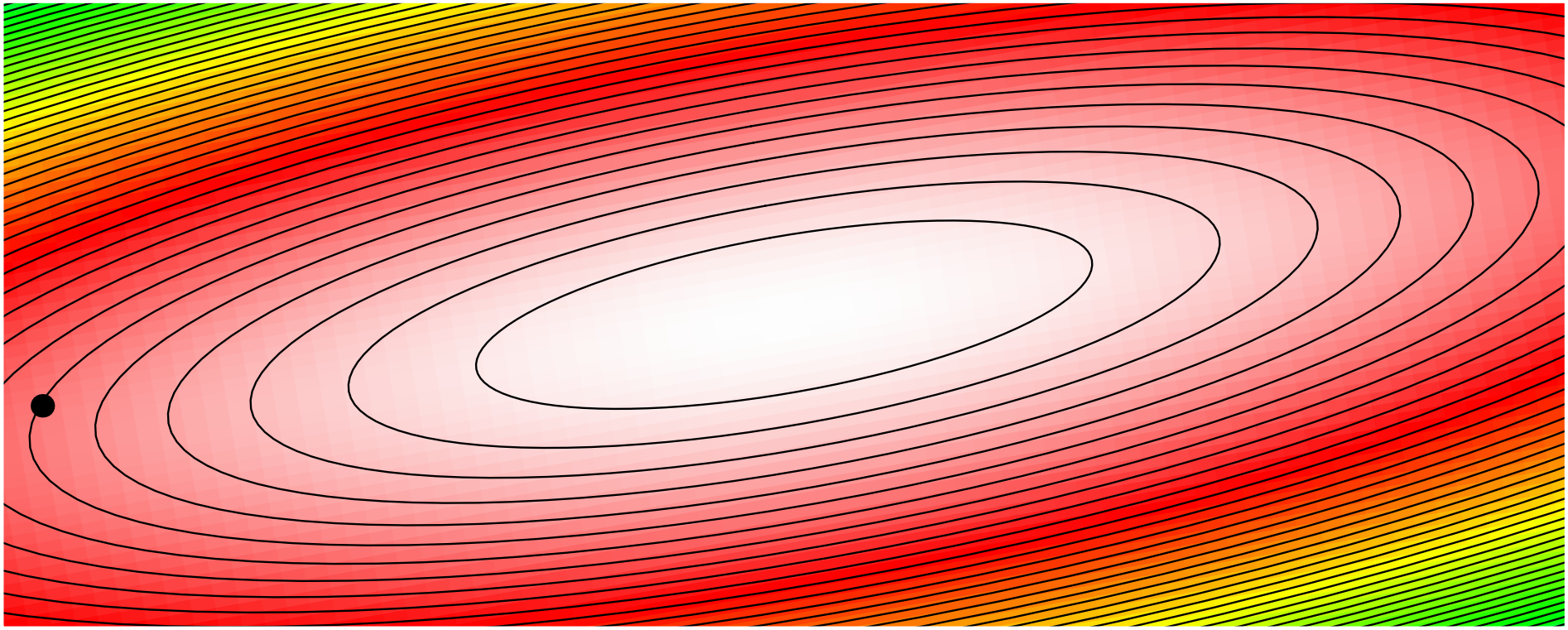

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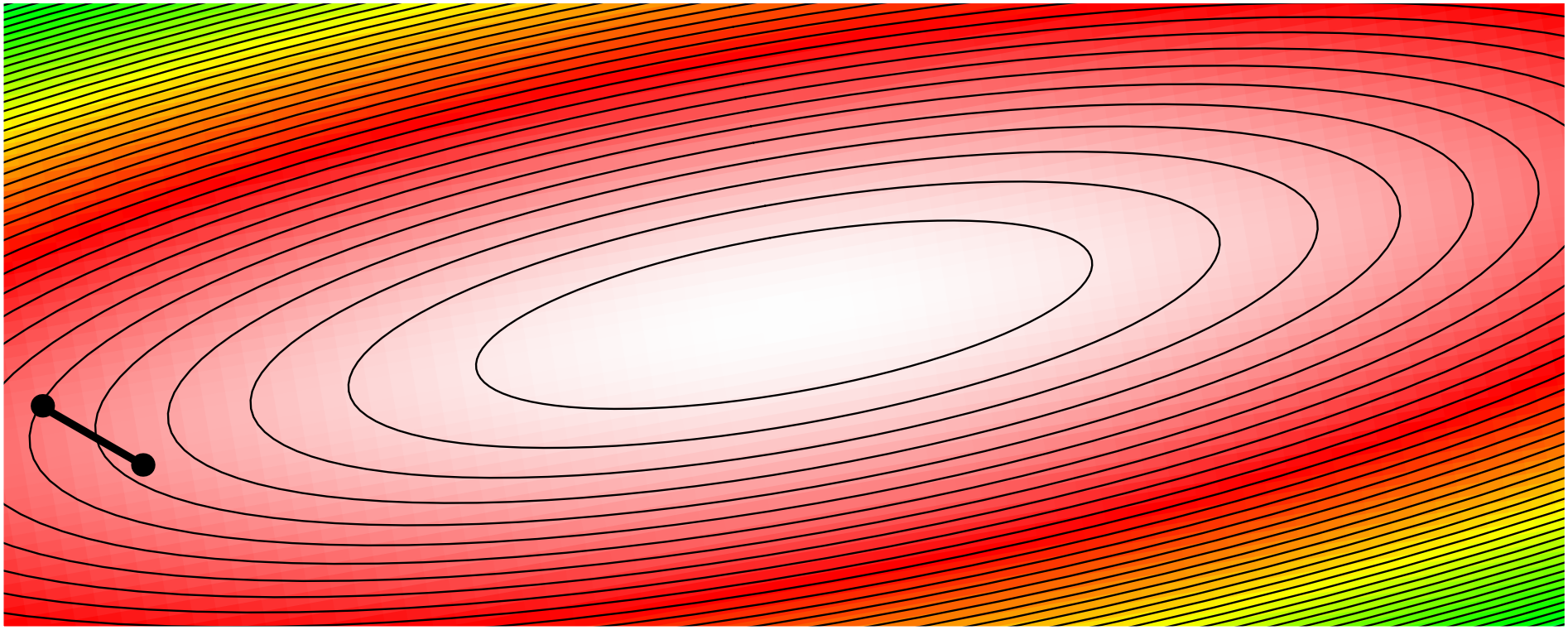

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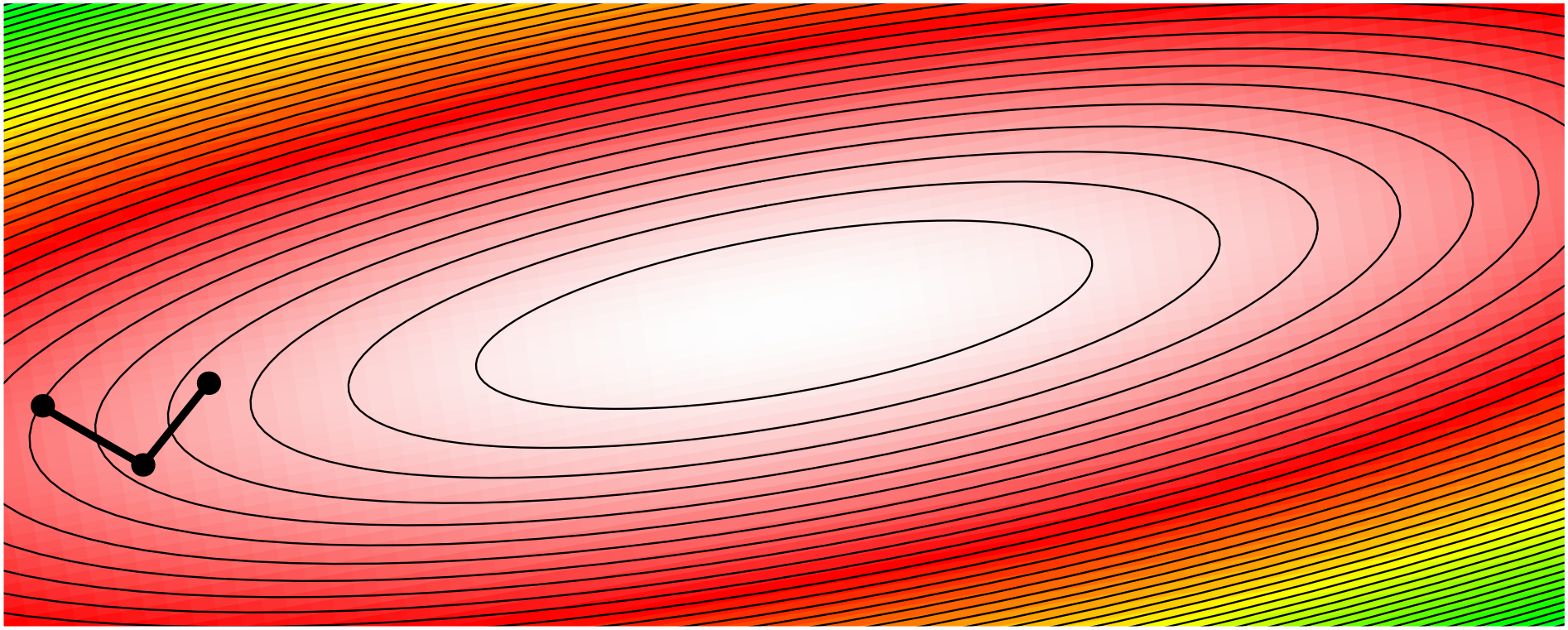

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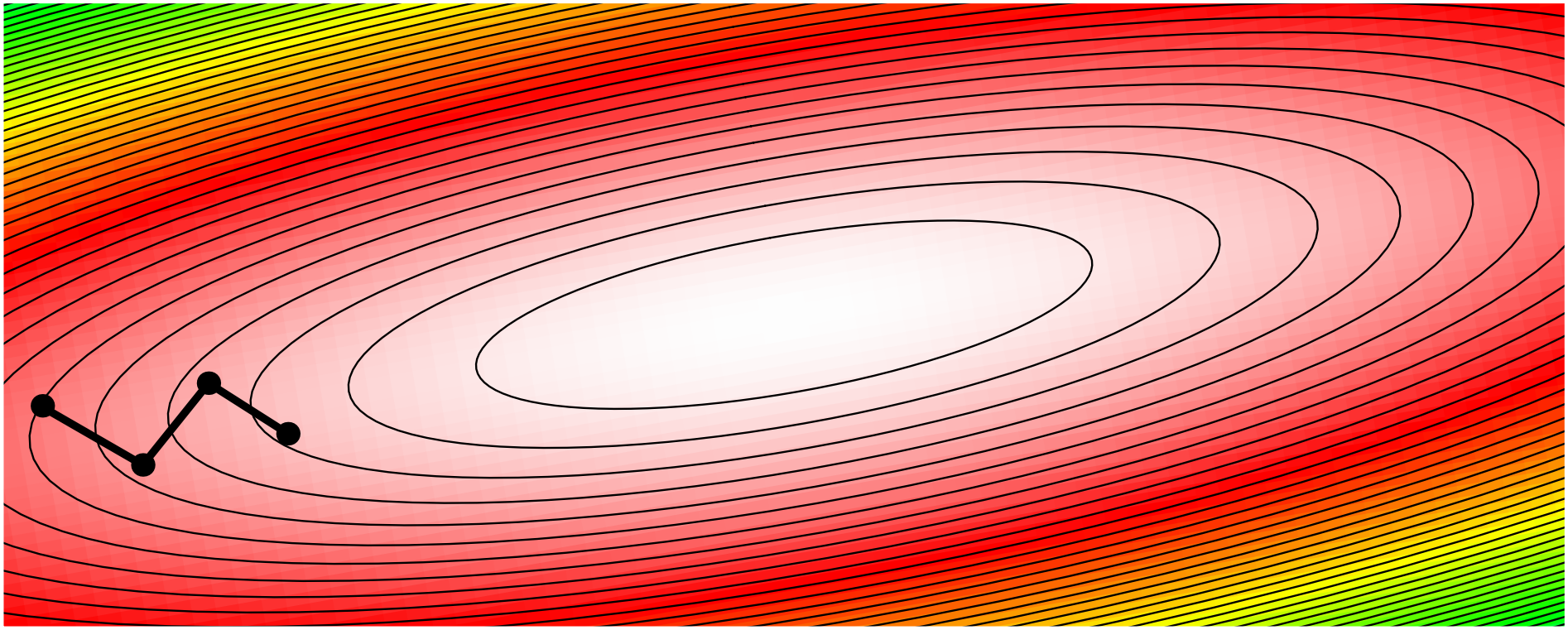

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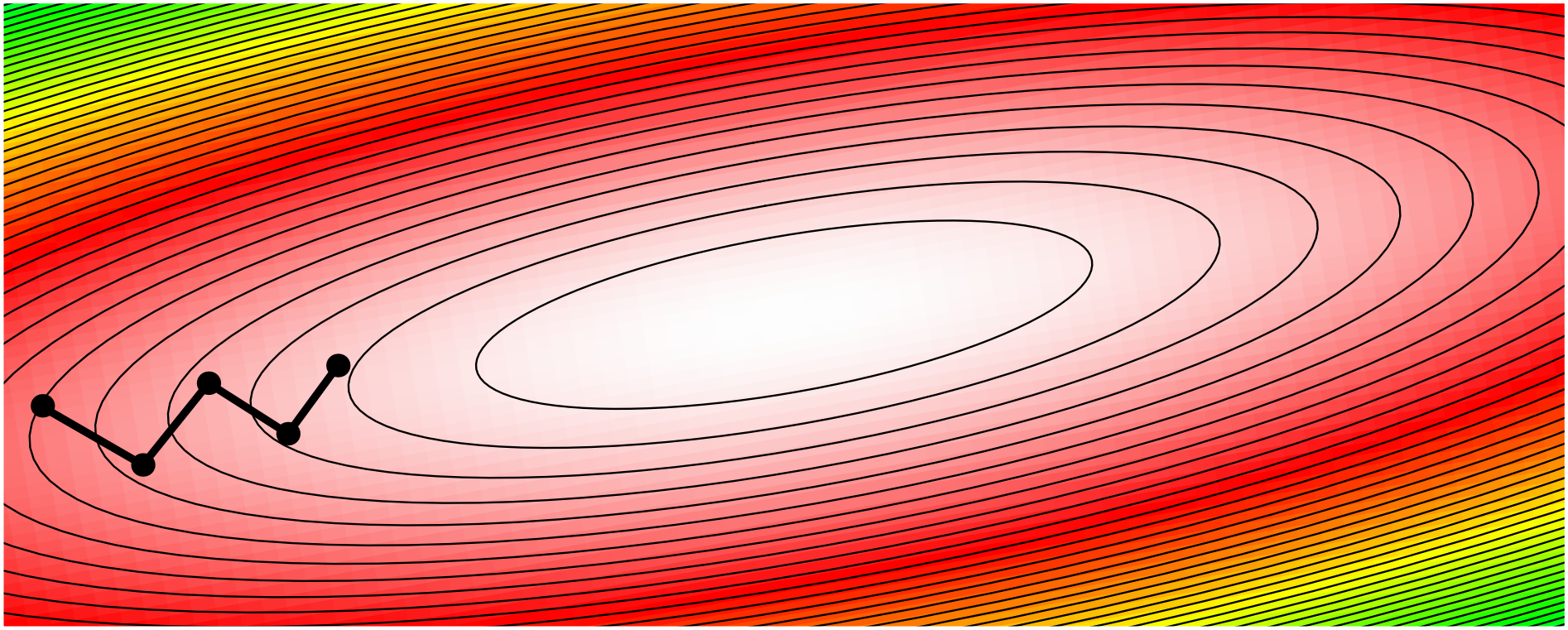

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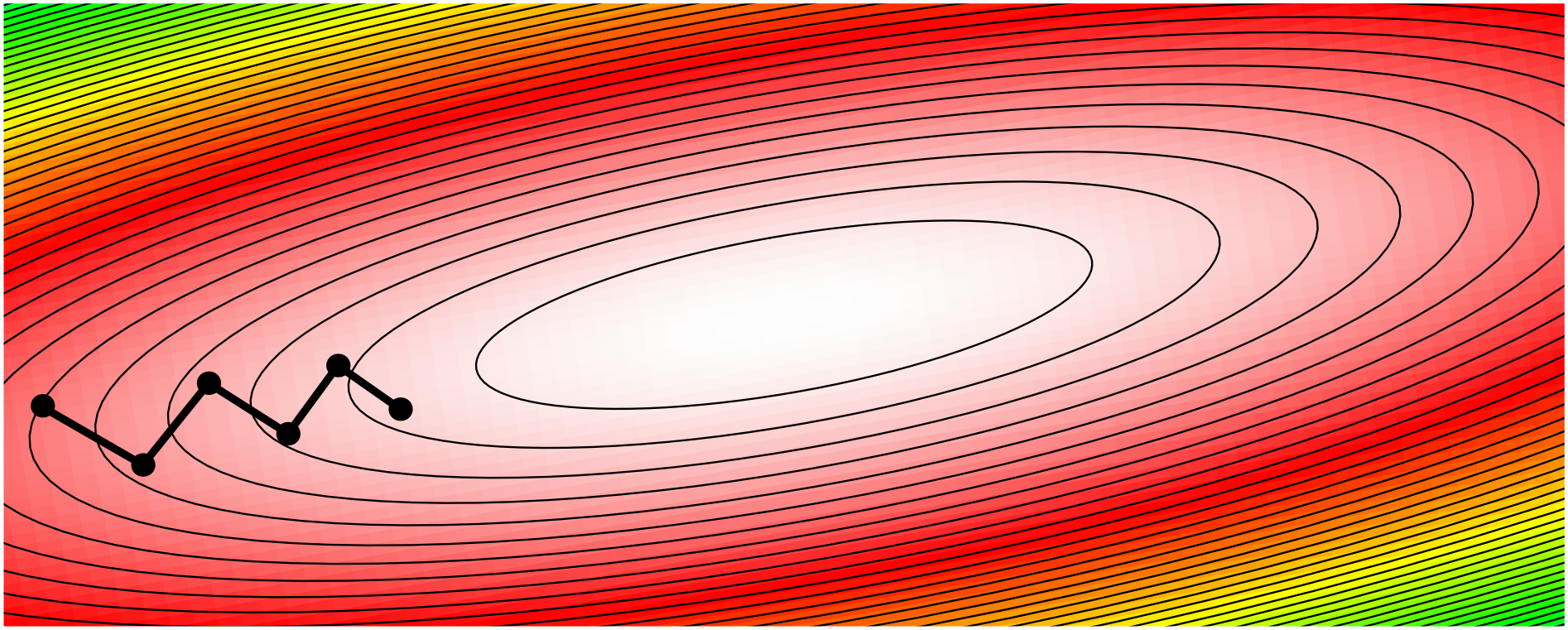

