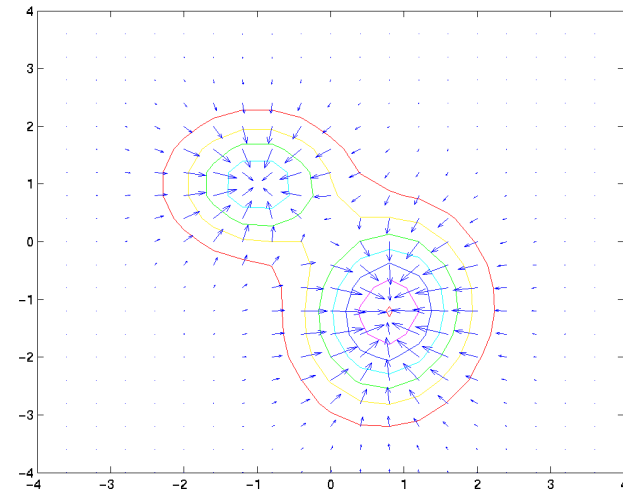
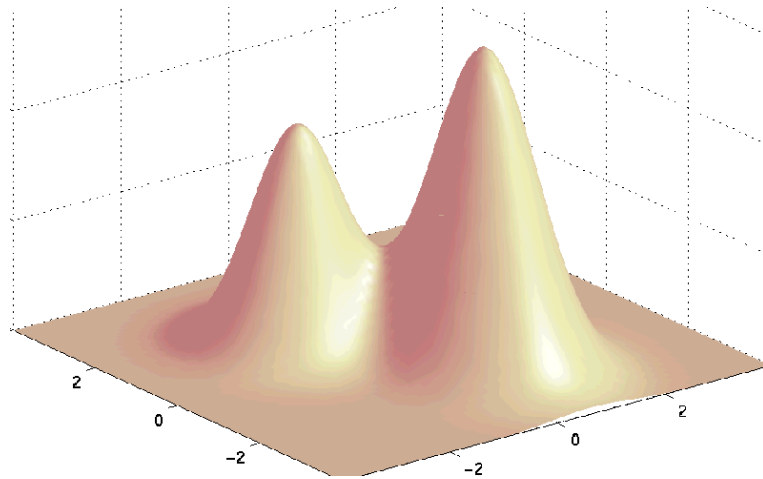


Advanced Machine Learning

Optimisation

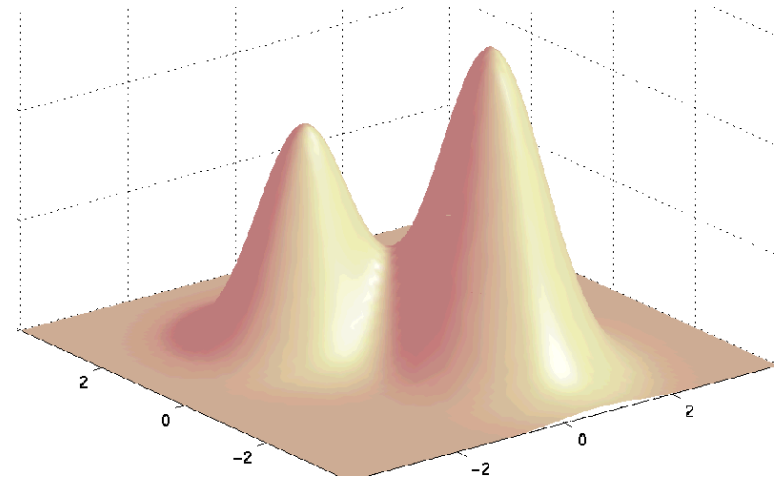


$$z = e^{-(x+1)^2 - (y-1)^2} + 0.6e^{-(x-1)^2 - 0.5(y+1)^2 + 0.1(x-3)(y-3)}$$

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

$$\hat{y} = f(x|w)$$

(or more generally $\hat{y} = f(x|w)$)

- Given an input pattern (set of features) x the learning machine makes a prediction \hat{y}
- We try to choose the parameters w so that the predictions are good
- In practice training a learning machine comes down to optimising some loss function

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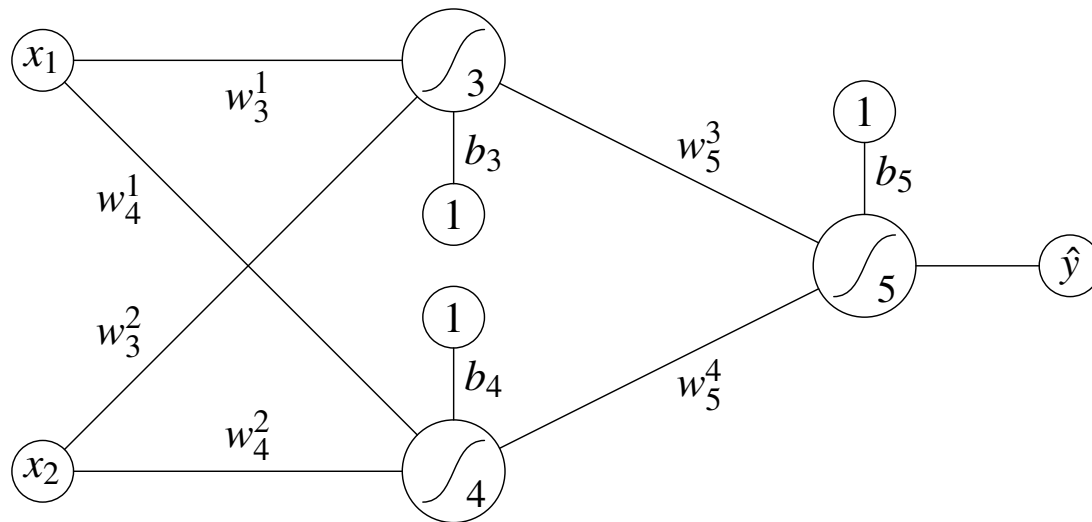
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MLP

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



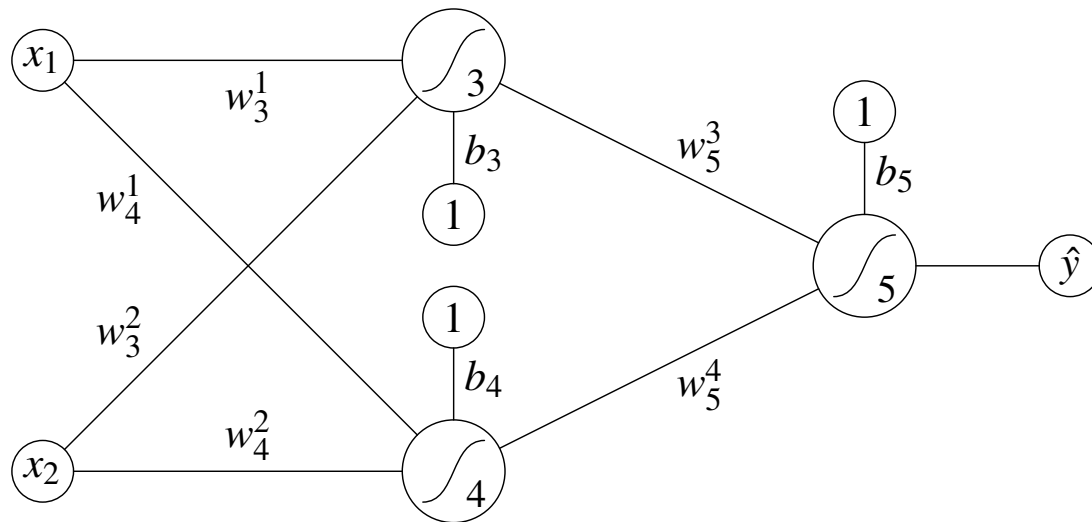
- Stands for the function $(\hat{y} = f(\mathbf{x}|\mathbf{w}))$