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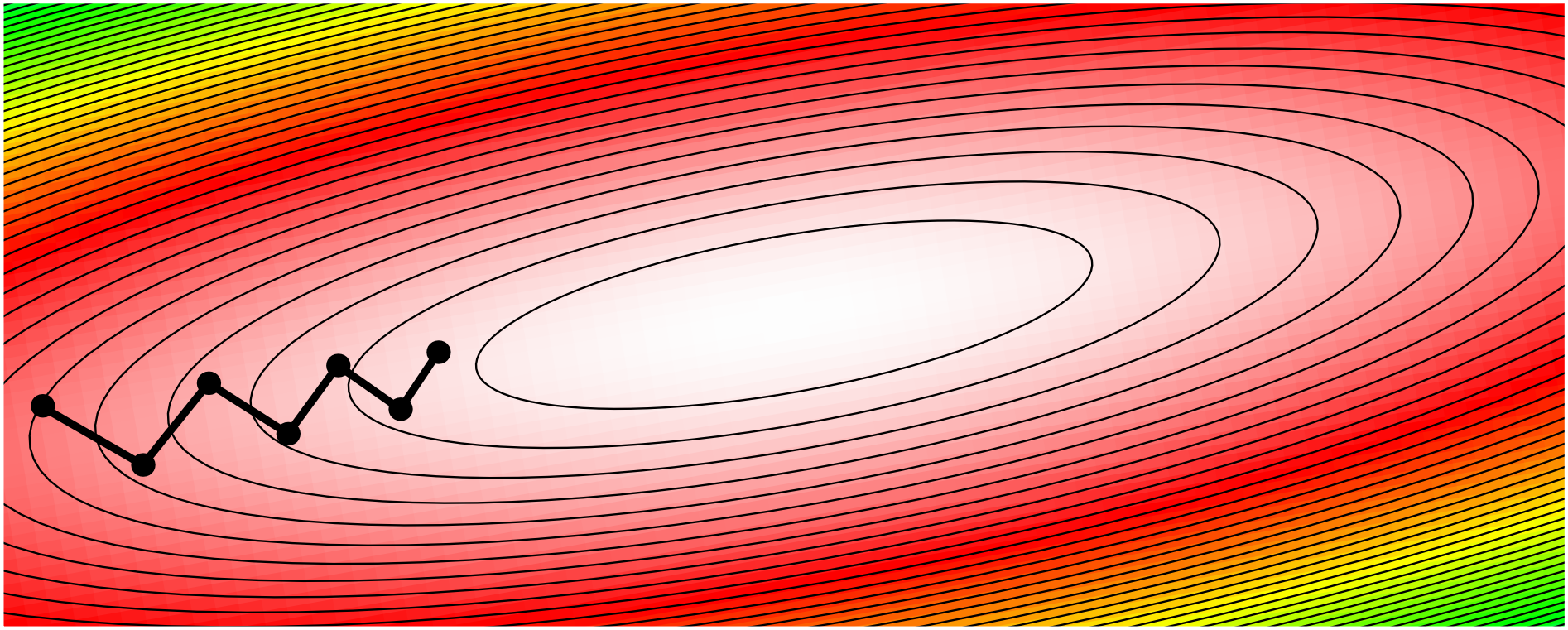

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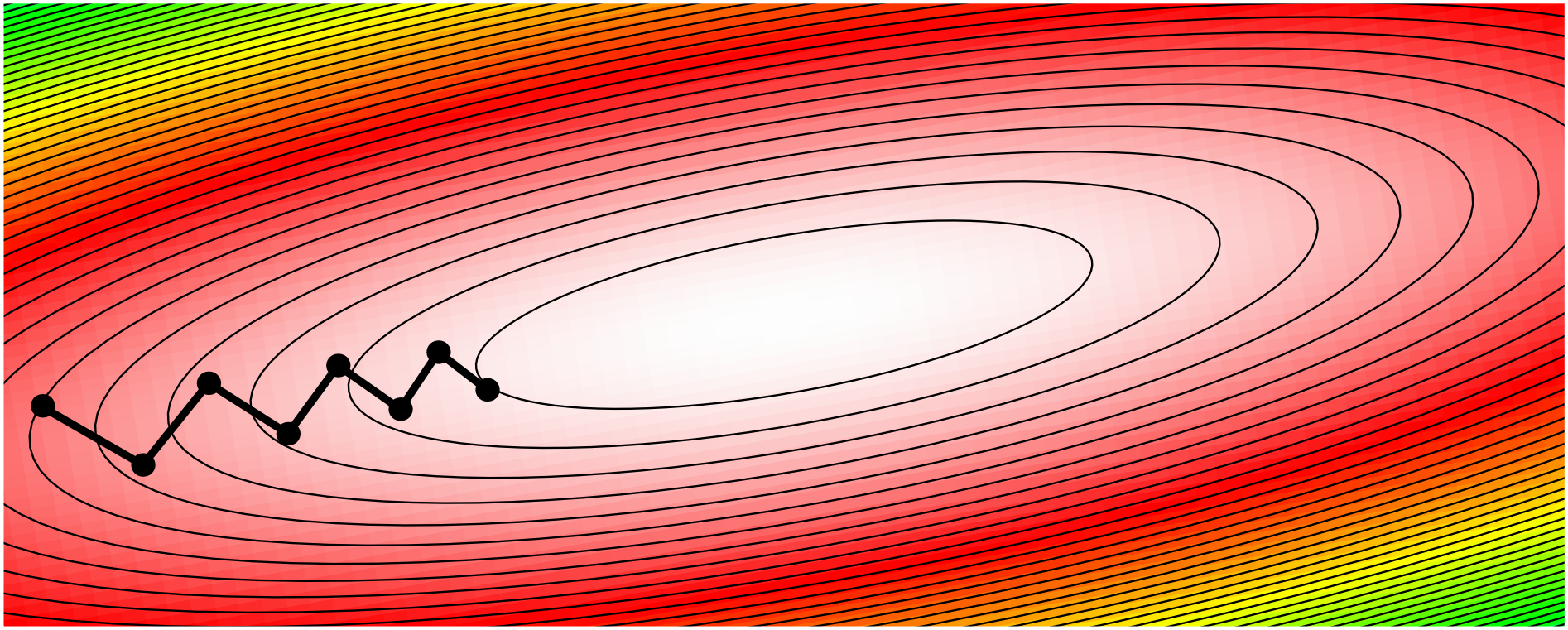

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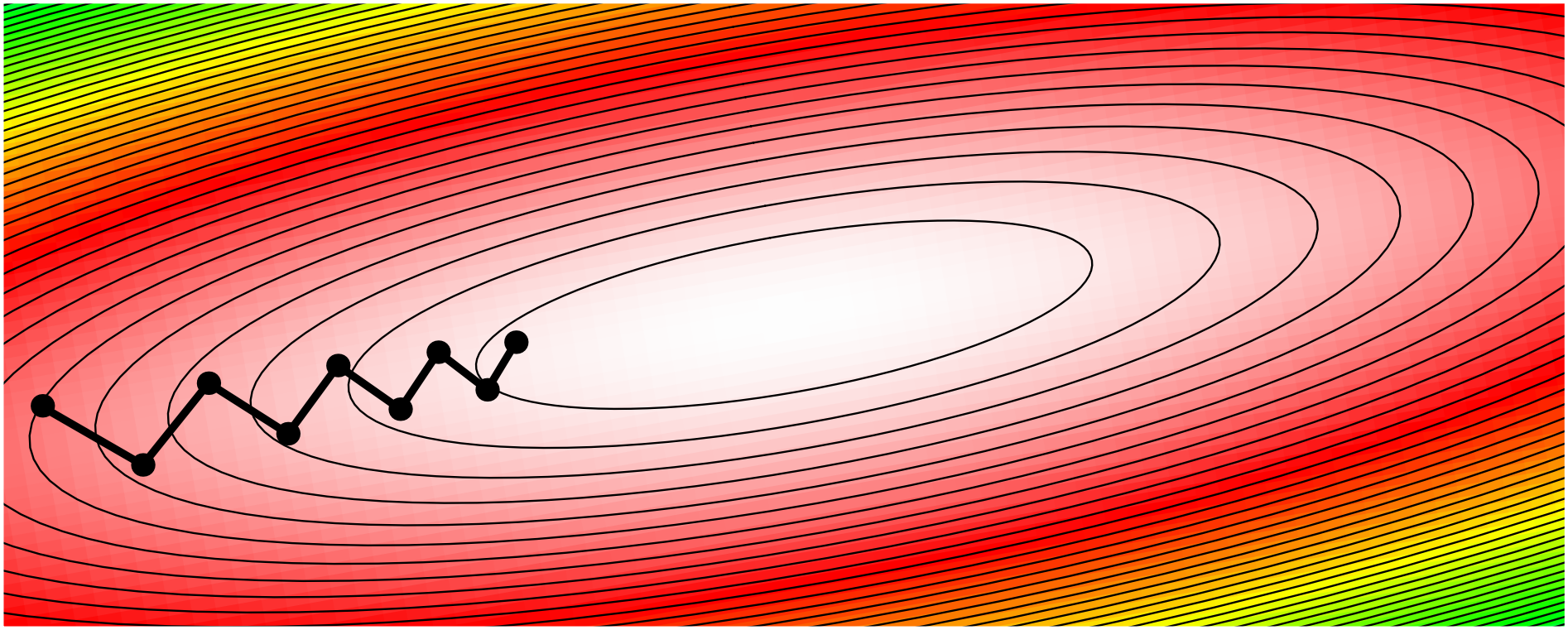

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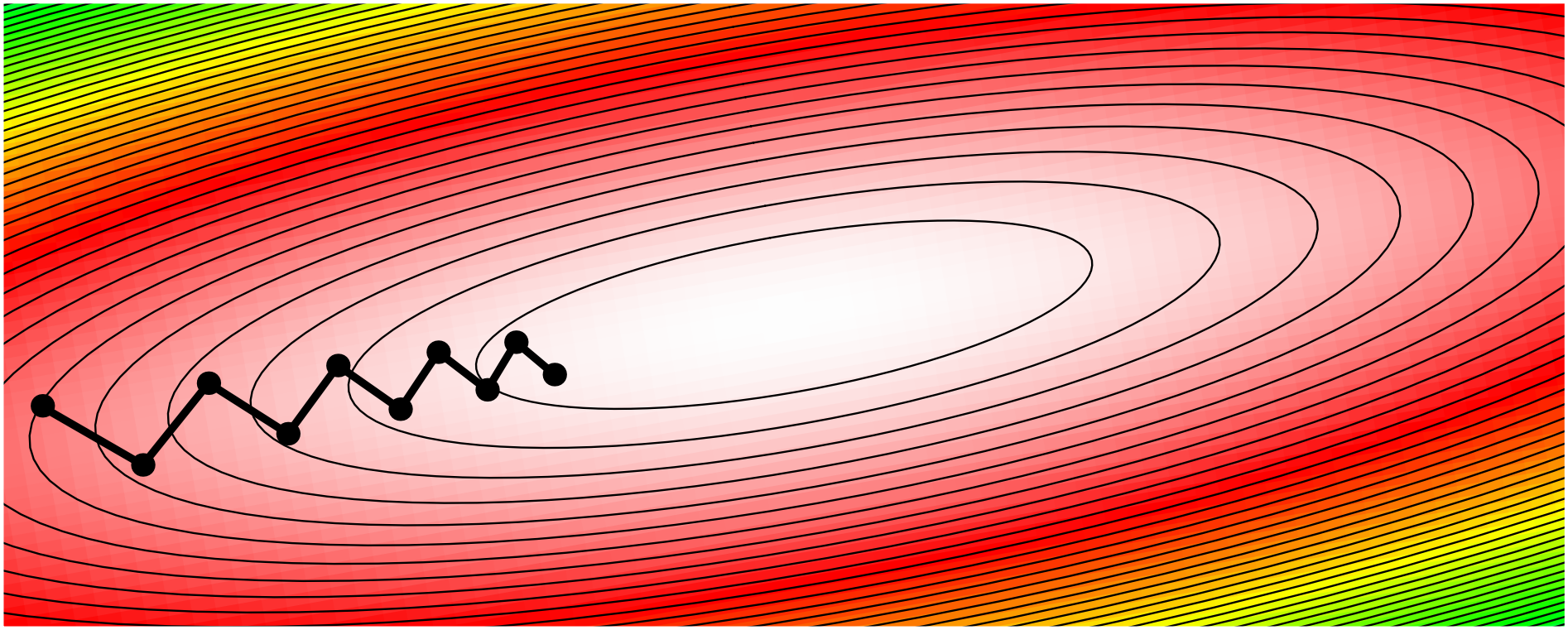

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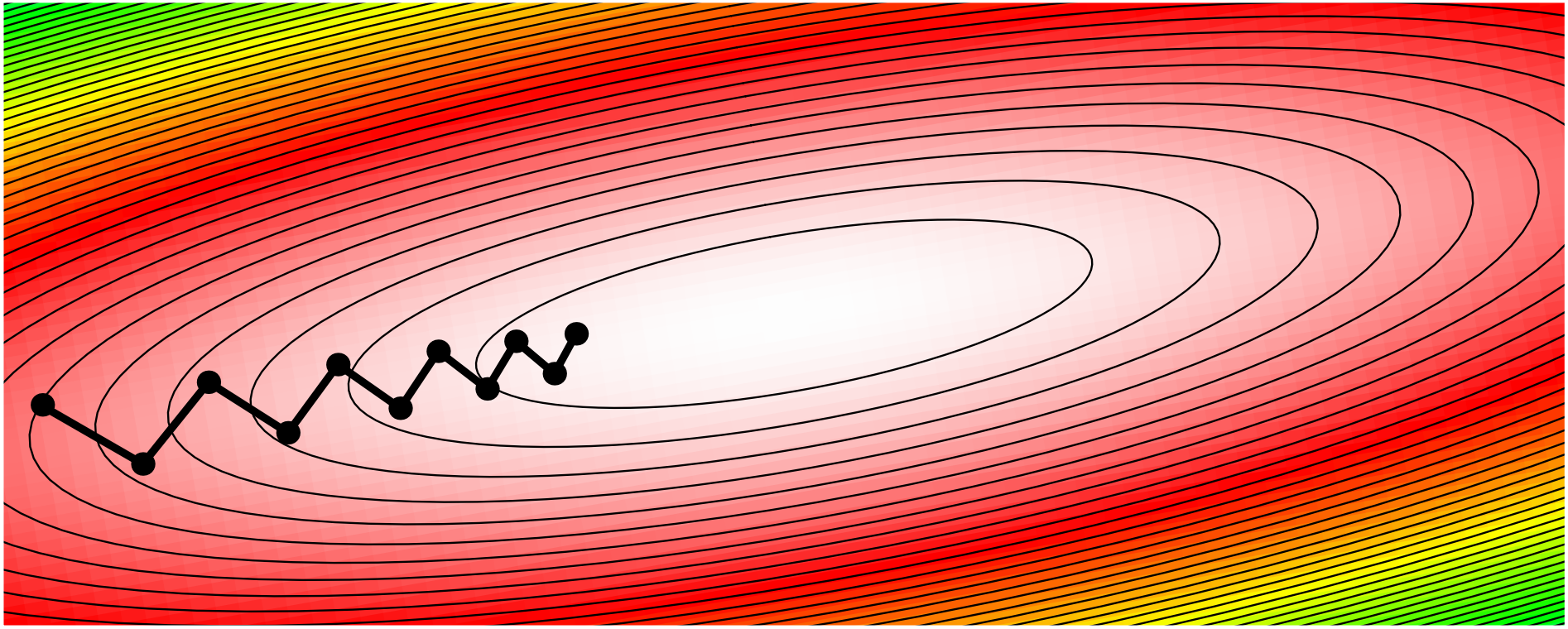

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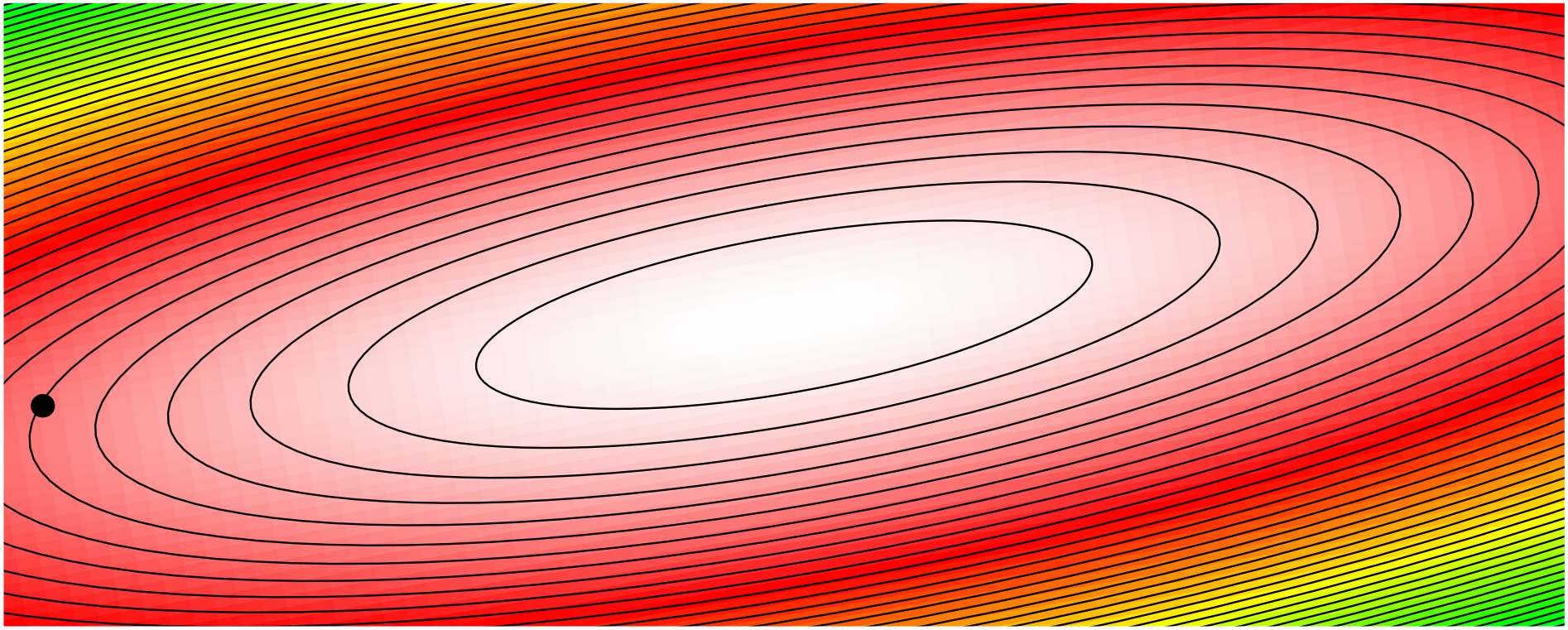

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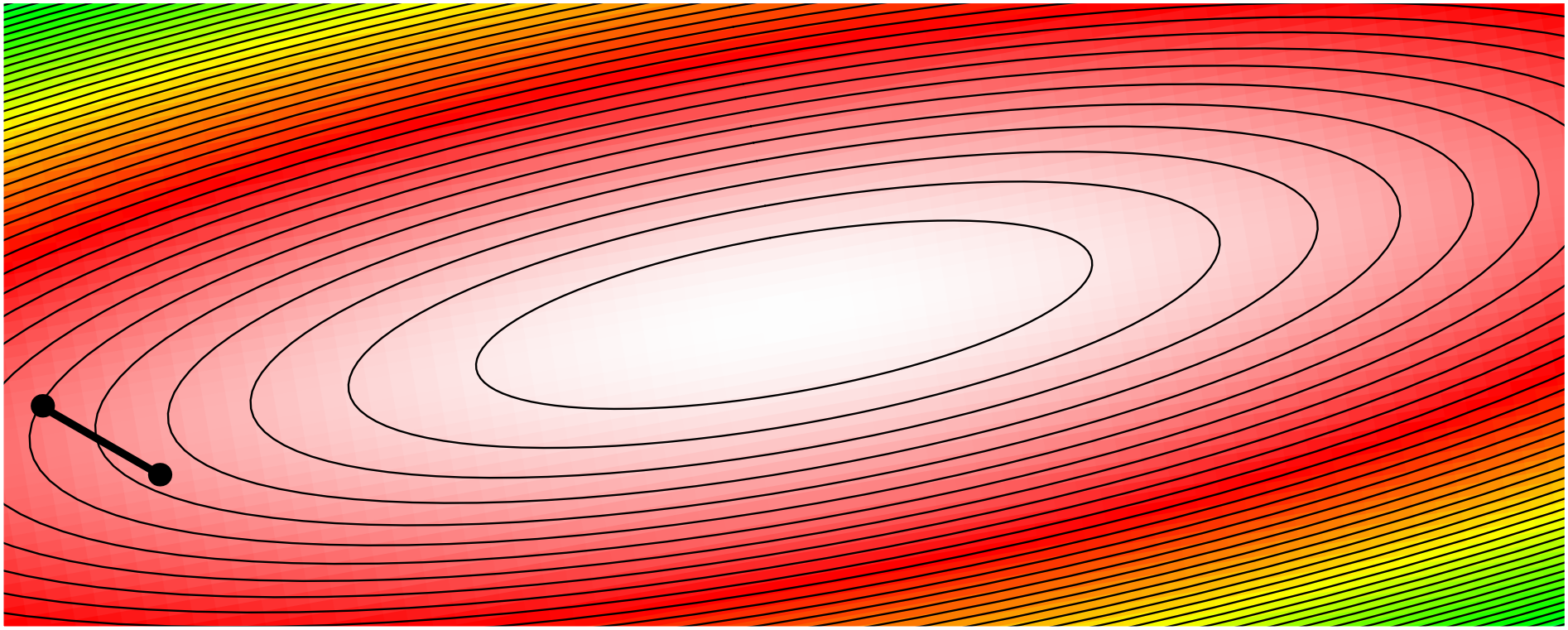

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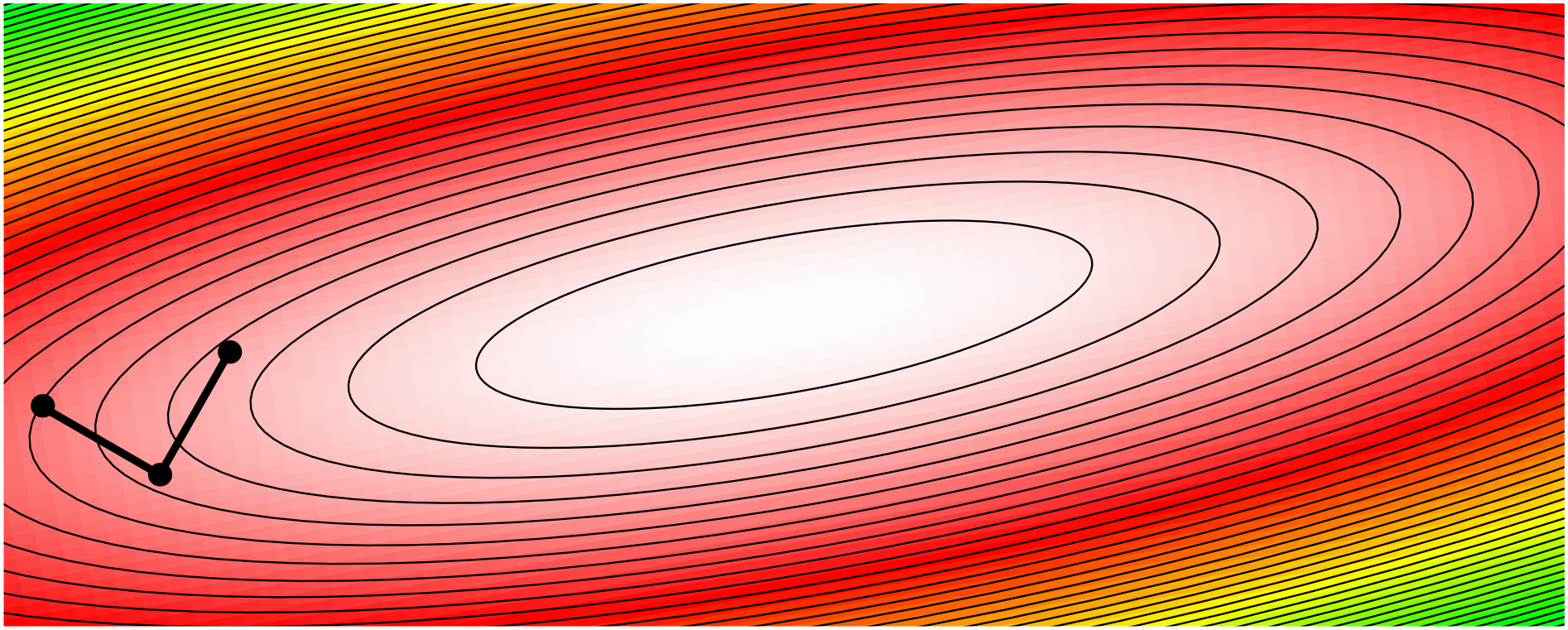

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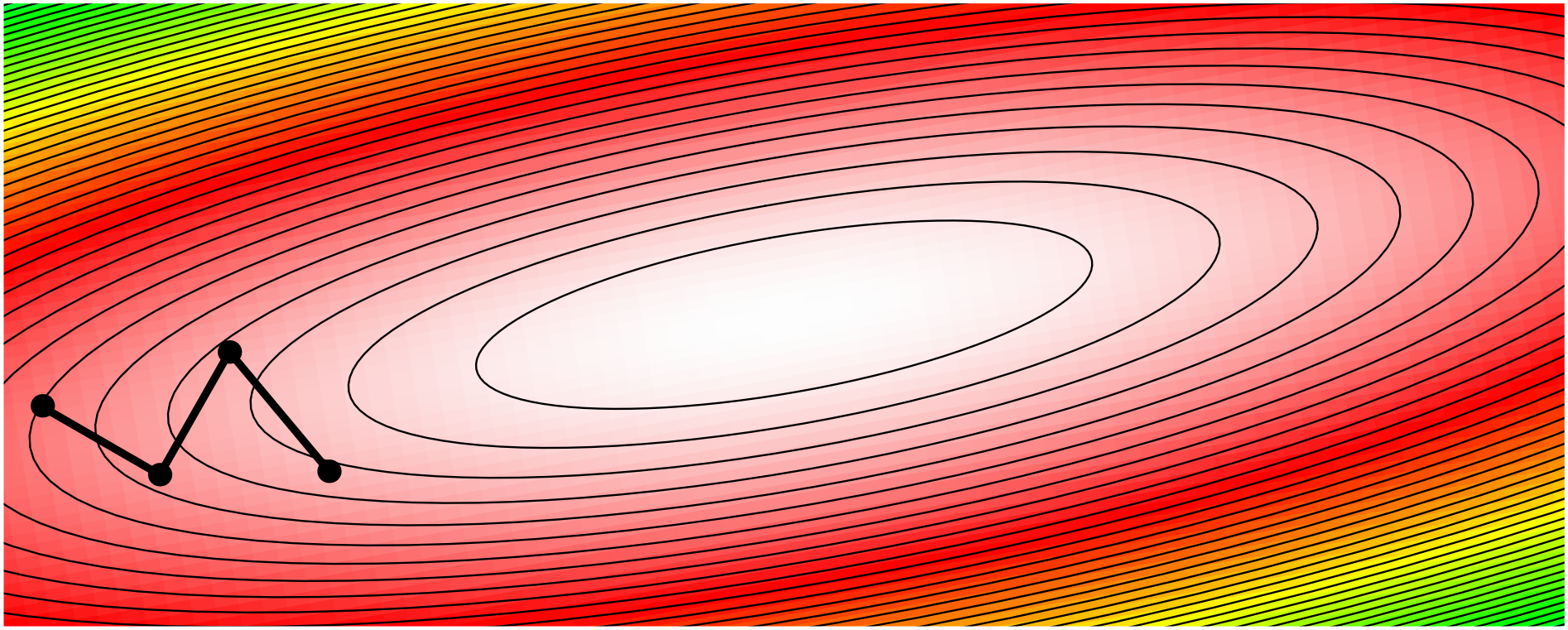

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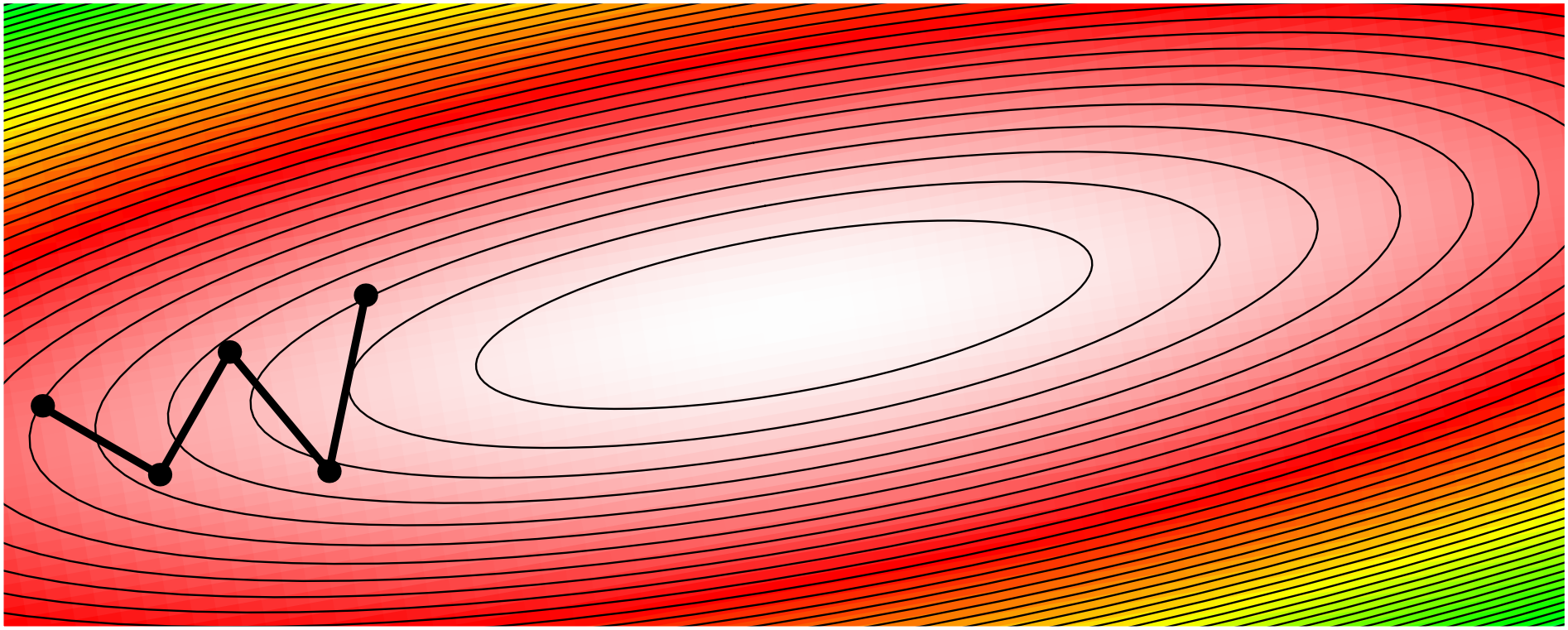

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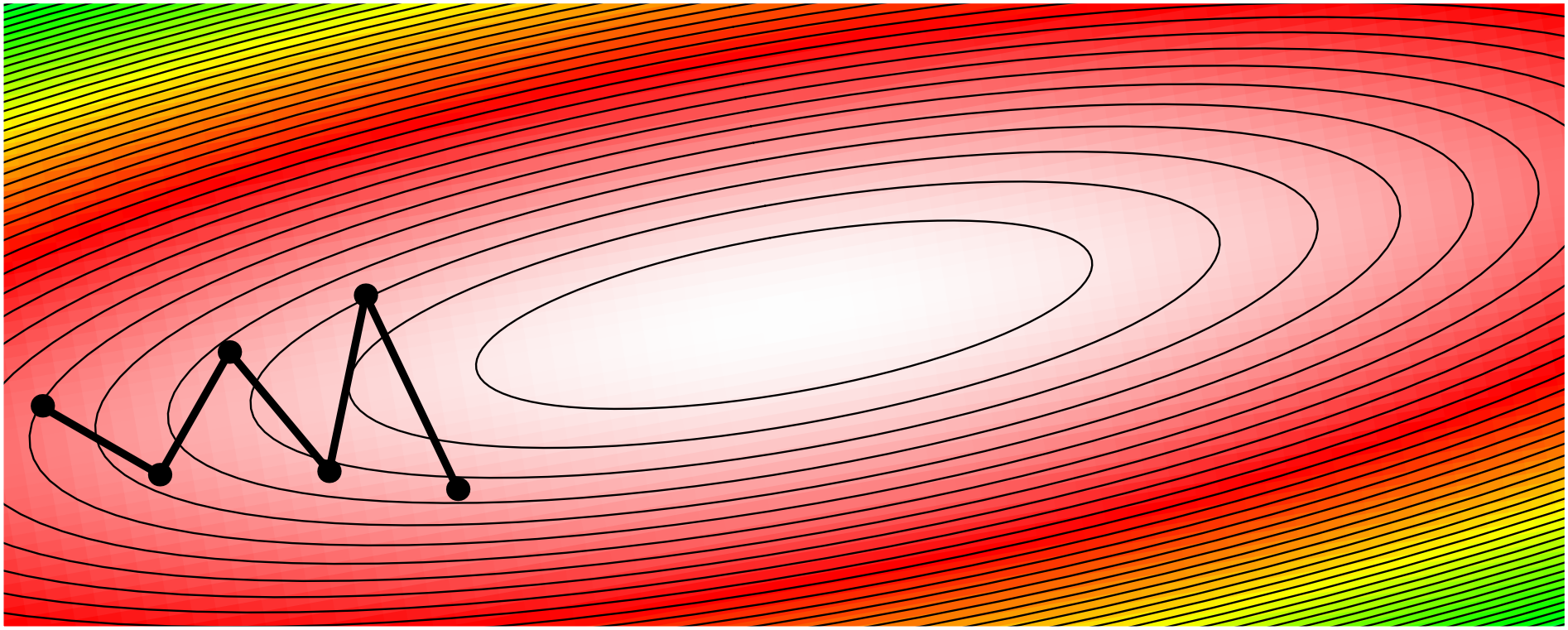