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

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Training

- Given a (labelled) training dataset

$$\mathcal{D} = \{(\mathbf{x}_k, y_k) \mid k = 1, \dots, m\}$$

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

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

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

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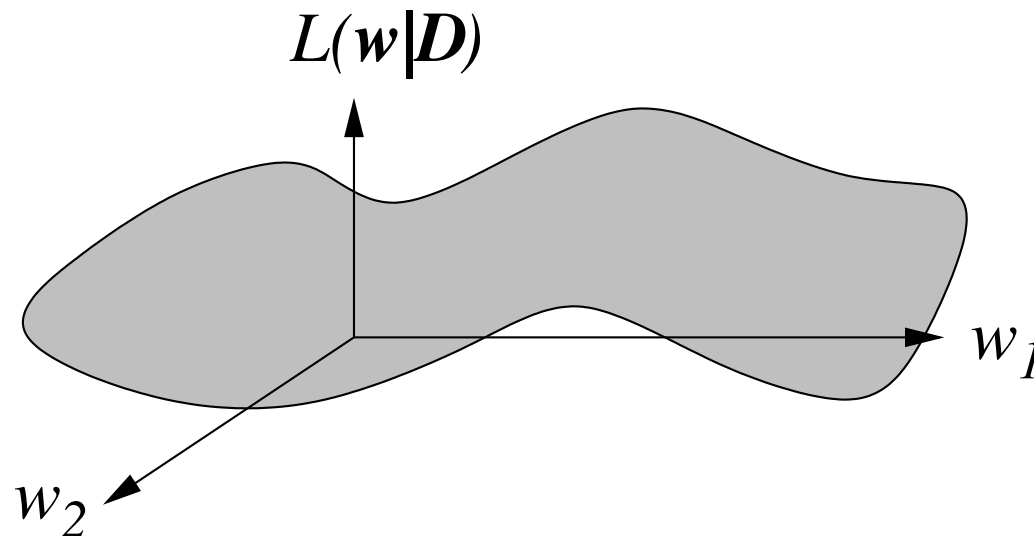
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Computing Gradients

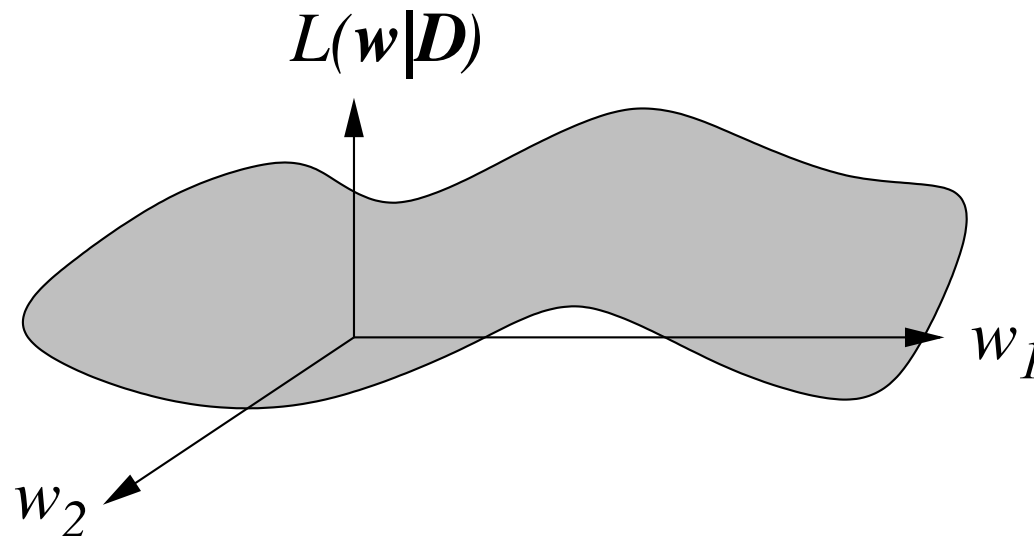
- $L(\mathbf{w}|\mathcal{D})$ is a complex function of the weights \mathbf{w}



- To minimise we $L(\mathbf{w}|\mathcal{D})$ we compute the gradient $\nabla L(\mathbf{w}|\mathcal{D})$
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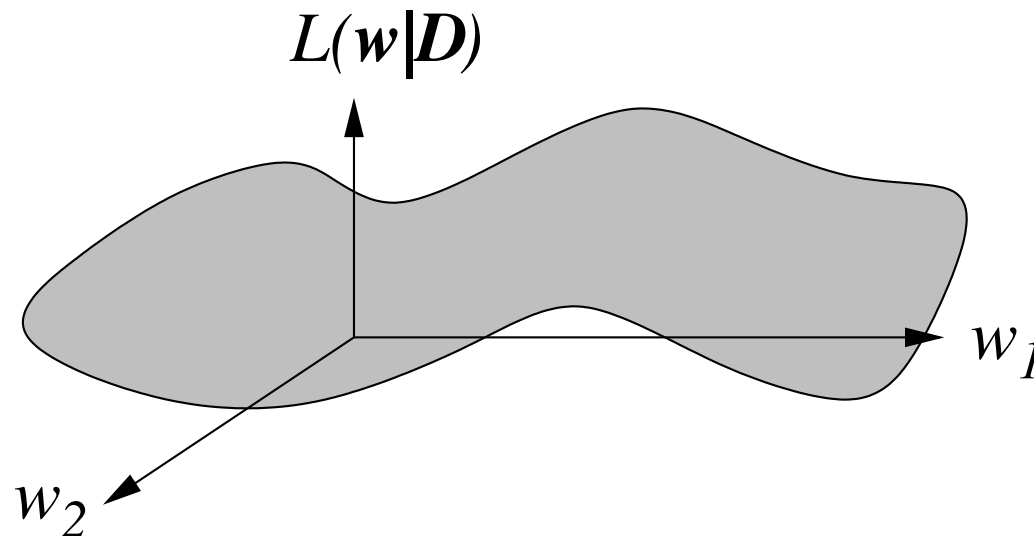
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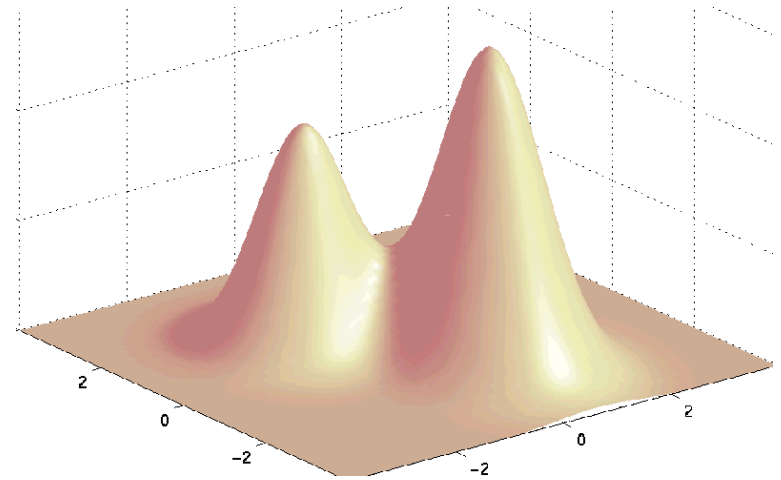
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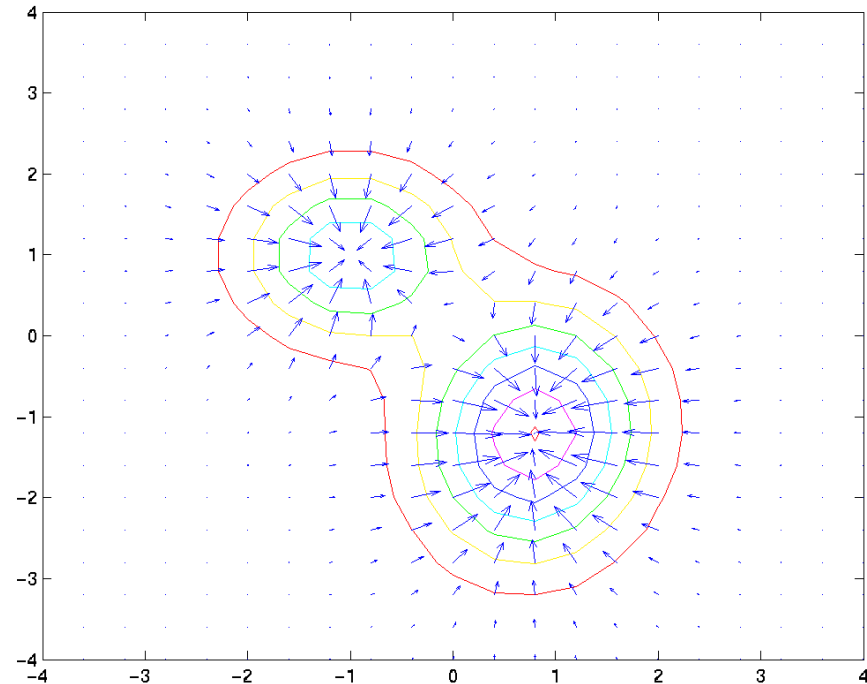
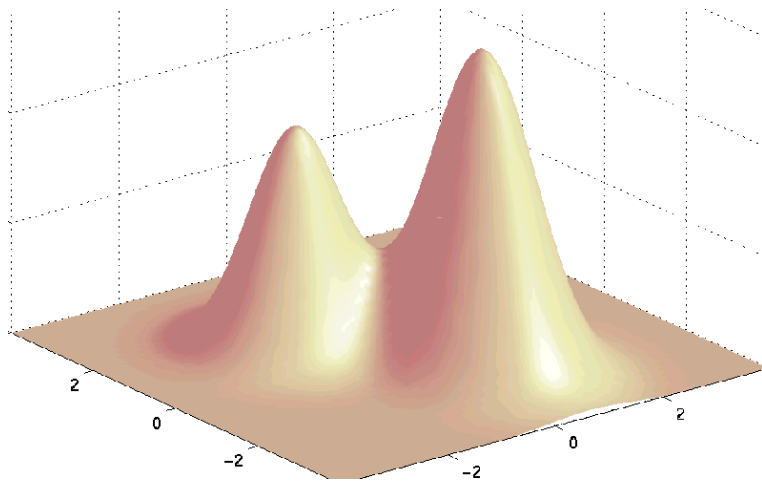
1. Motivation
2. **Gradient Descent**
3. Why Gradient Descent is Difficult