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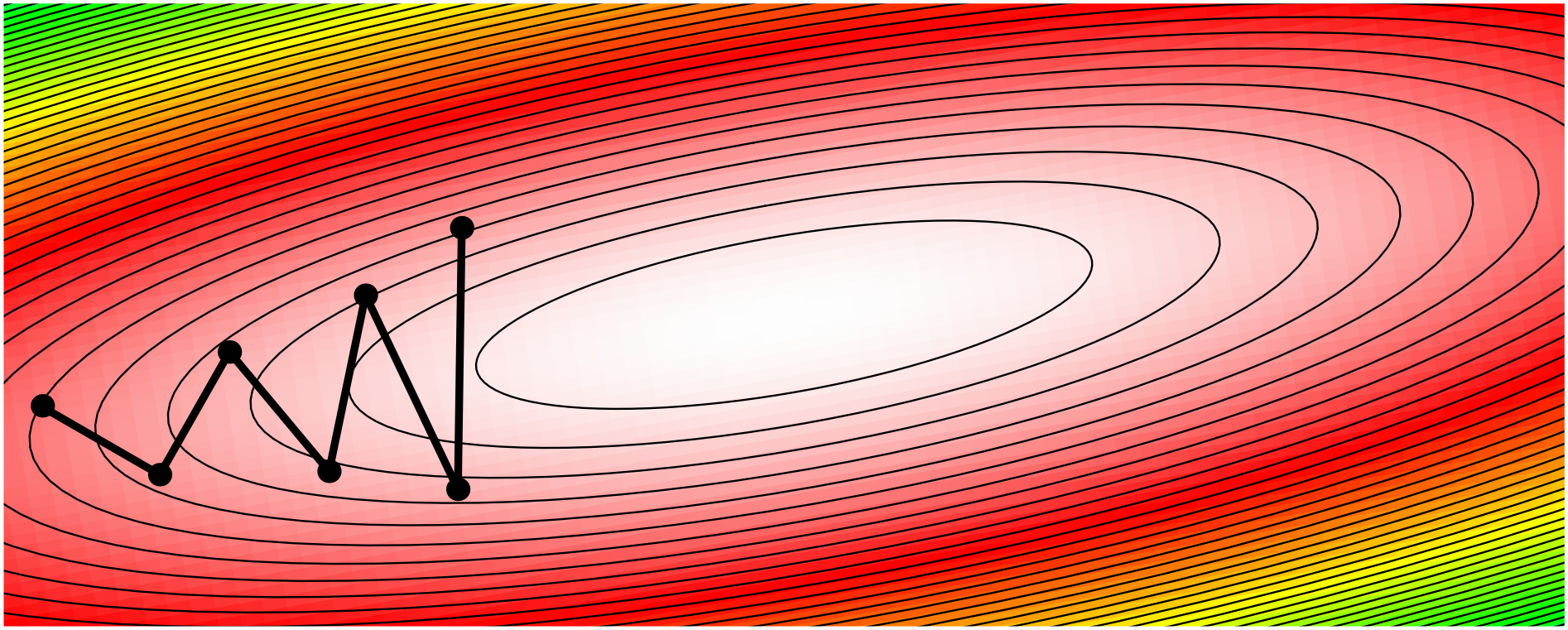

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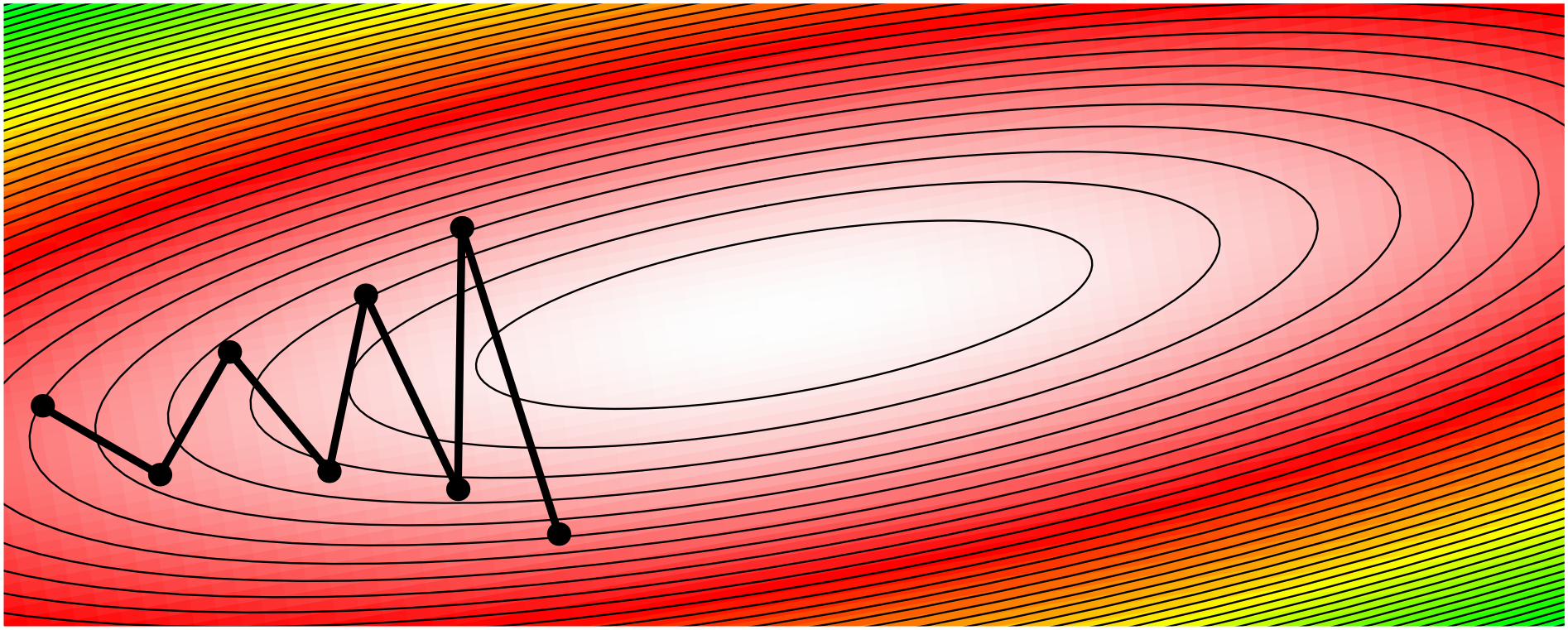

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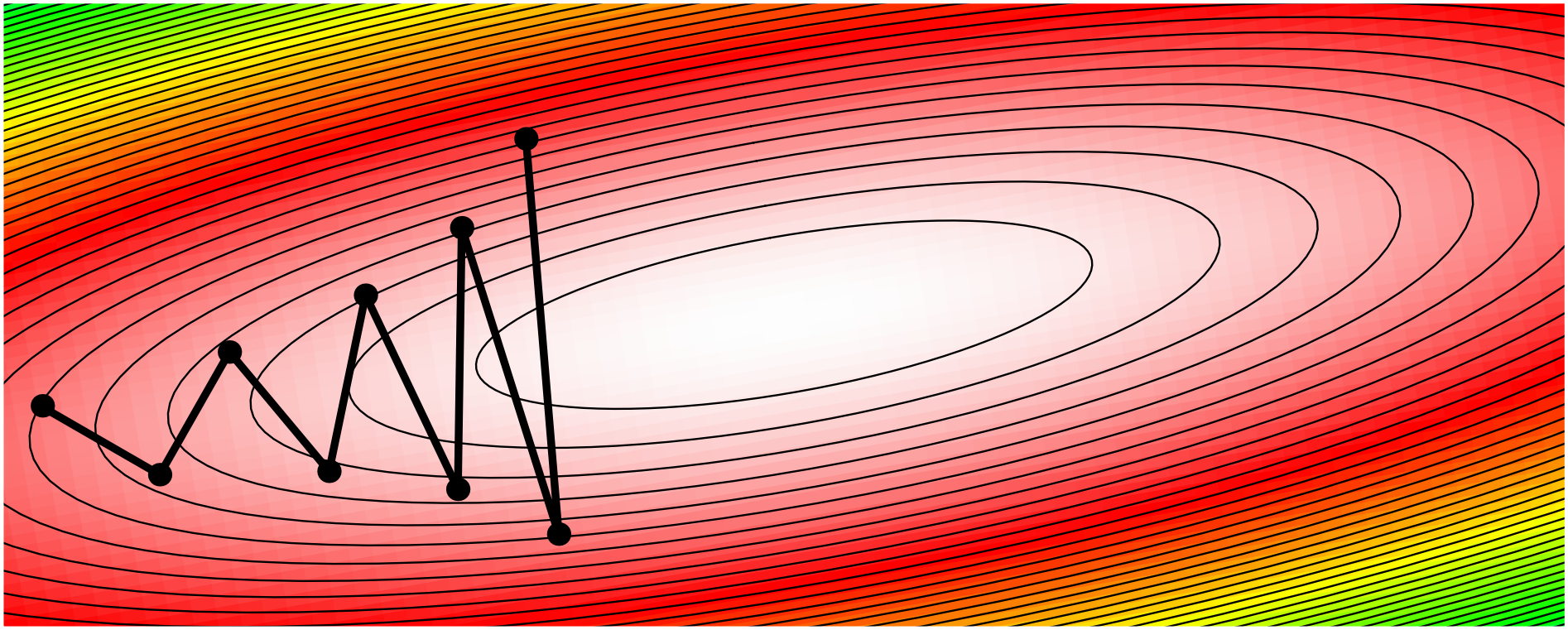

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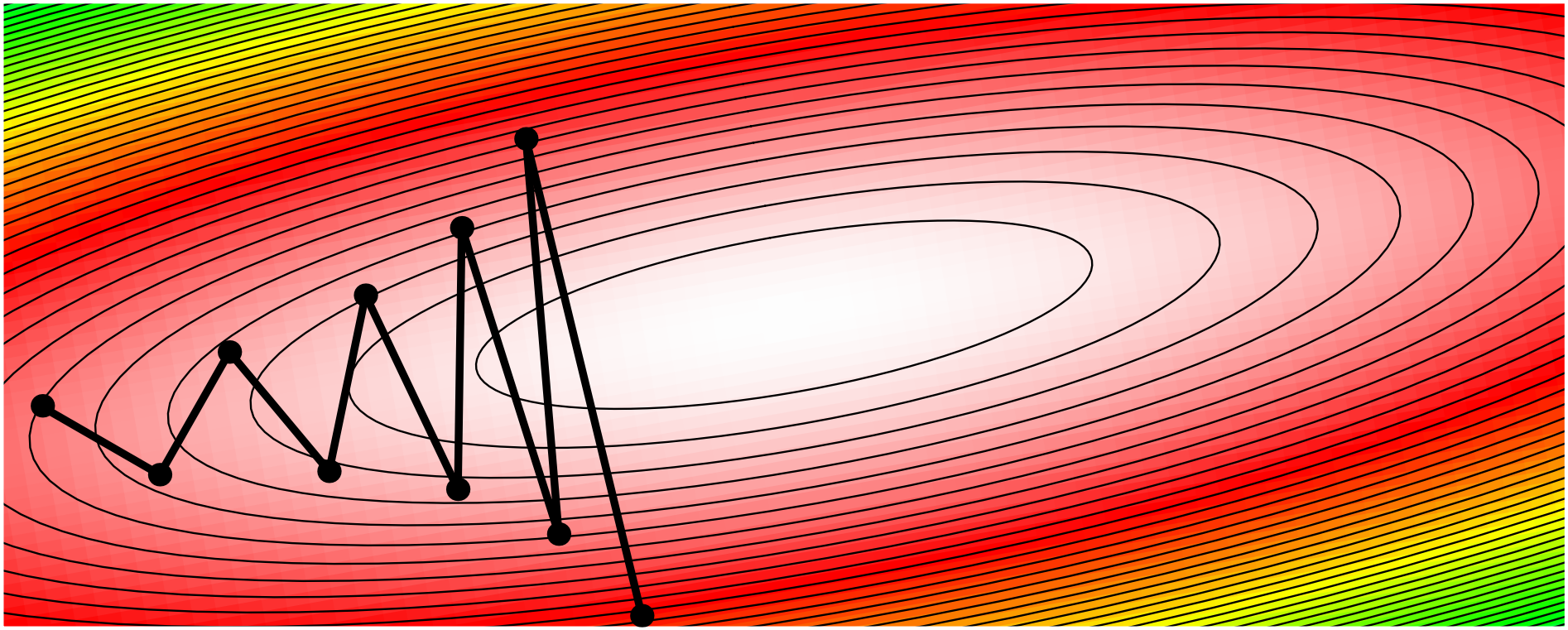

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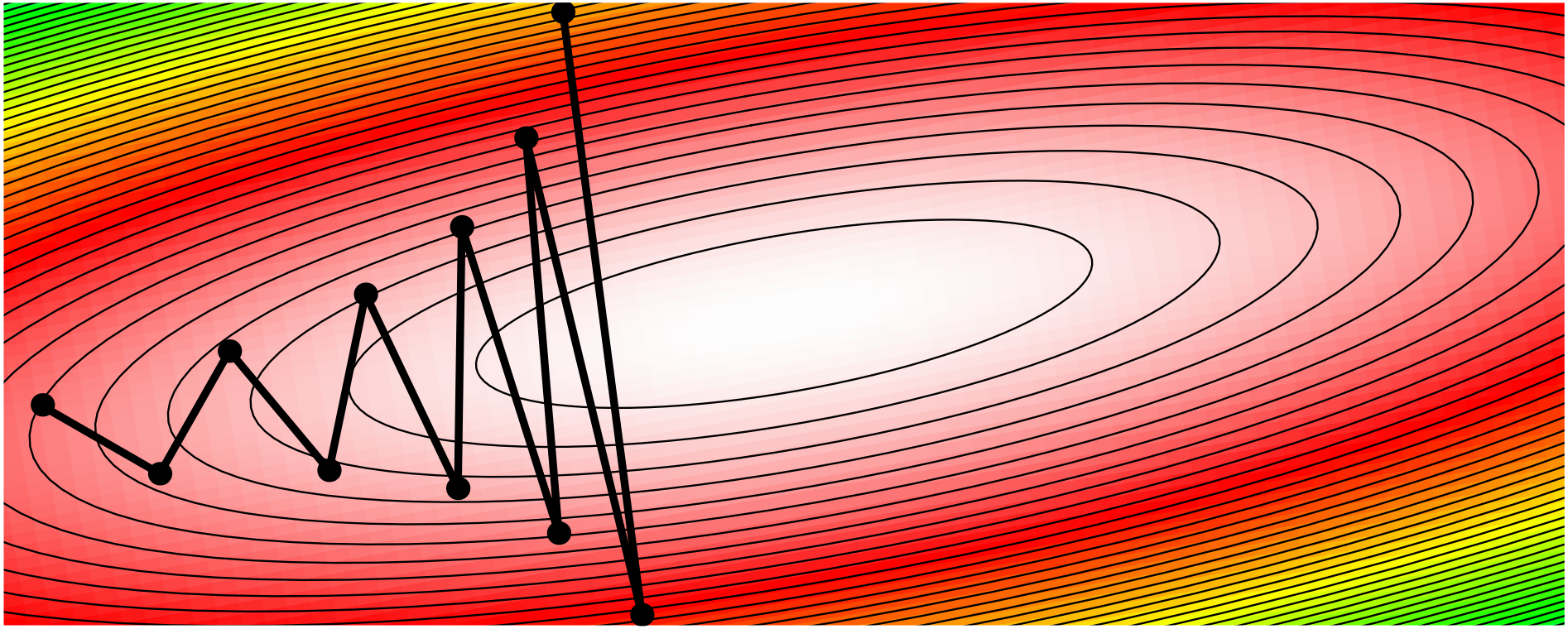

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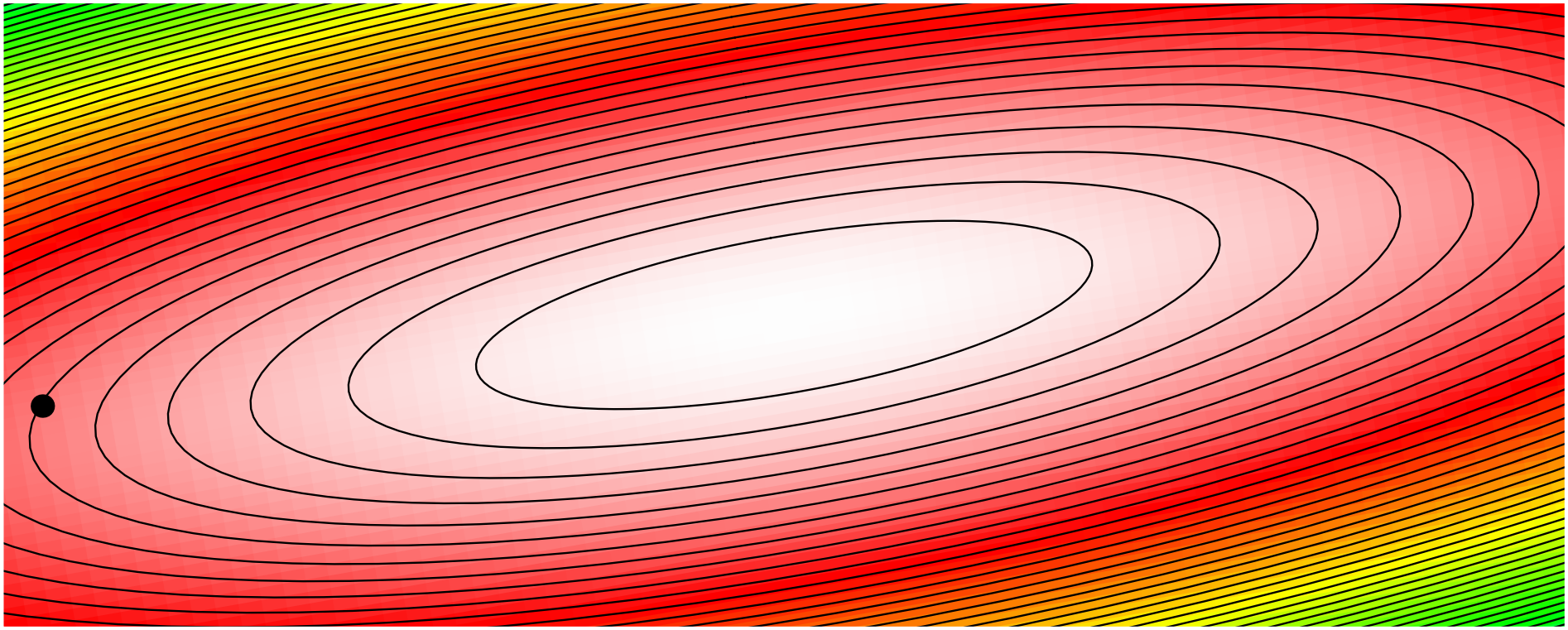

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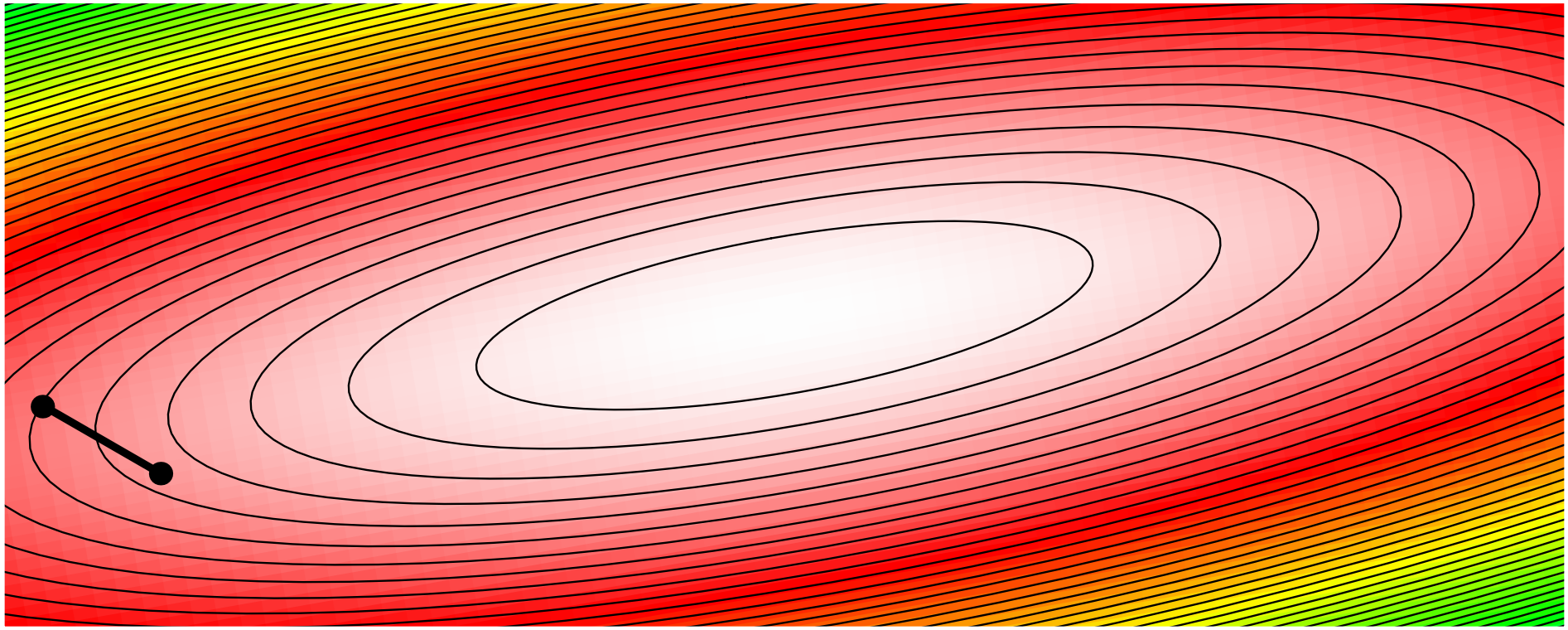

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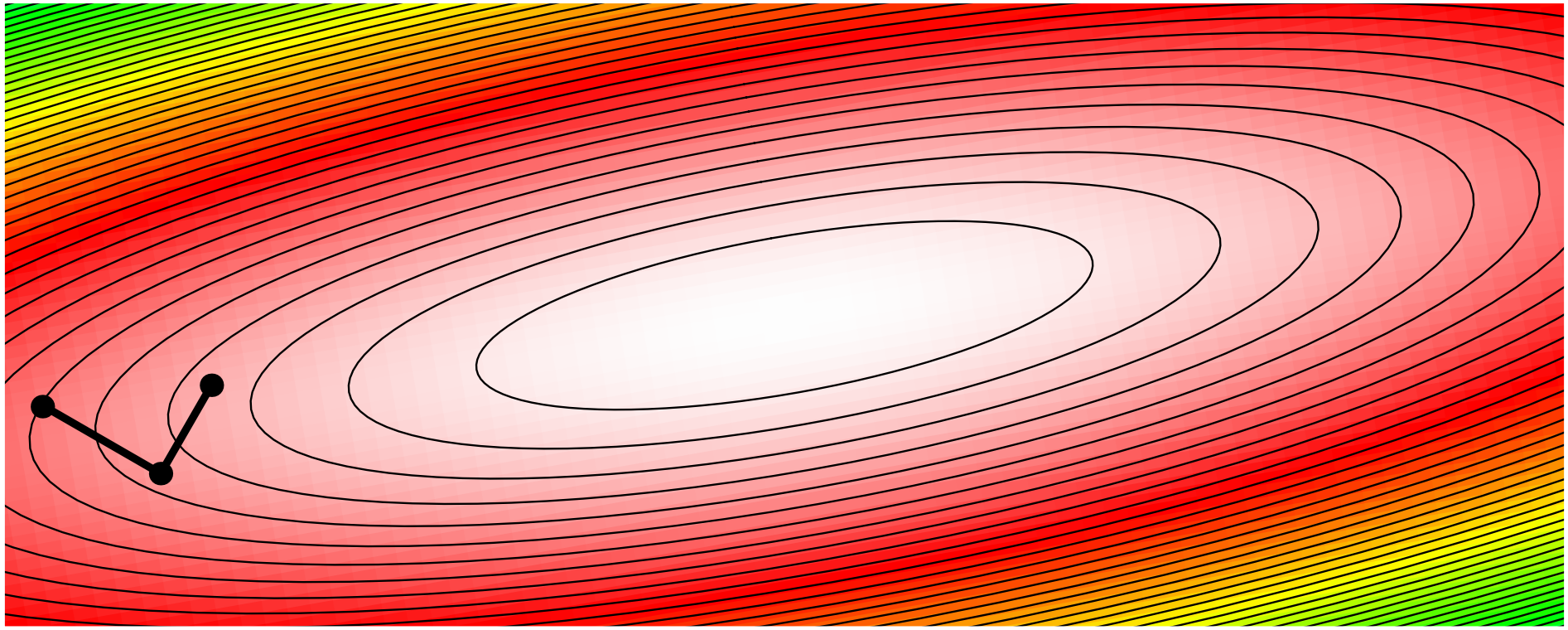

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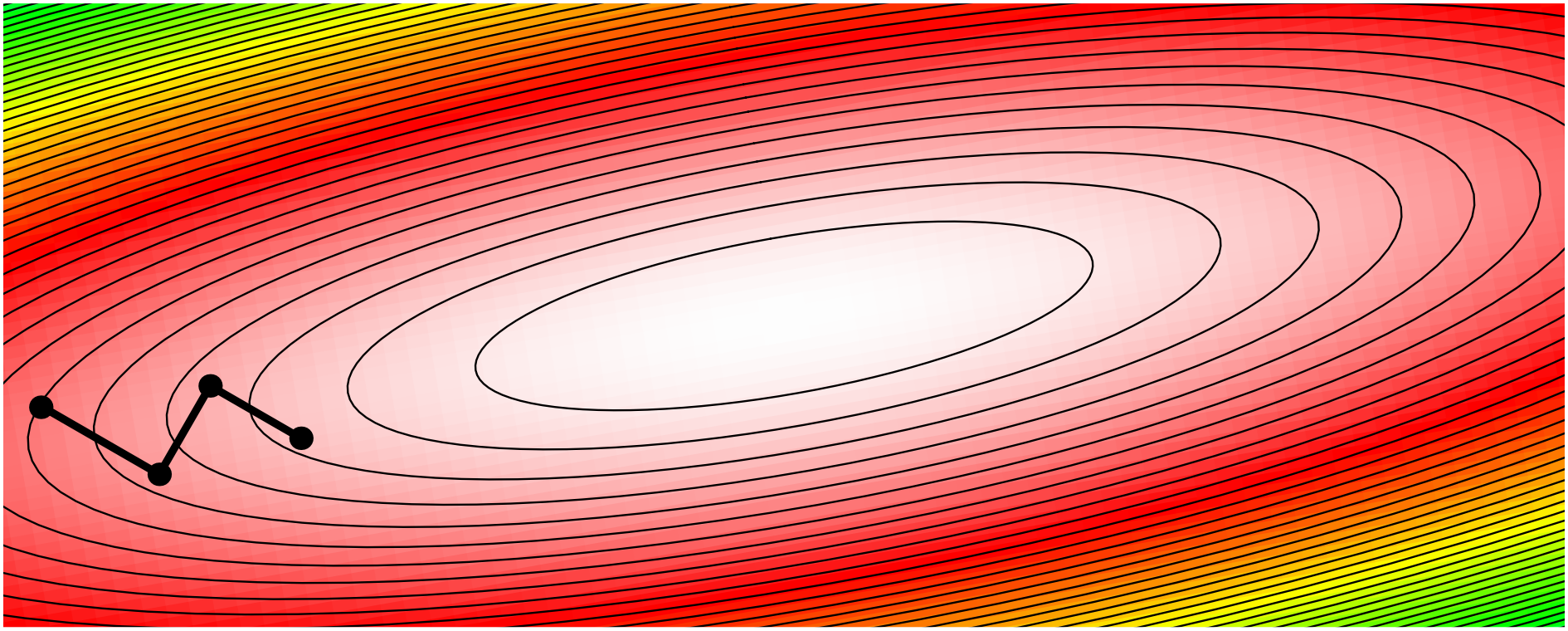

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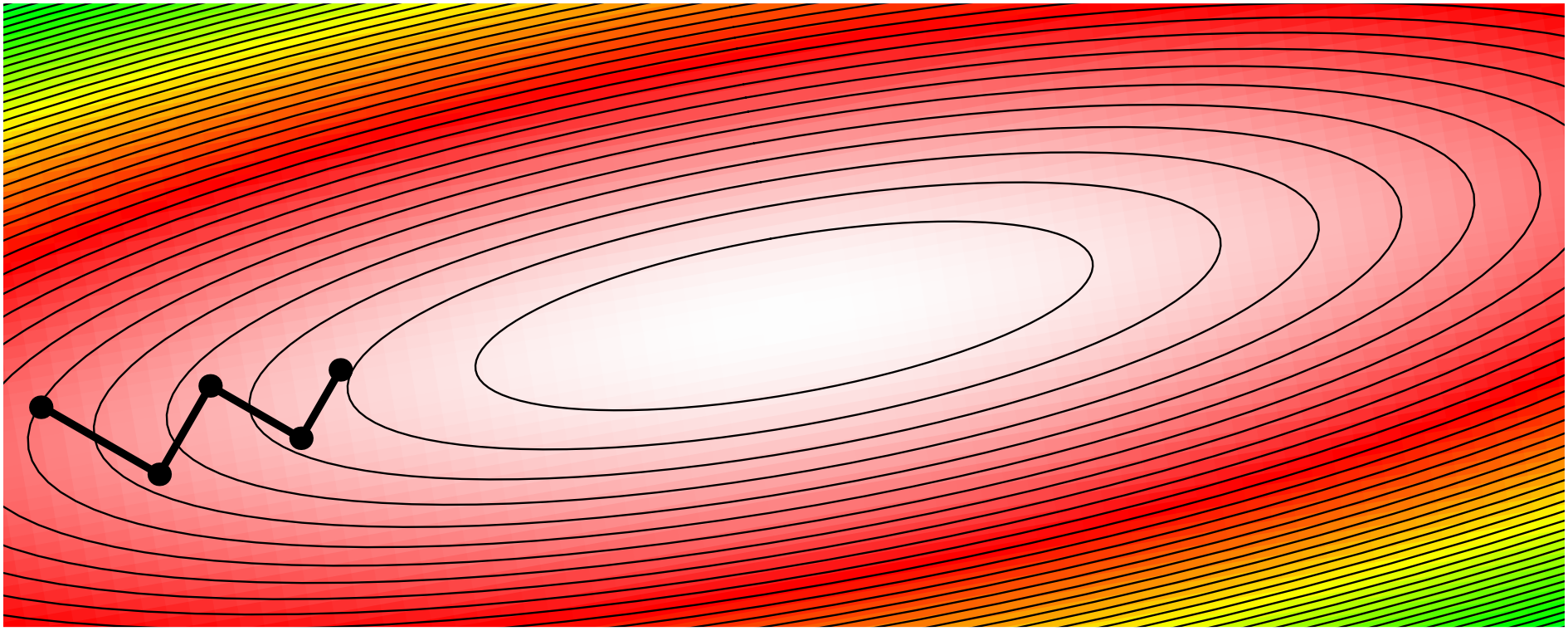

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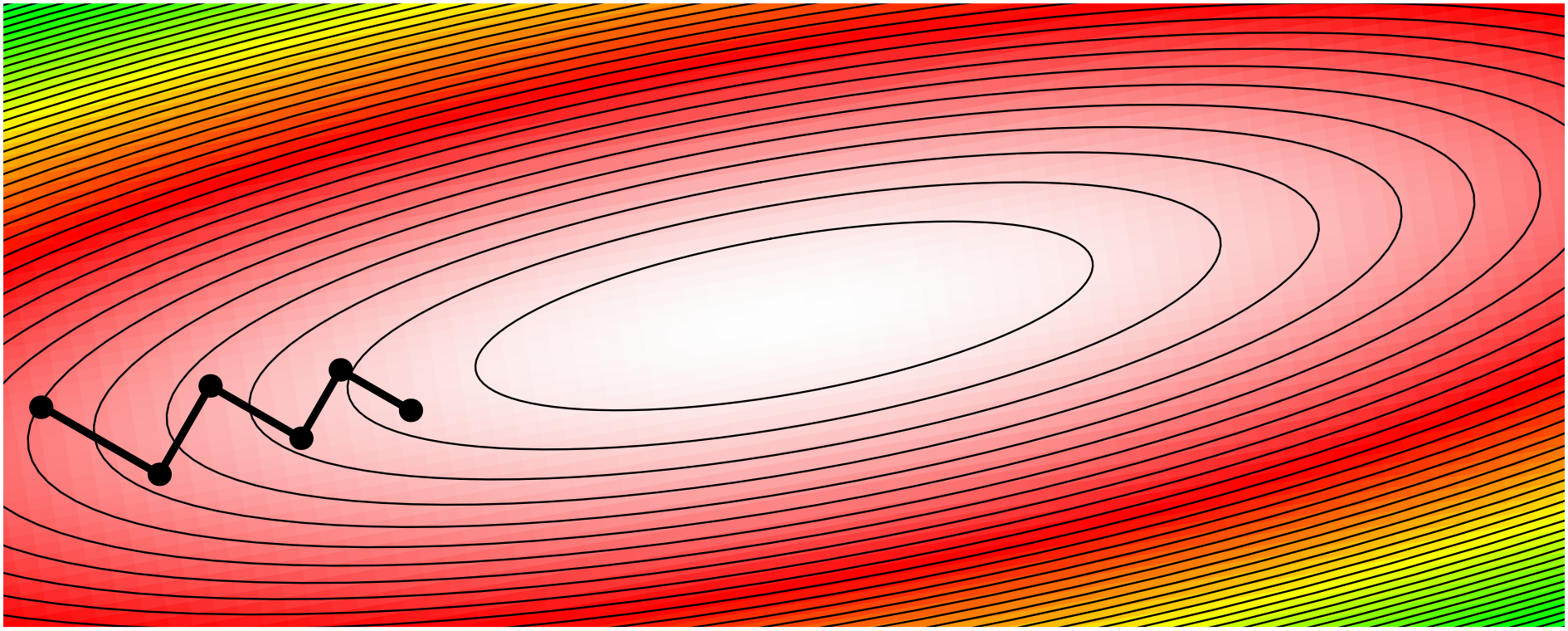

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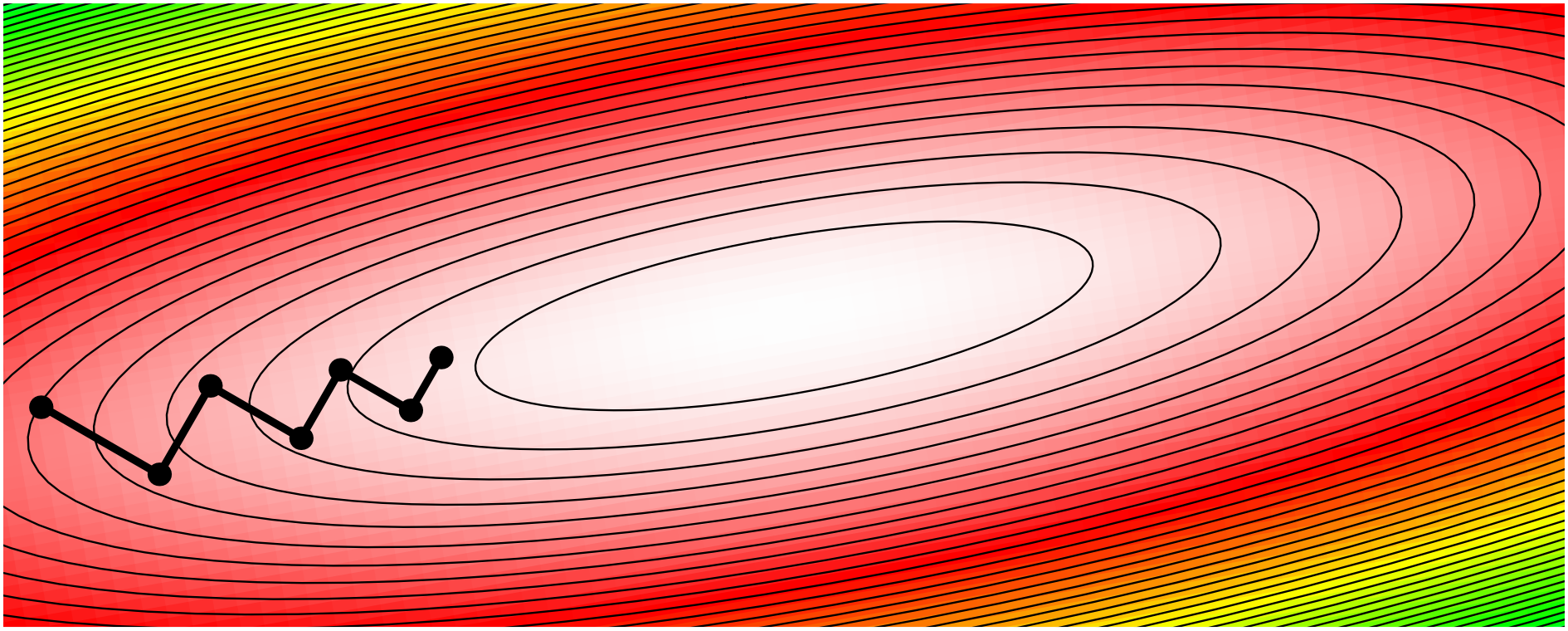