Gradient Optimisation

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

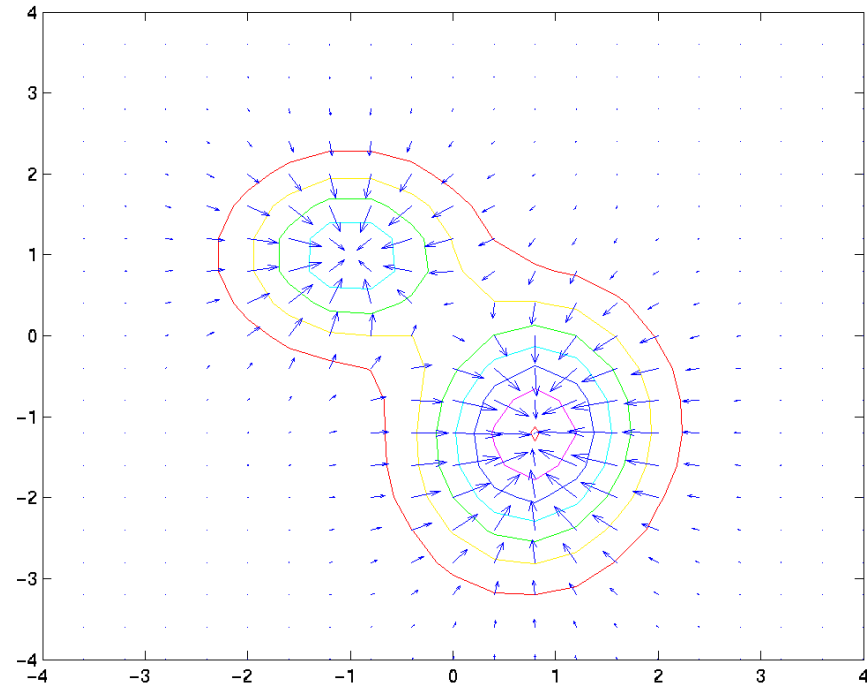
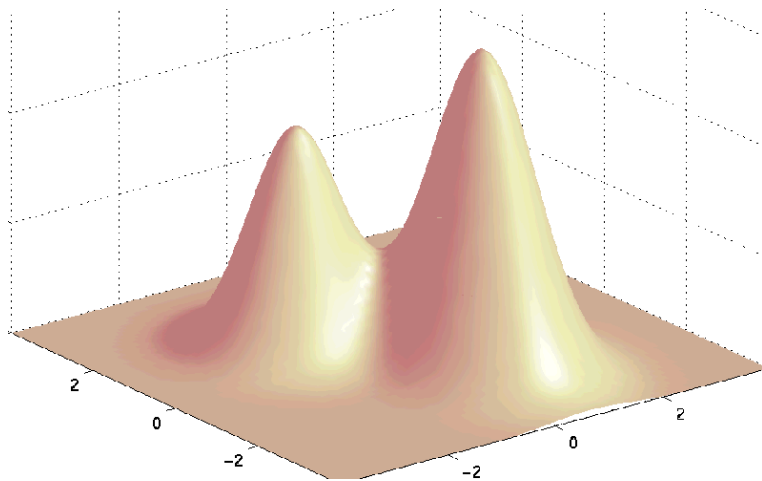
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- For a simple function $L(\mathbf{w}|\mathcal{D})$ we can solve $\nabla L(\mathbf{w}|\mathcal{D}) = \mathbf{0}$ explicitly. E.g. the linear perceptron
- For a non-linear functions we usually can't solve this set of simultaneous equations
- We can find a maximum or minimum **iteratively**
- If we know the gradient then we can follow the gradient
 - ★ Maximisation: $\mathbf{w} \rightarrow \mathbf{w}' = \mathbf{w} + r \nabla L(\mathbf{w}|\mathcal{D})$
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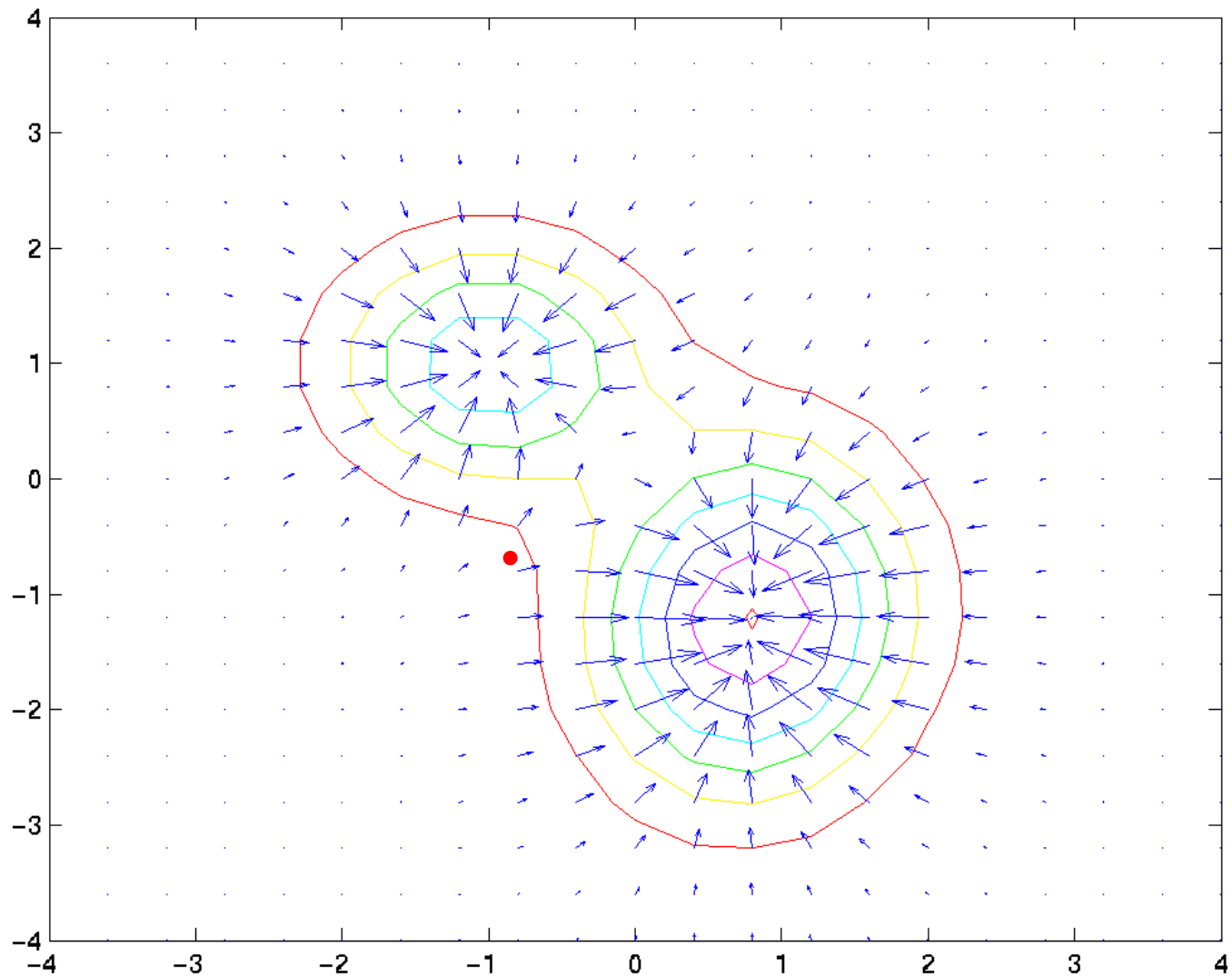
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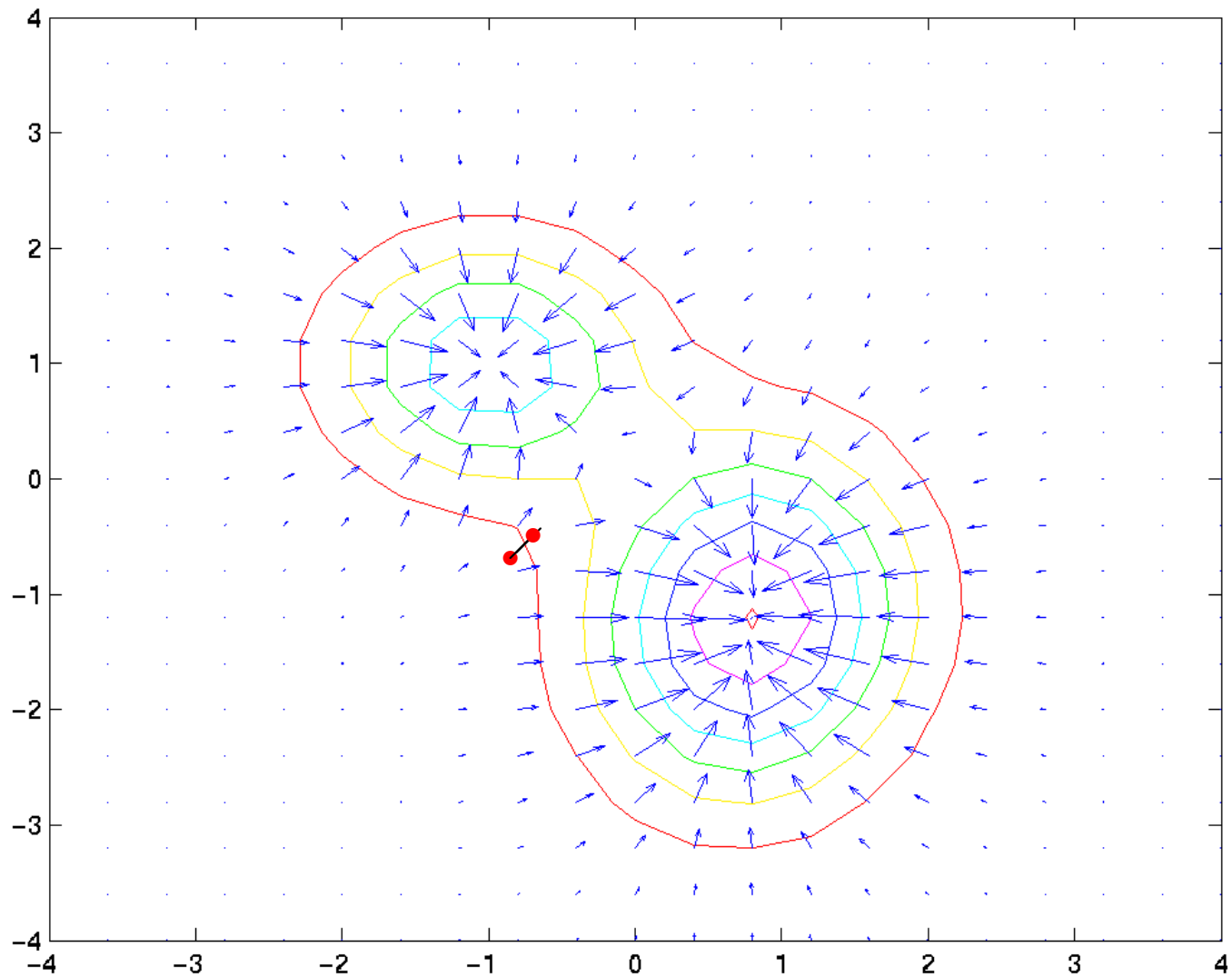
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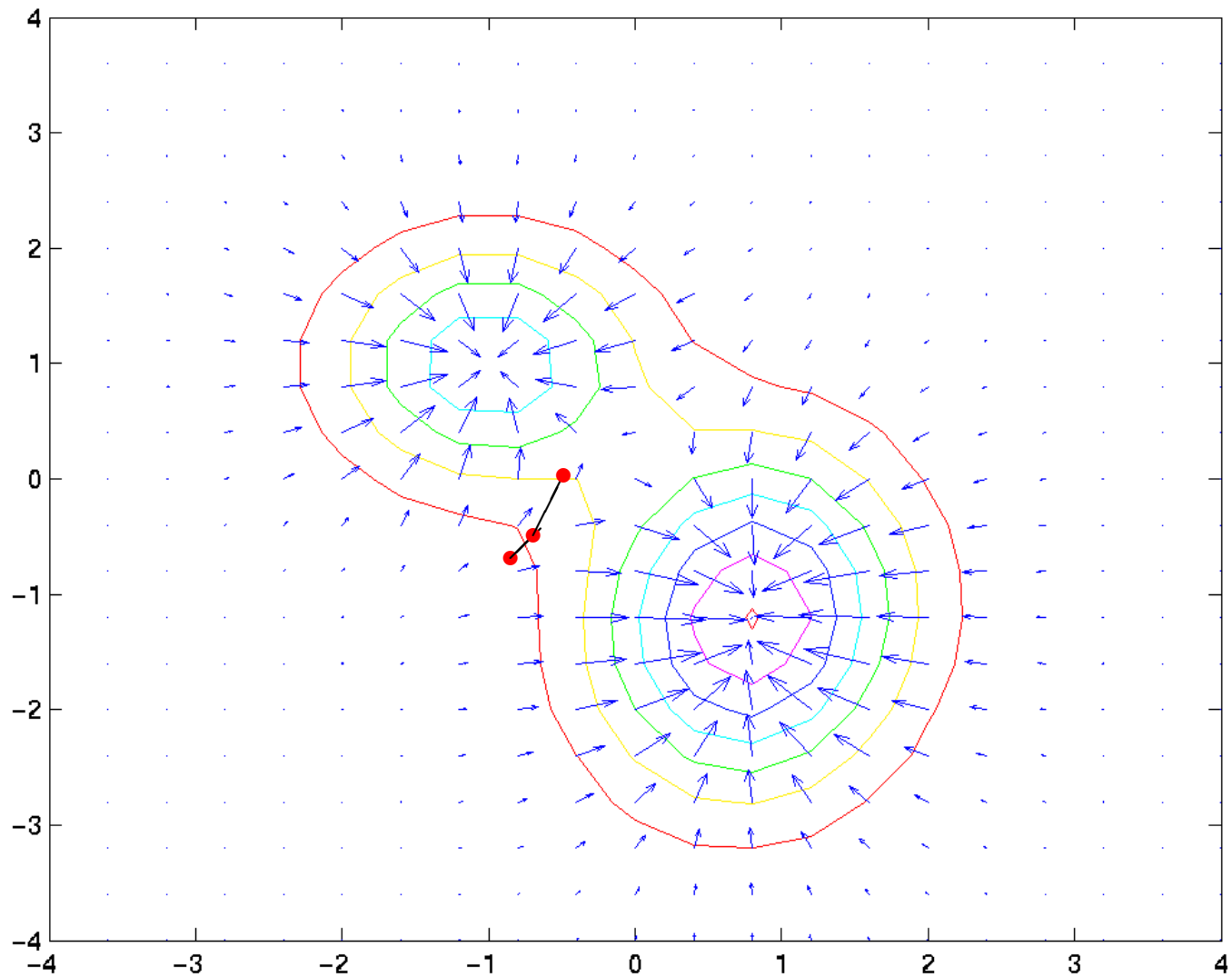
Hill-Climbing