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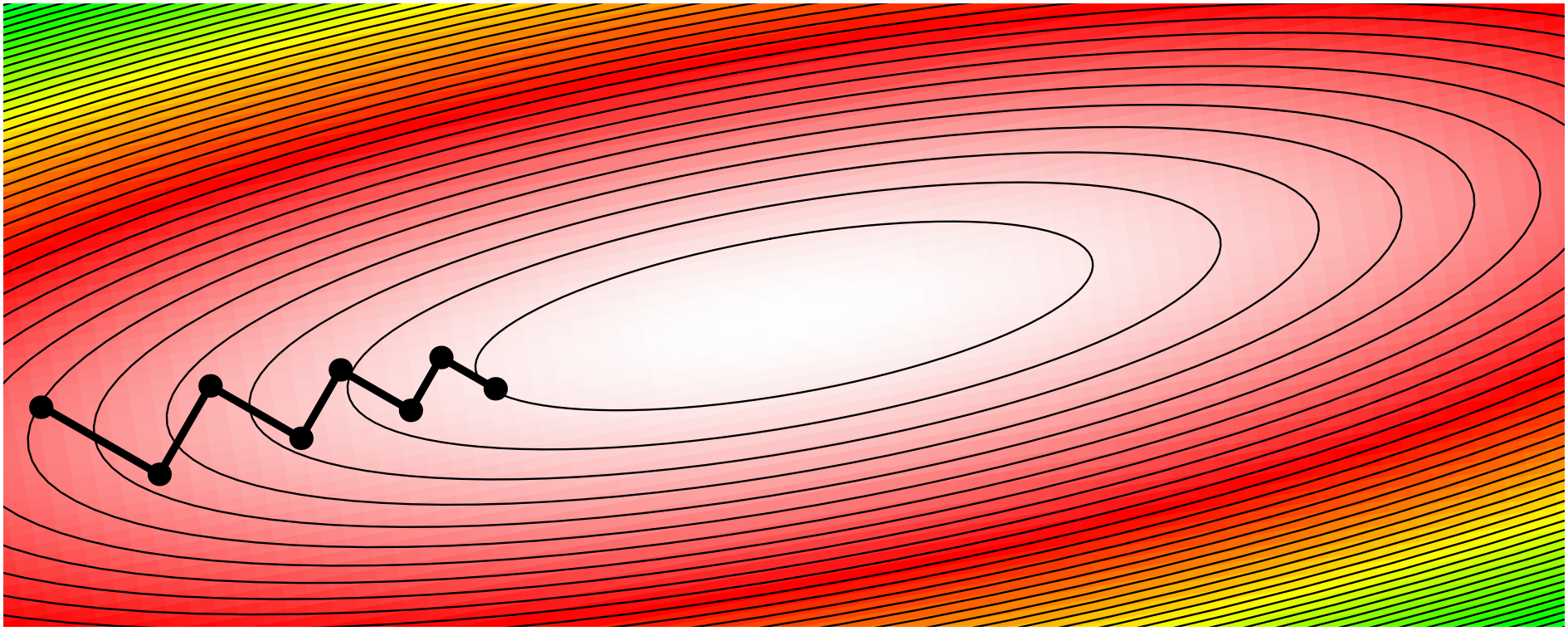

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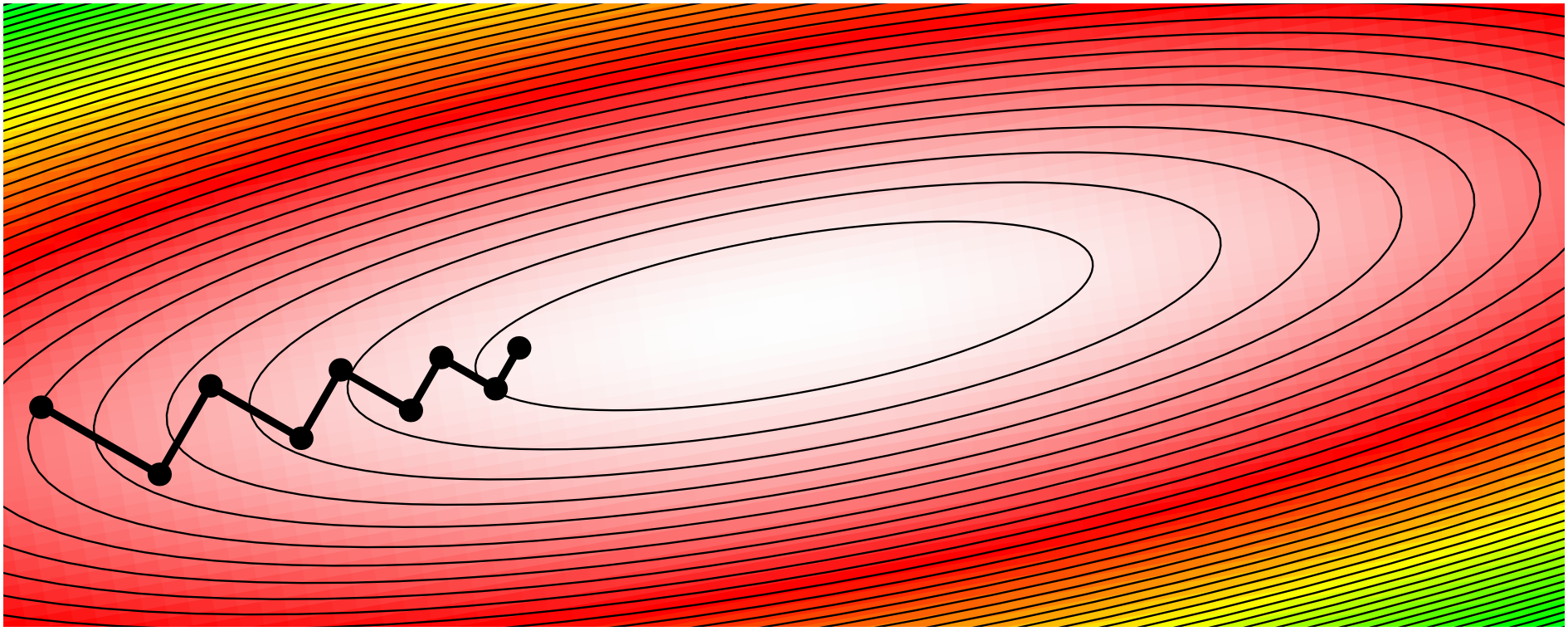

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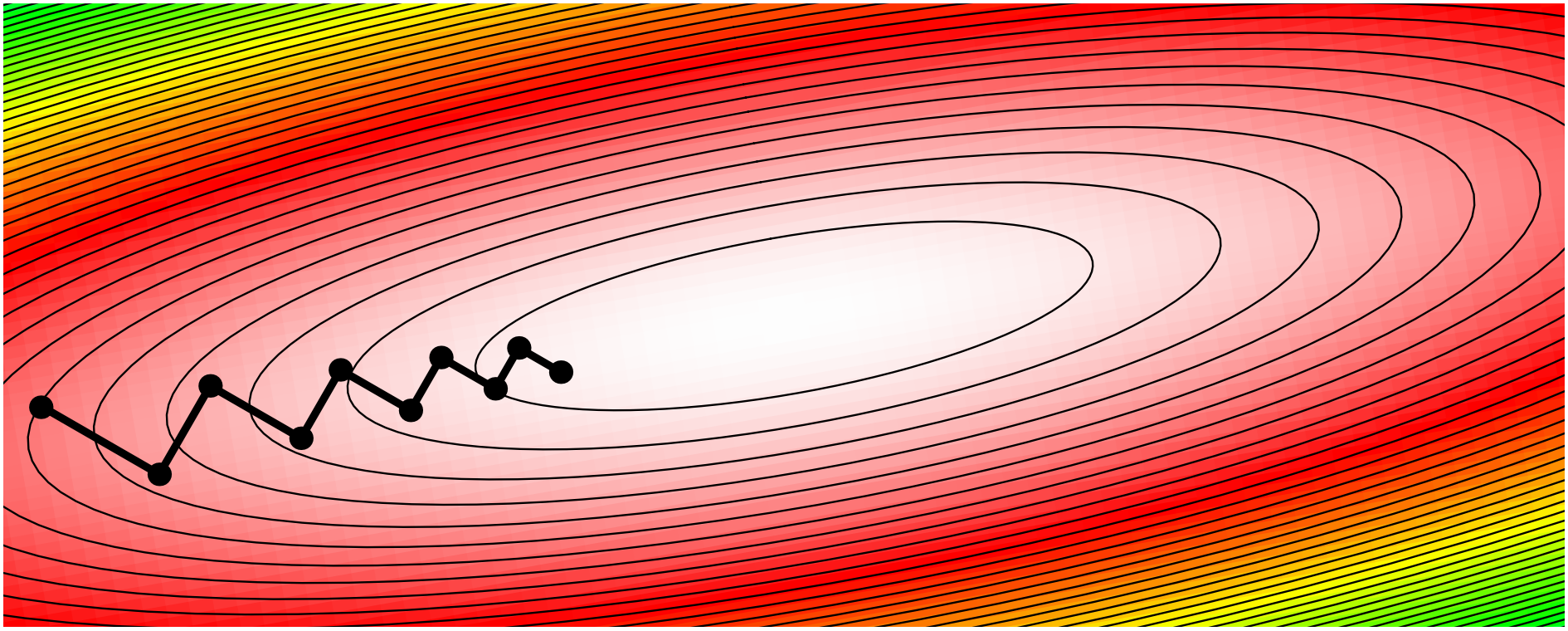

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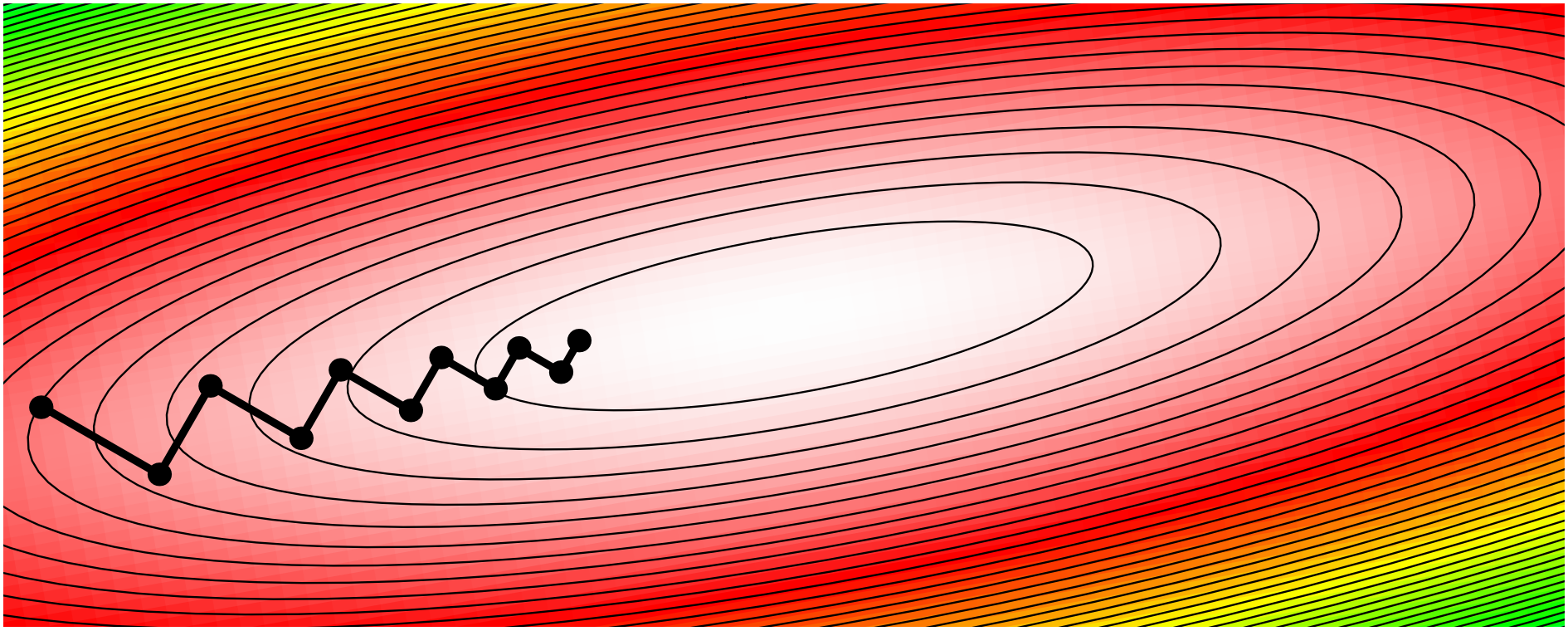
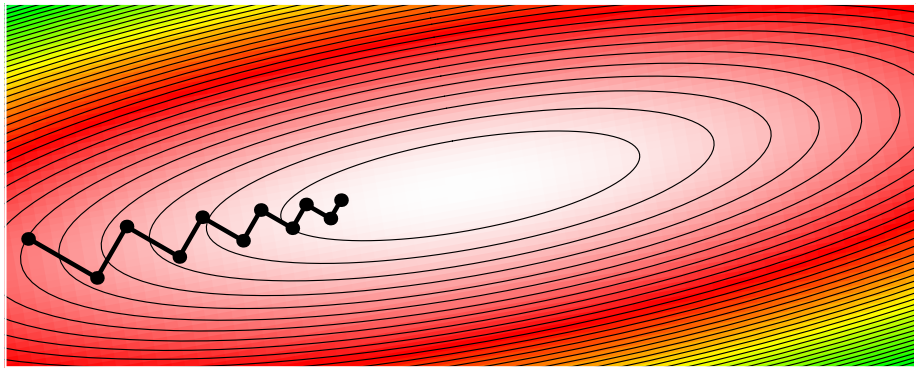


# Zig-Zag

- Note that in high dimensions gradient descent tends to zigzag



- If we computed the Hessian and used Newton's method we would jump straight to the minimum if we were in a quadratic potential

- However computing the Hessian is time consuming and misleading if we are not in a quadratic potential (i.e. far from the optimum)

# Zig-Zag

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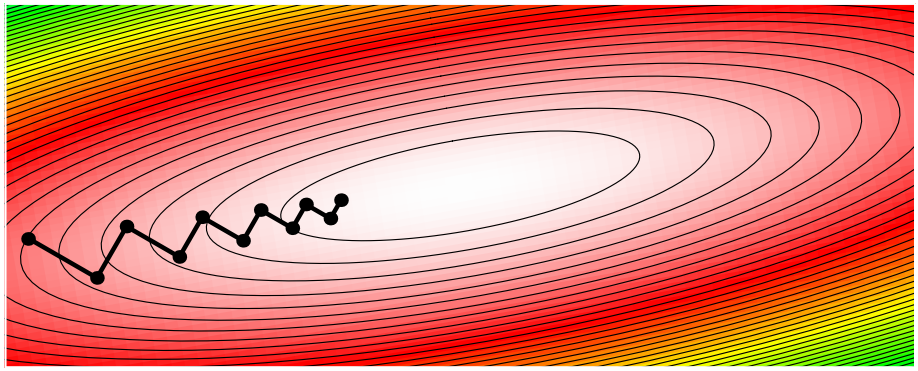

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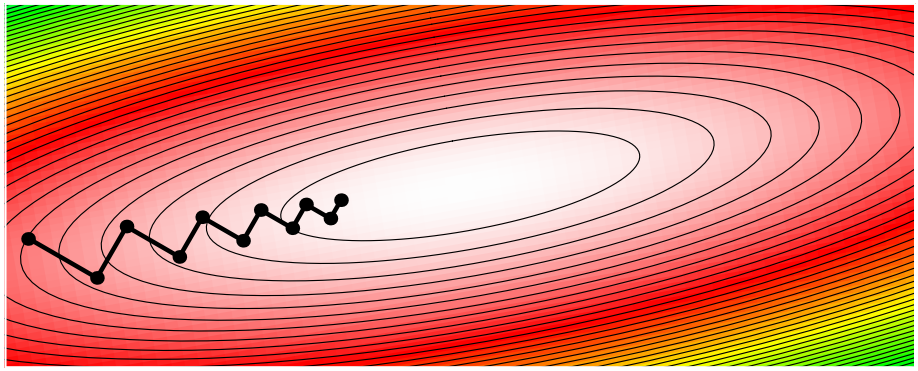

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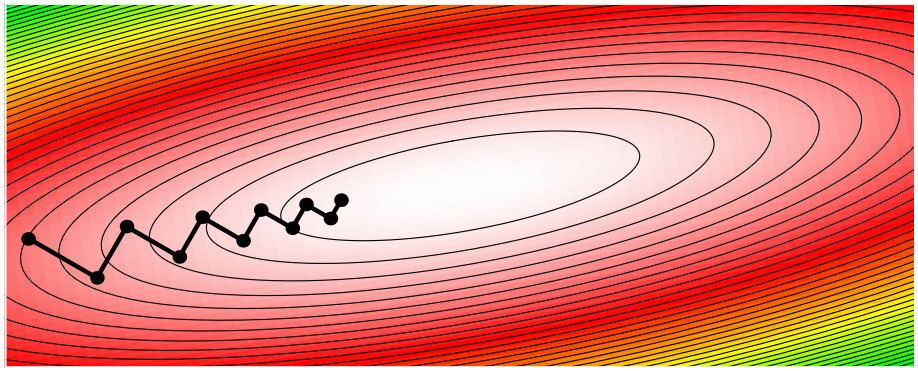

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- The best optimisation algorithms compute an approximation of the Hessian

- E.g. Conjugate gradient
  - ⋆ Performs Line Minimisation
  - ⋆ Uses gradient, but does not go along it
  - ⋆ Reaches quadratic minimum in $N$ steps

- E.g. Levenberg-Marquardt
  - ⋆ Used on least squares problem only
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# Levenberg-Marquardt

- Want to minimise $\|\boldsymbol{\epsilon}(\boldsymbol{w})\|^2$ where $\epsilon_i(\boldsymbol{w}) = f(\boldsymbol{x}_i|\boldsymbol{w}) - y_i$
- Use linear approximation

$$\epsilon_i(\boldsymbol{w}) \approx \epsilon_i(\boldsymbol{w}^{(k)}) + (\boldsymbol{w} - \boldsymbol{w}^{(k)})\boldsymbol{\nabla}\epsilon_i(\boldsymbol{w}^{(k)})$$

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- Solve quadratic minimisation of approximate error $\operatorname{argmin}_{\boldsymbol{w}} L_{approx}(\boldsymbol{w})$ with $\mathbf{J} = \boldsymbol{\nabla}\boldsymbol{\epsilon}(\boldsymbol{w}^{(k)})$