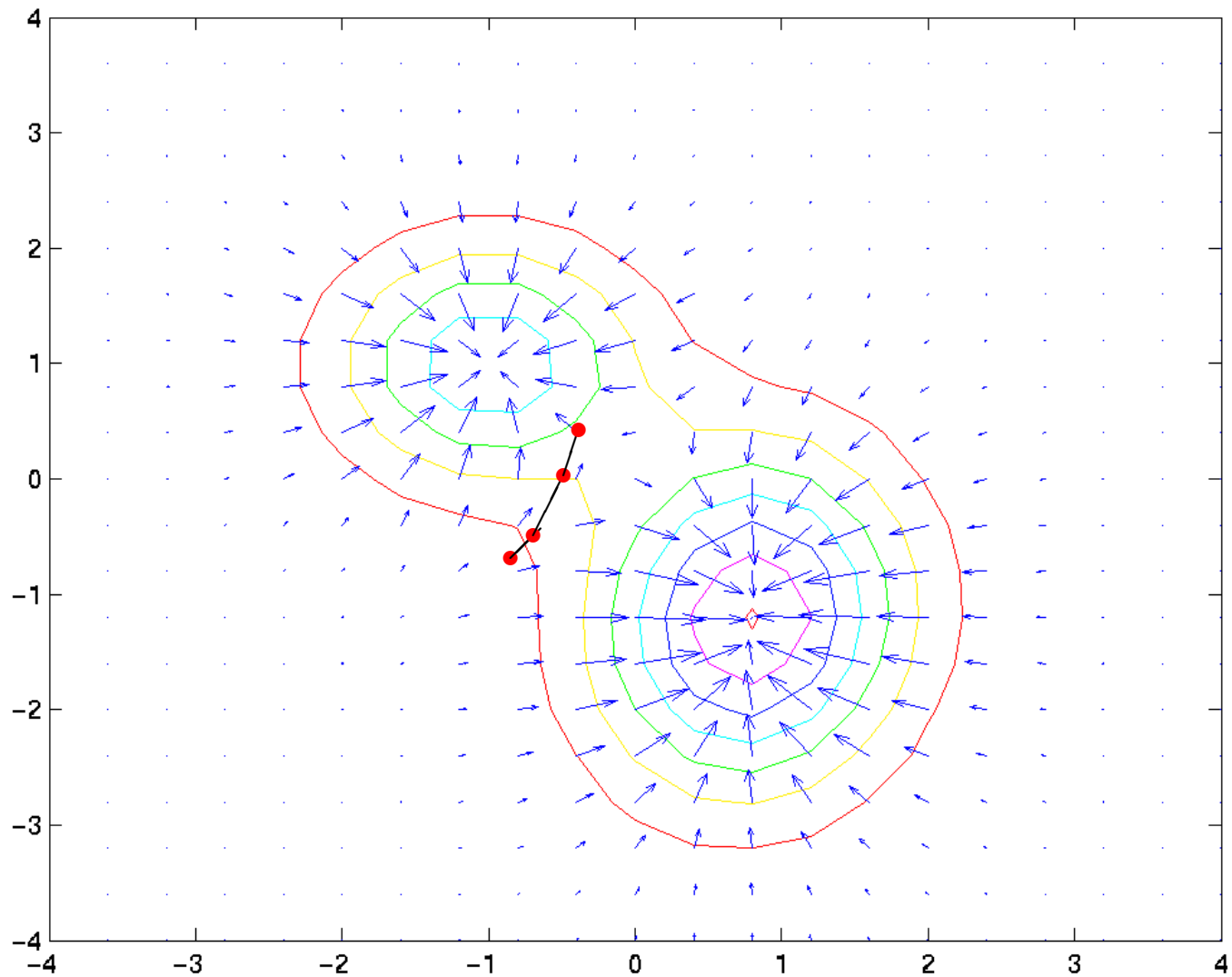
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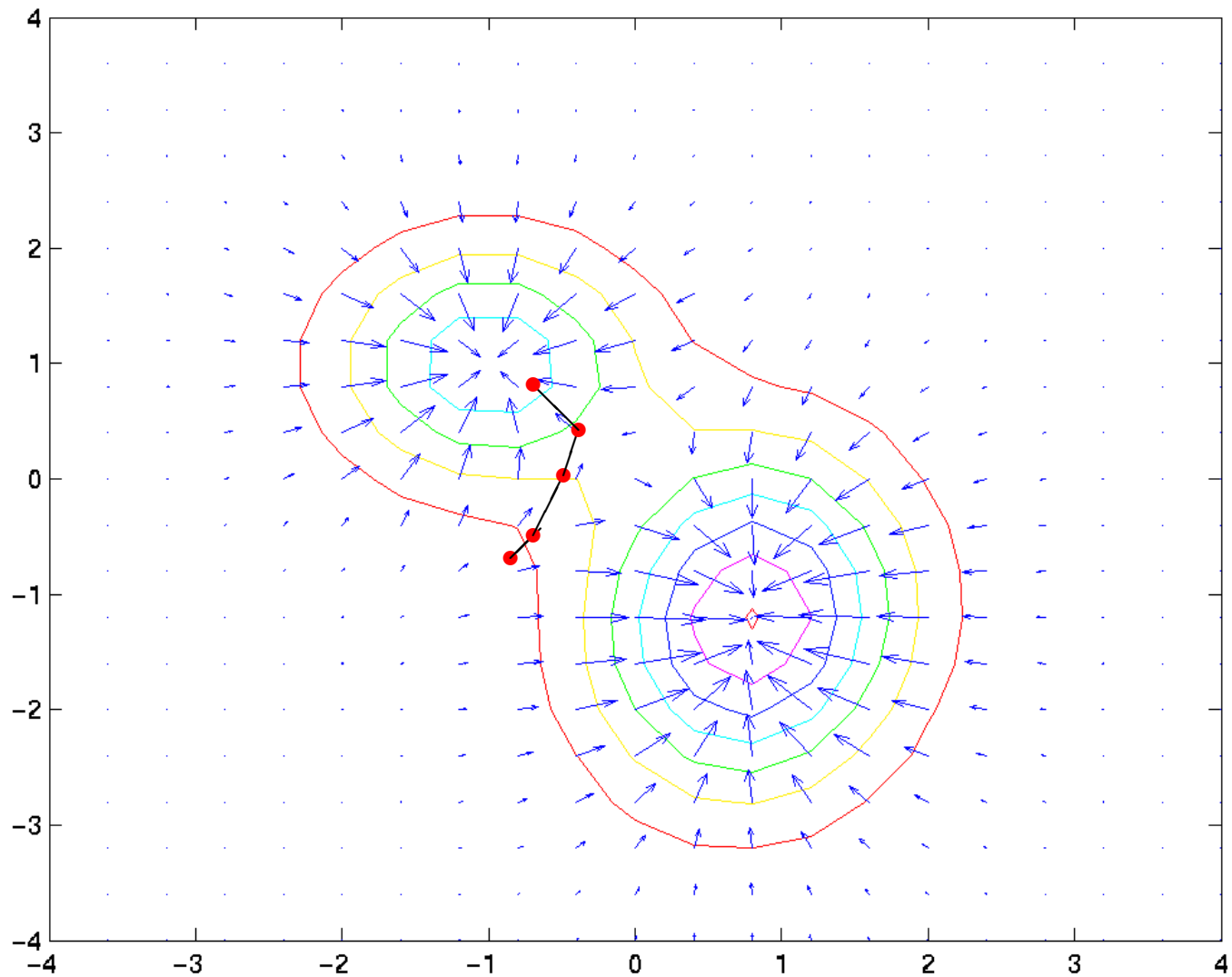
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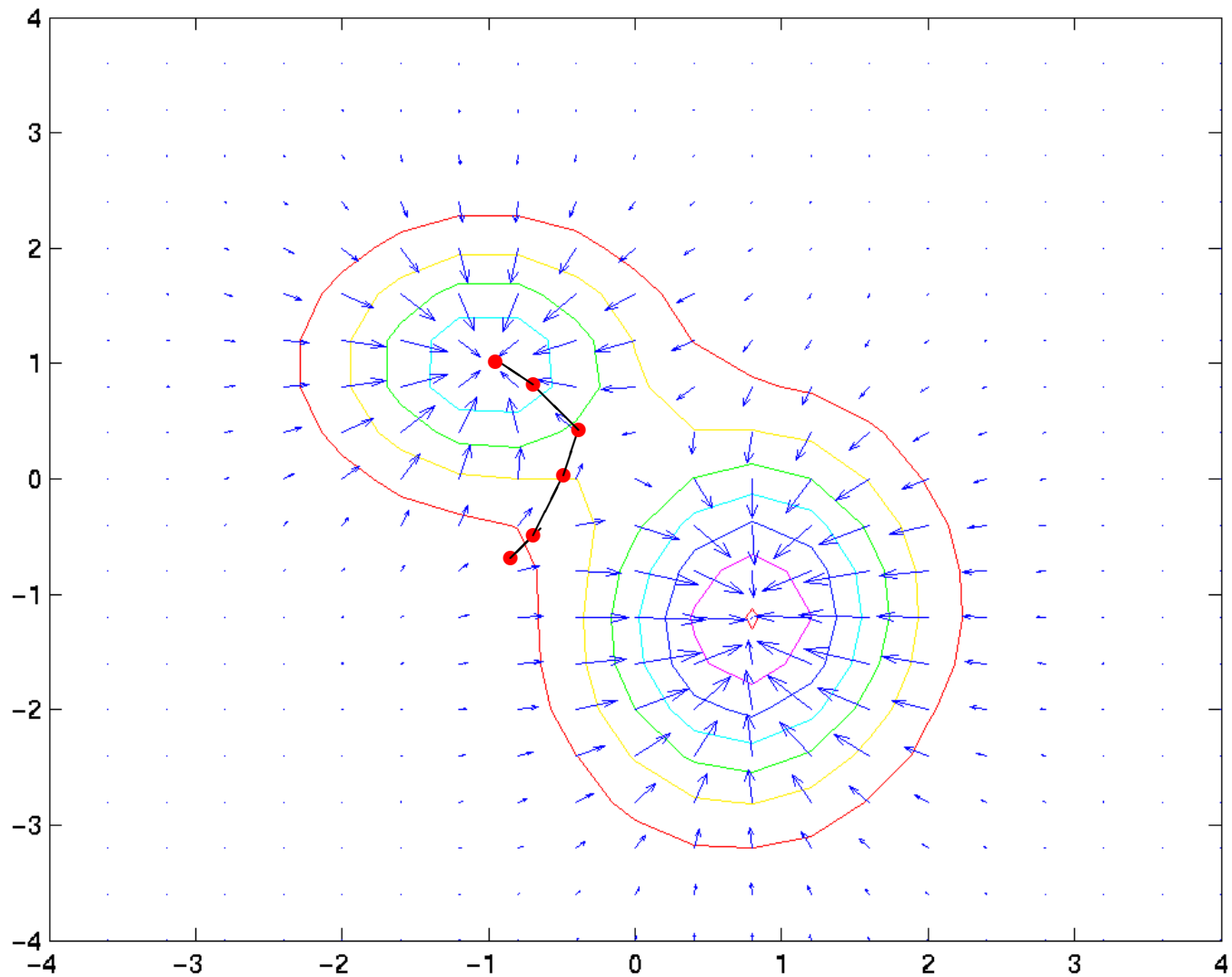
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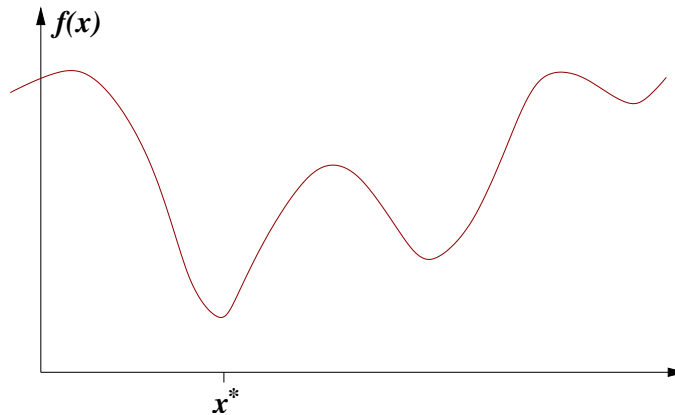