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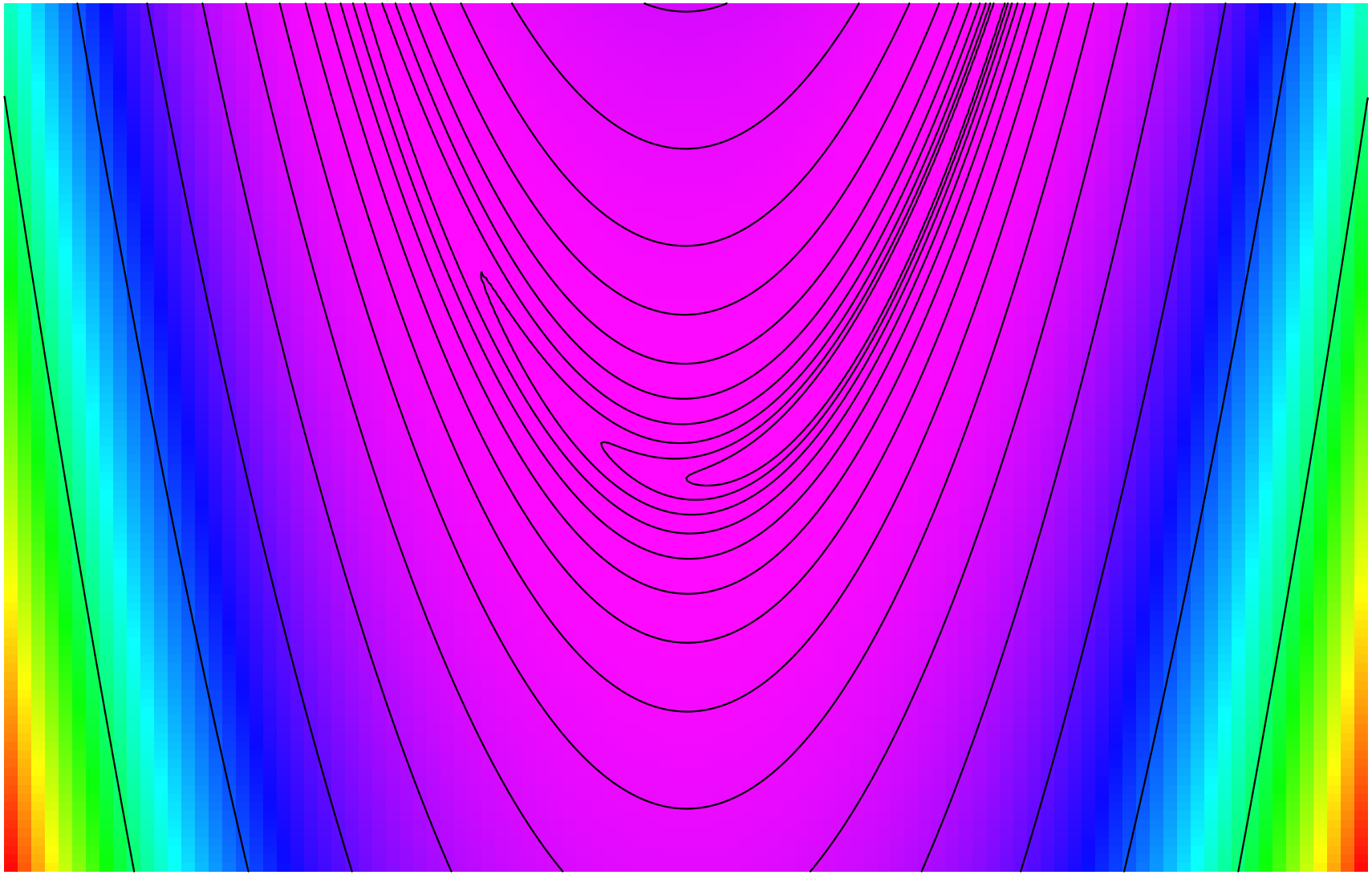

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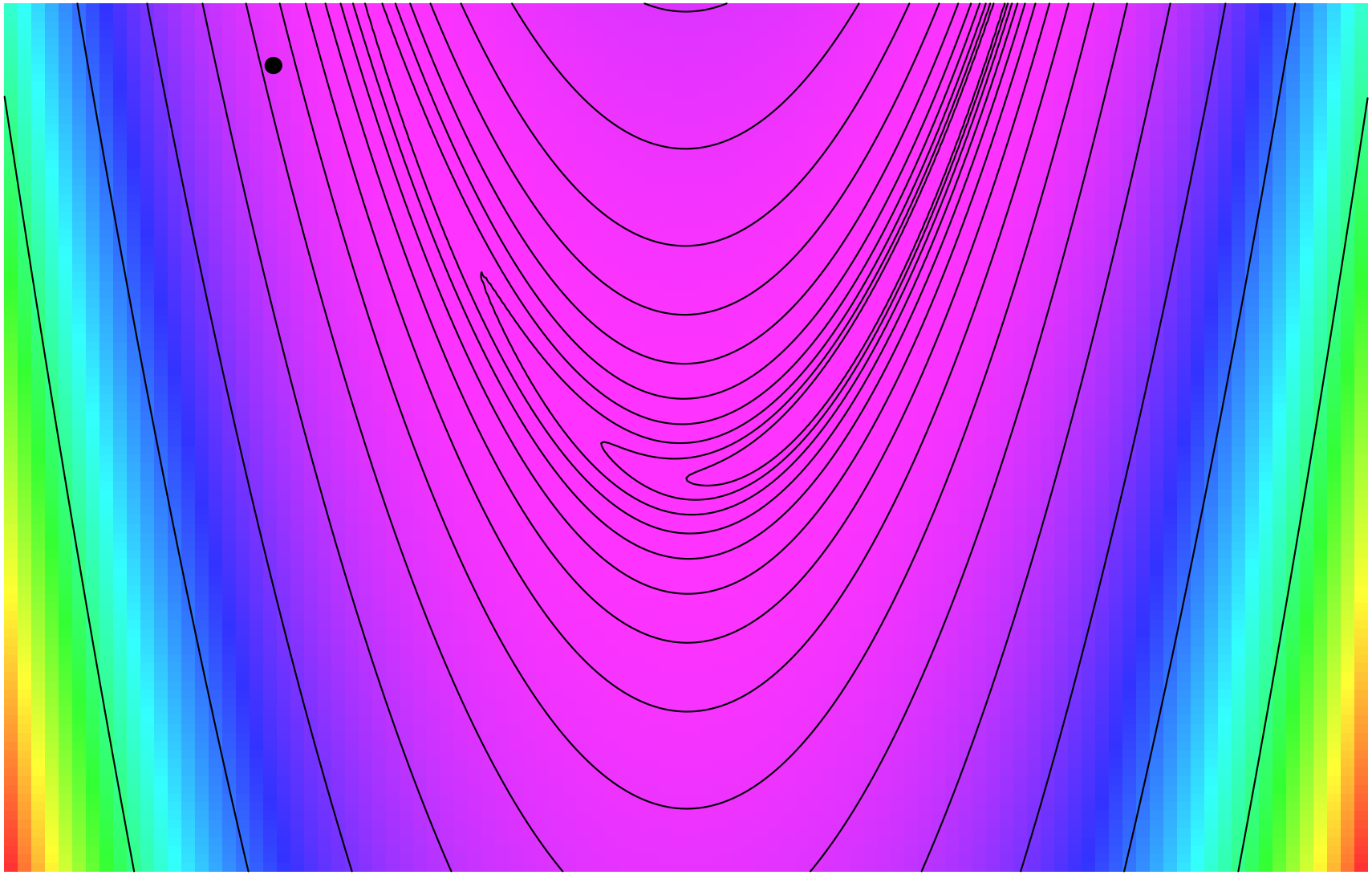

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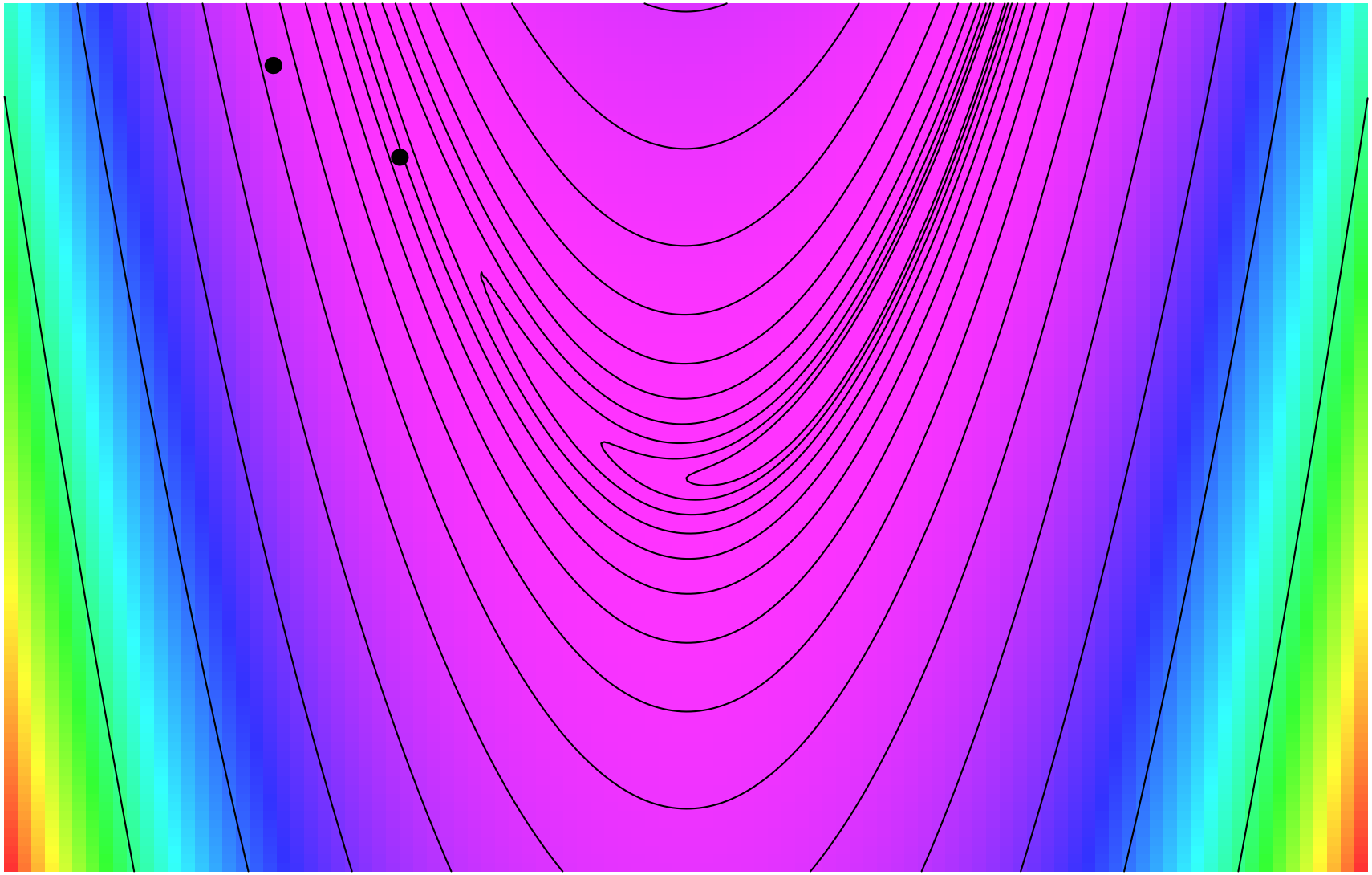

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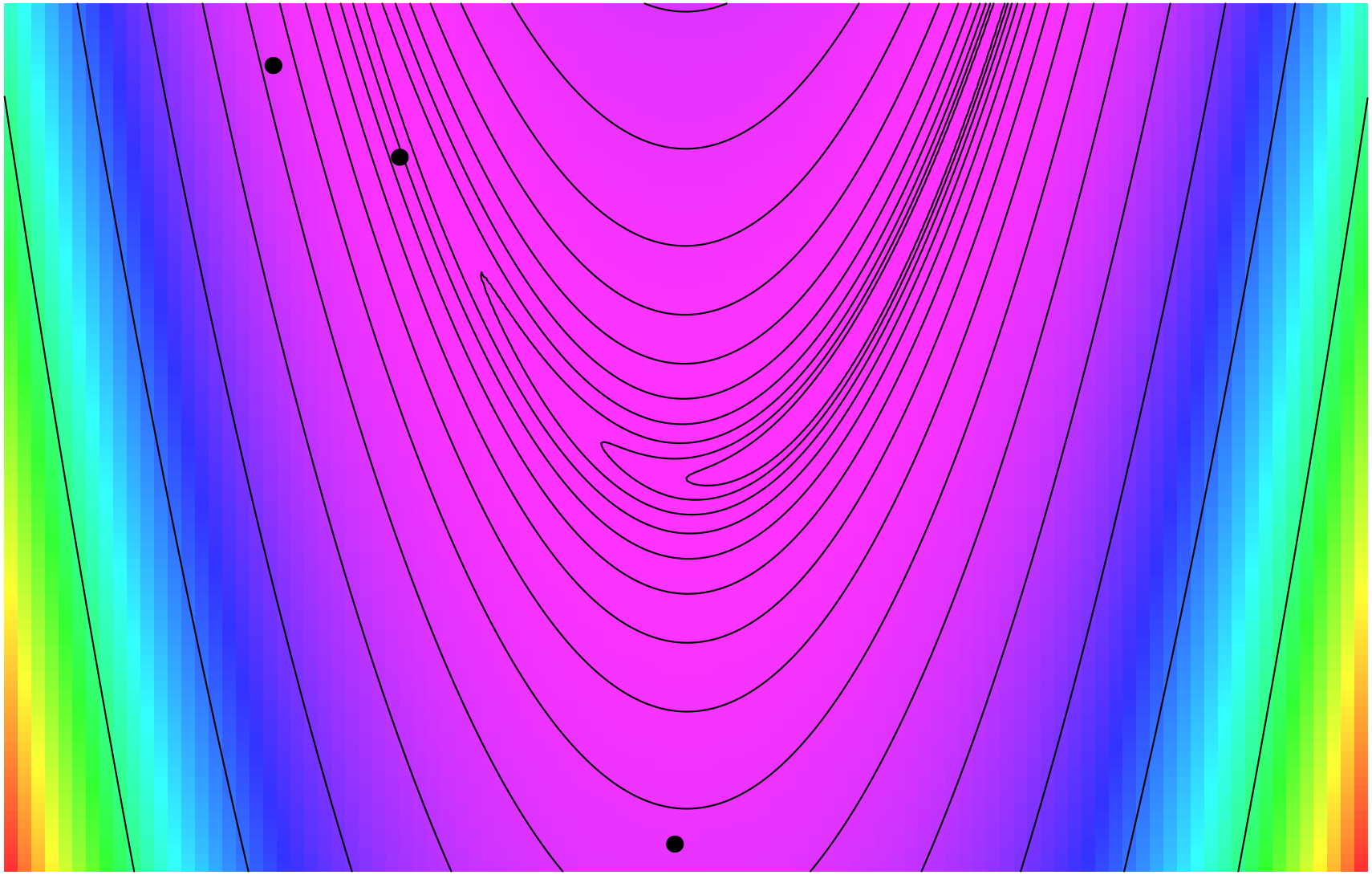

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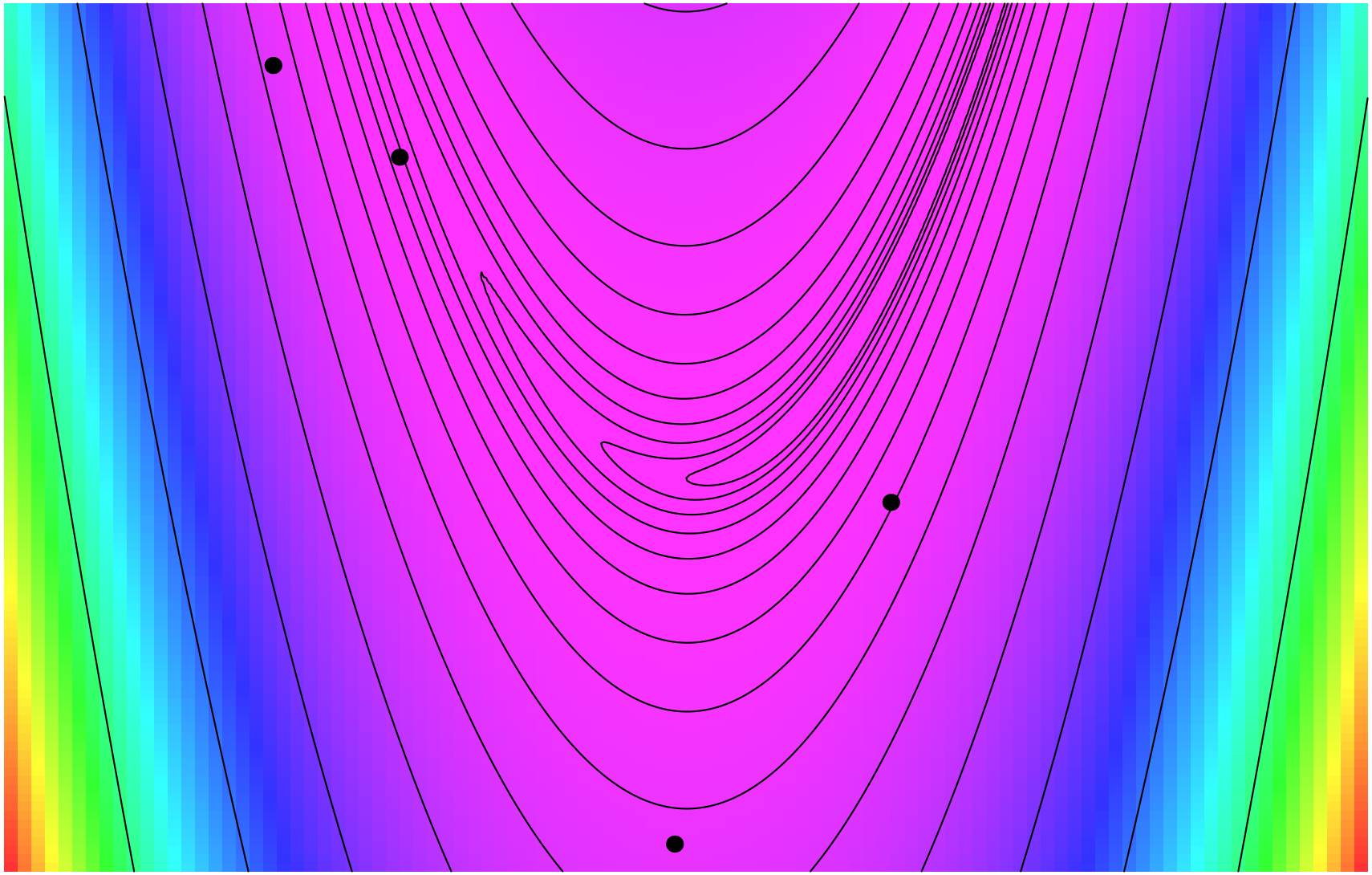