Hill-Climbing



What Goes Right

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



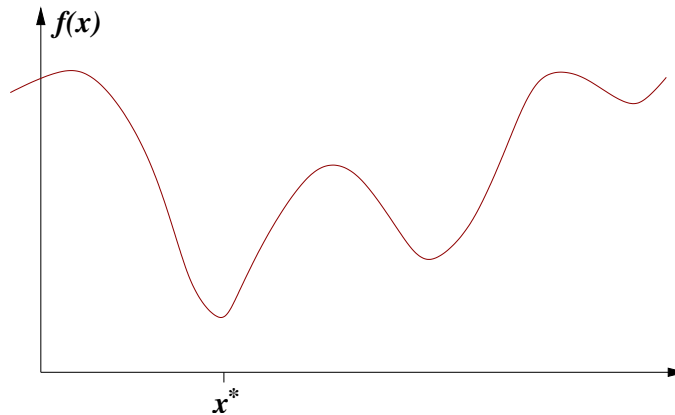
- Taylor expanding around a minimum x^*

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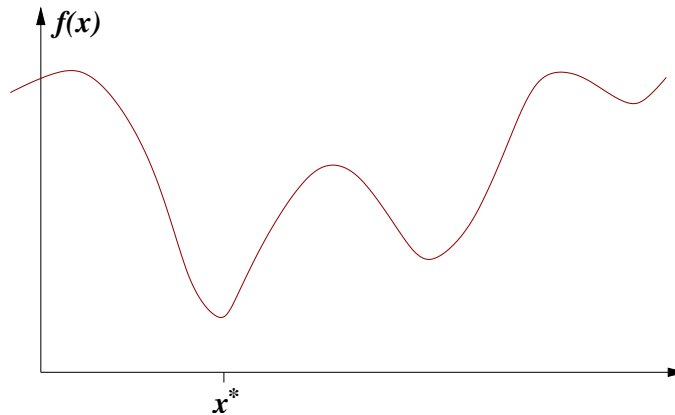
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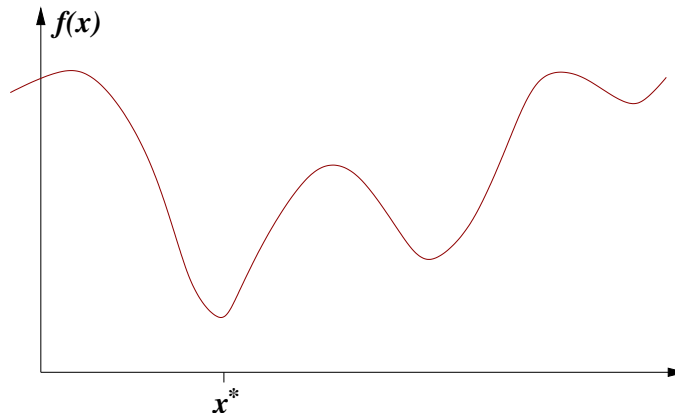
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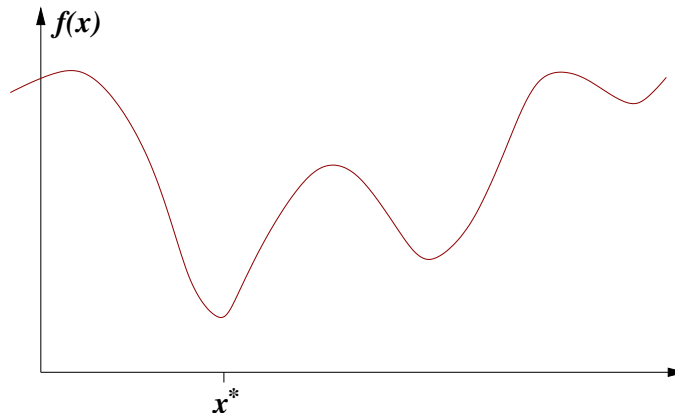
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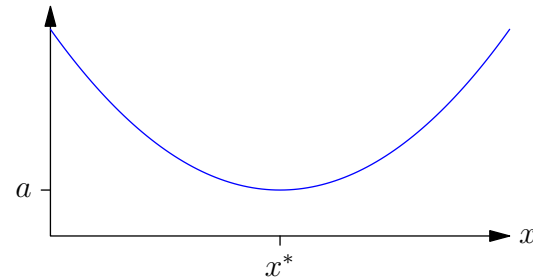
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Newton's Method

- If we were in a quadratic minimum

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



- then

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

- so

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

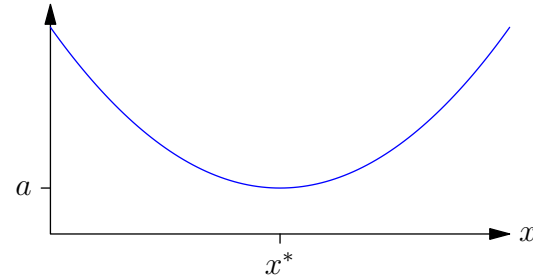
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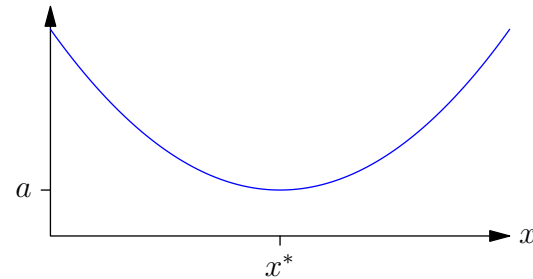
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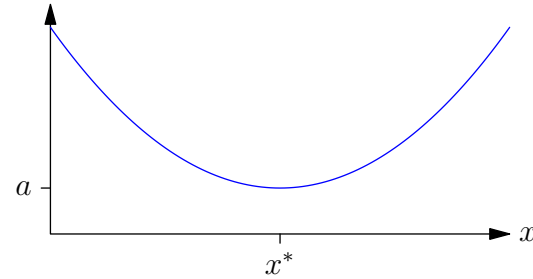
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Taylor's Expansion in High Dimensions

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

$$f(\mathbf{x}) = f(\mathbf{x}_0) + (\mathbf{x} - \mathbf{x}_0)^\top \nabla f(\mathbf{x}_0) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^\top \mathbf{H}(\mathbf{x} - \mathbf{x}_0) + \dots$$

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

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$$\mathbf{x}^* = \mathbf{x} - \mathbf{H}^{-1} \nabla f(\mathbf{x})$$

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$$f(\mathbf{x}) = f(\mathbf{x}_0) + (\mathbf{x} - \mathbf{x}_0)^\top \nabla f(\mathbf{x}_0) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^\top \mathbf{H}(\mathbf{x} - \mathbf{x}_0) + \dots$$

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

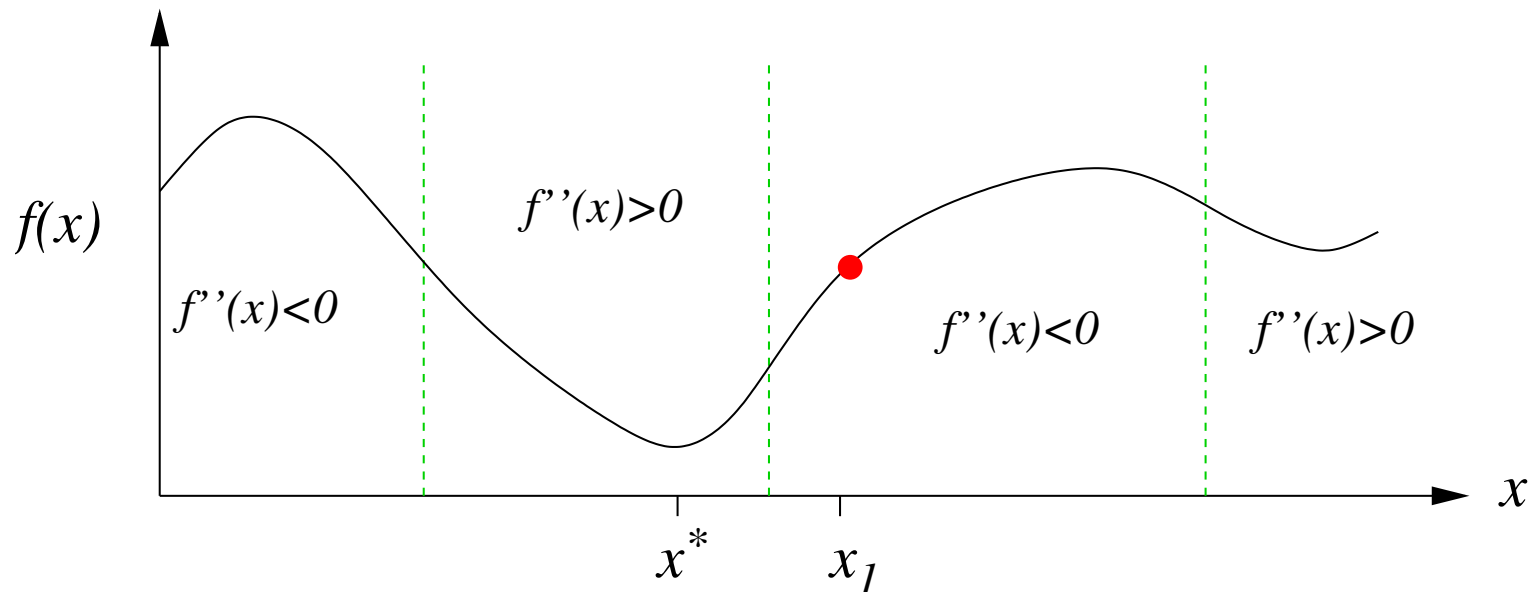
$$H_{ij} = \frac{\partial^2 f(\mathbf{x}_0)}{\partial x_i \partial x_j}$$