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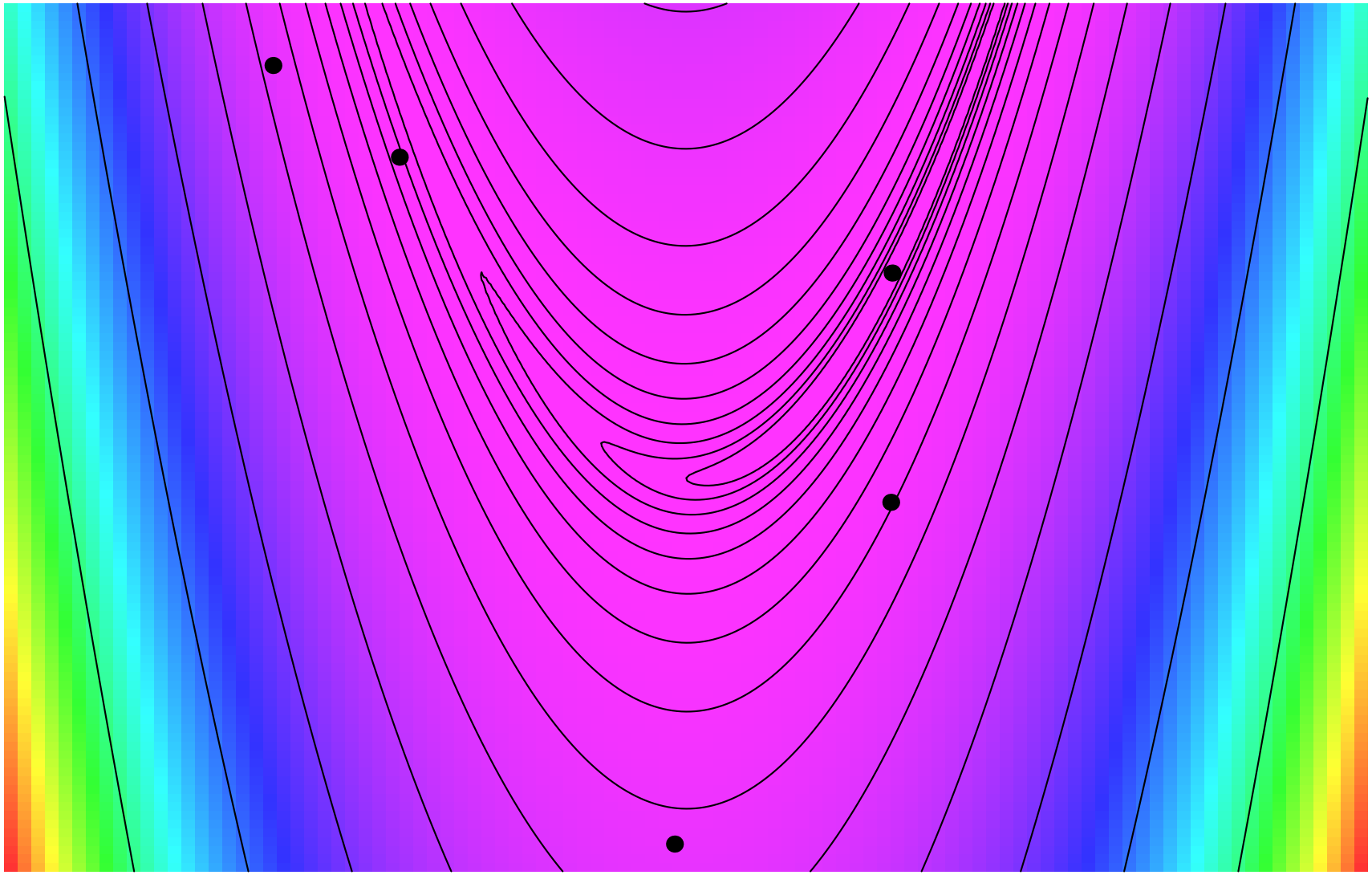

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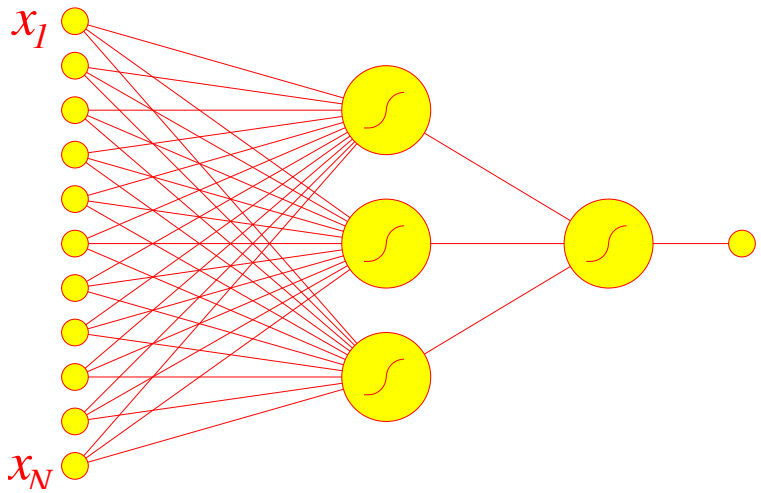
- Very little gradient information (can use momentum)
- Many local minima—not guaranteed to find global minimum
- Weight space is symmetric because of permutation symmetry



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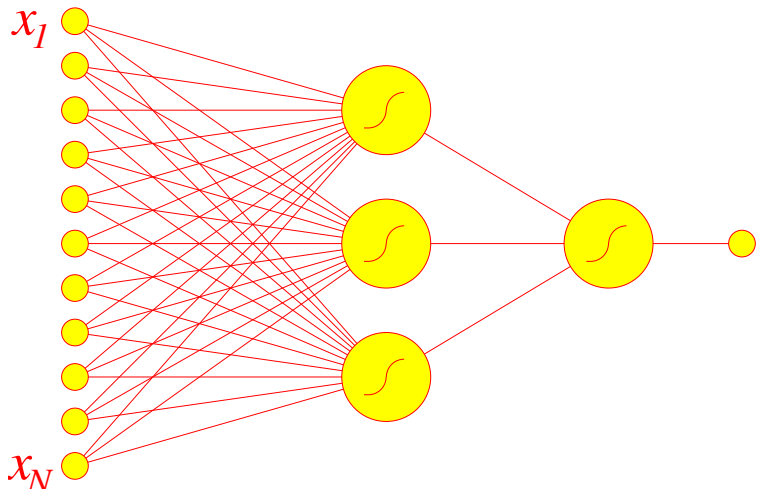

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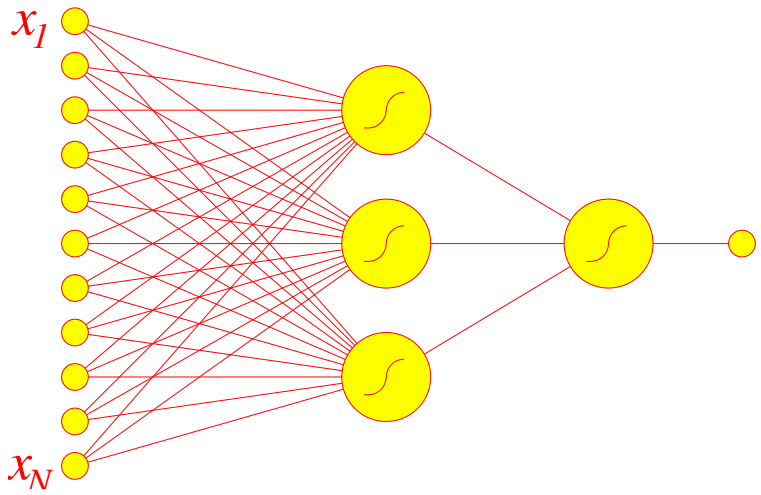

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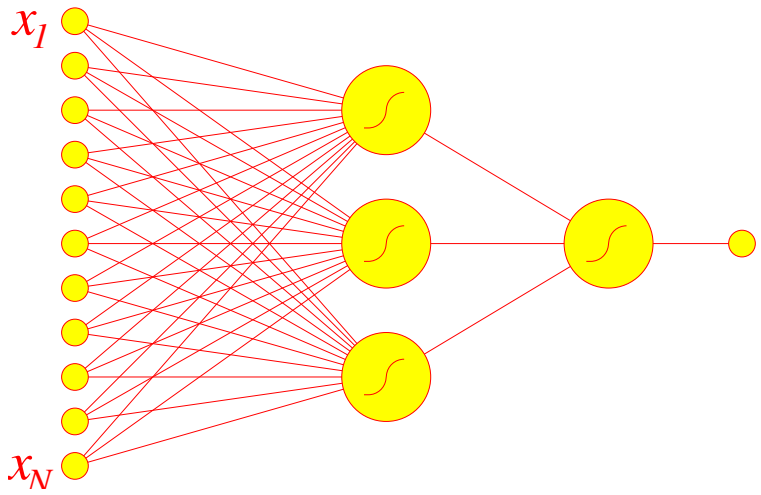

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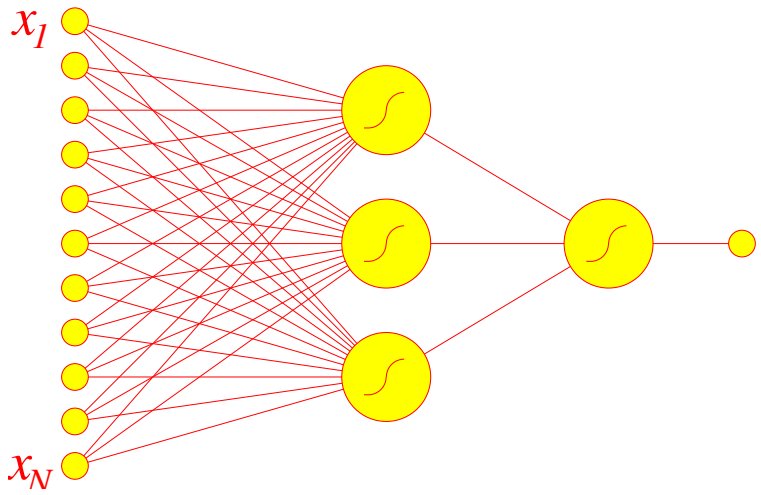

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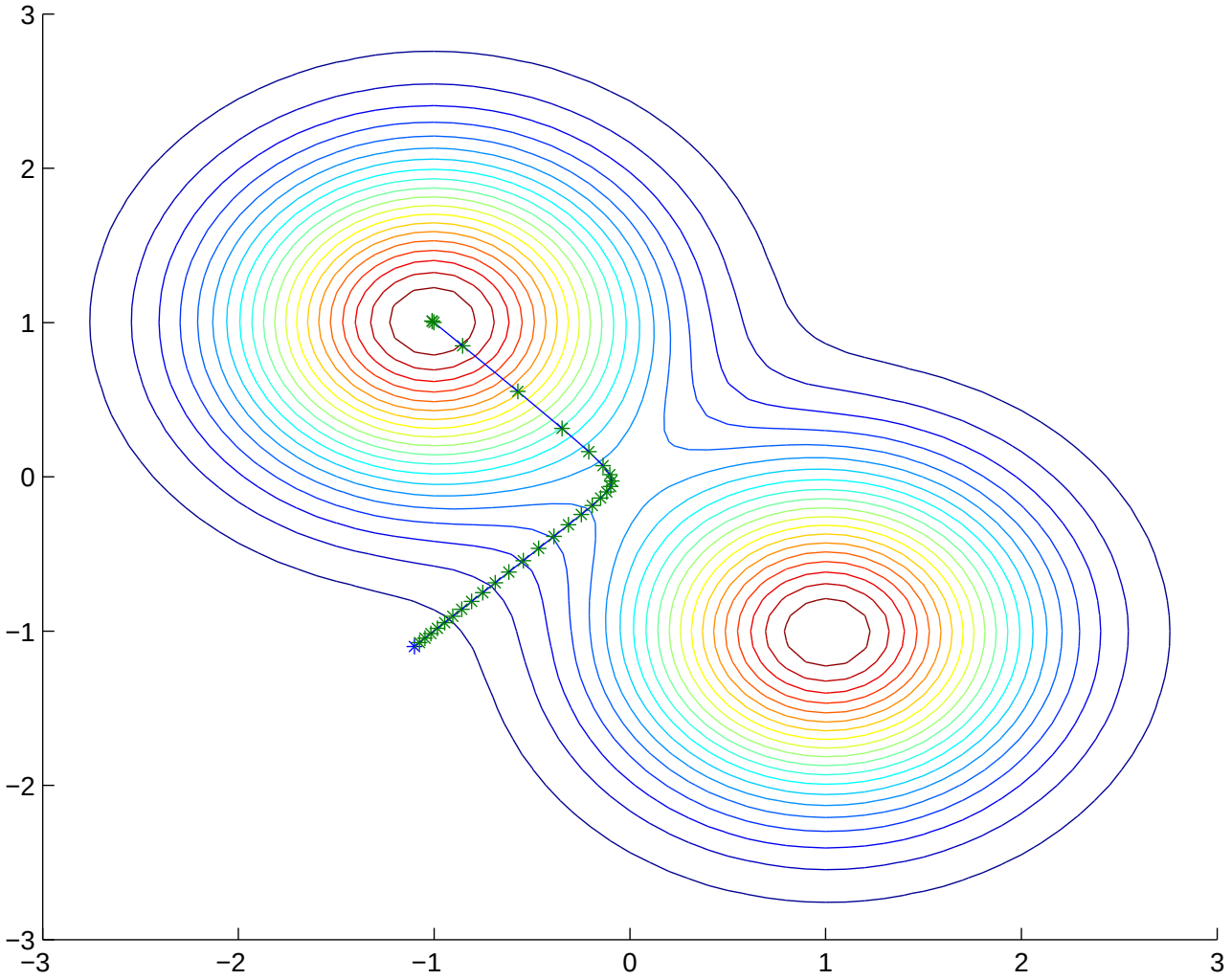

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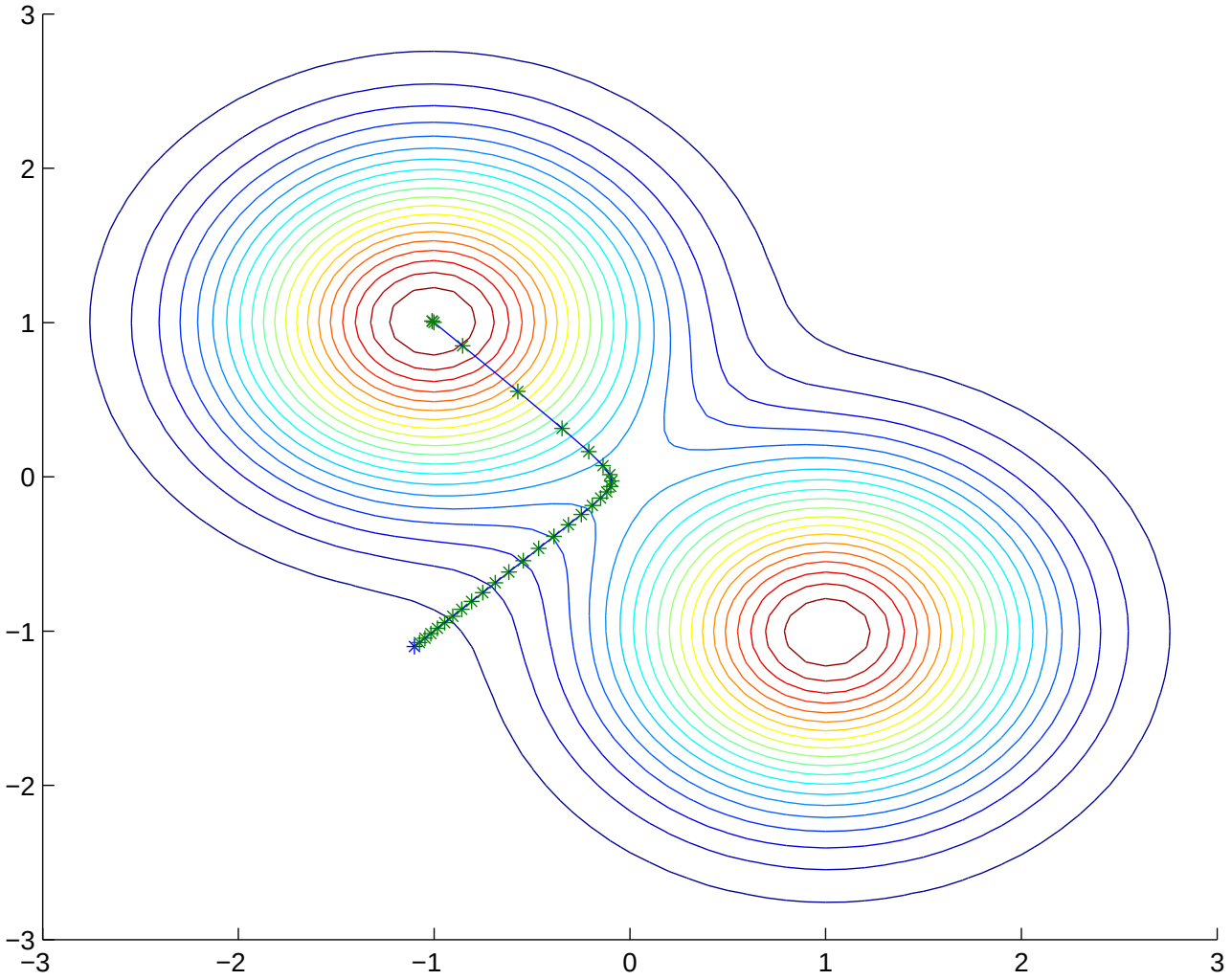

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