- Newton's method in high dimension is

$$\mathbf{x}^* = \mathbf{x} - \mathbf{H}^{-1} \nabla f(\mathbf{x})$$

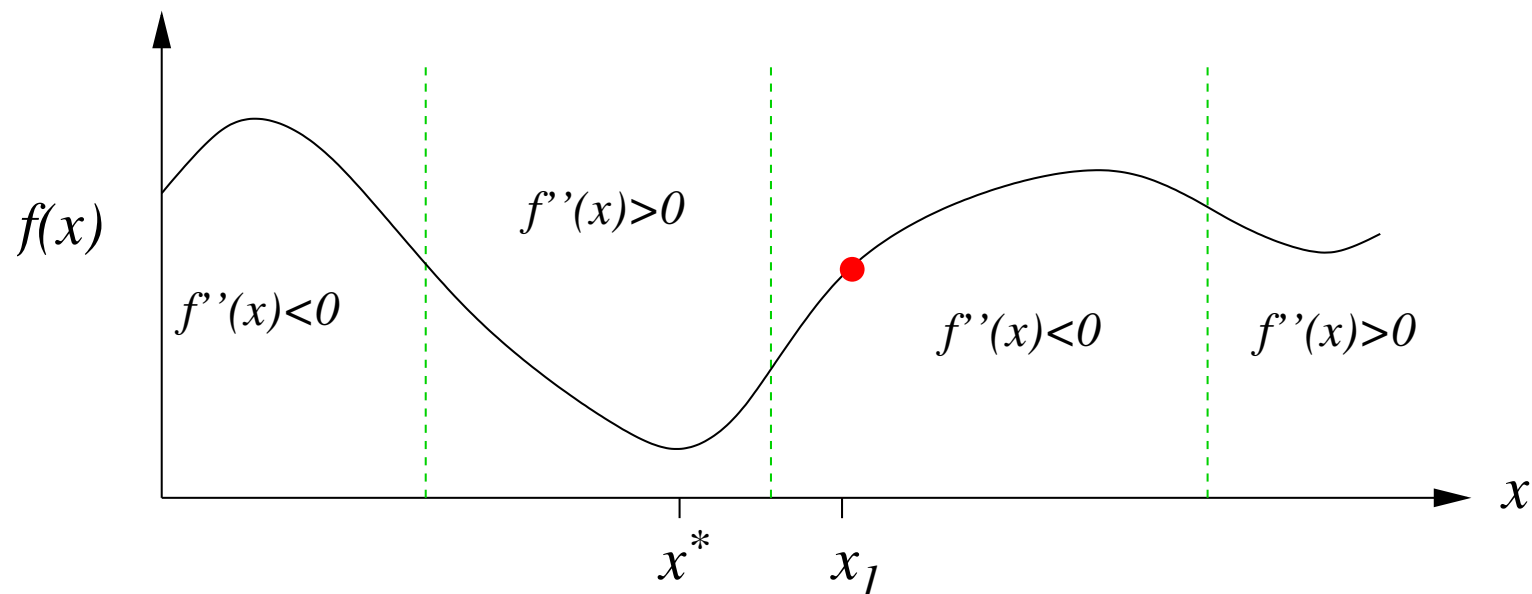
Using the Second Derivative

- 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



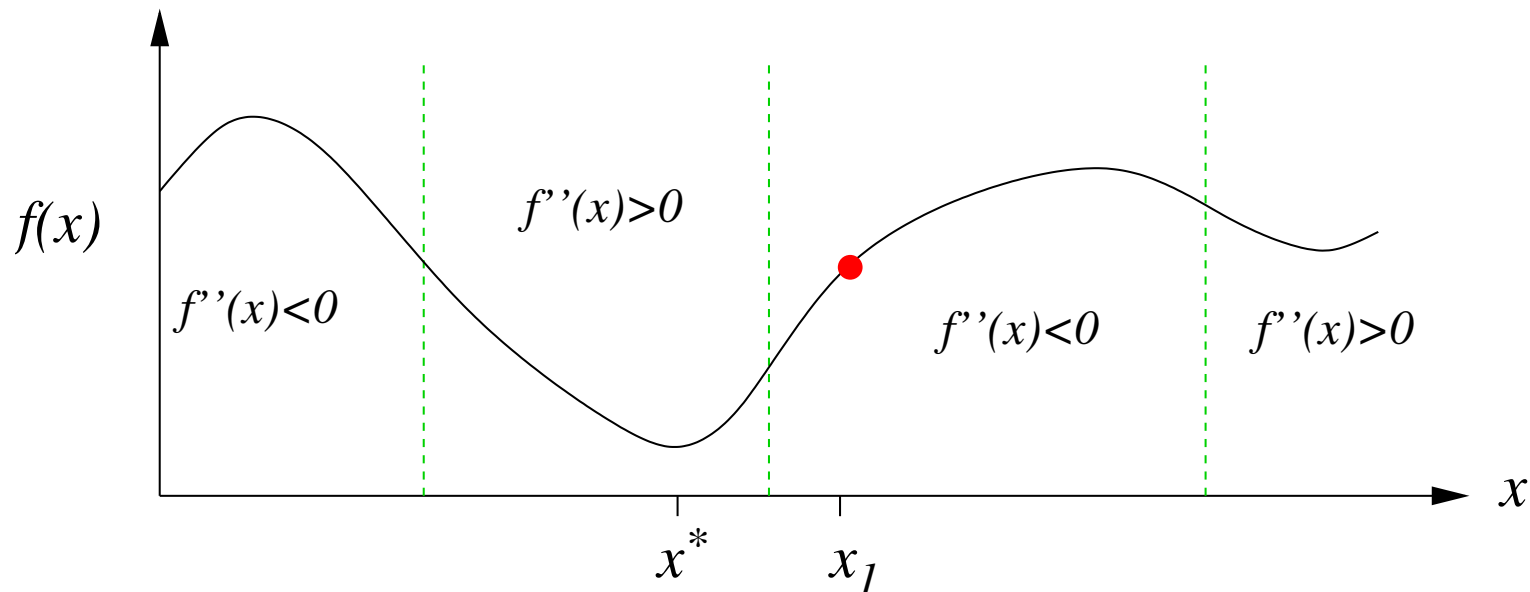
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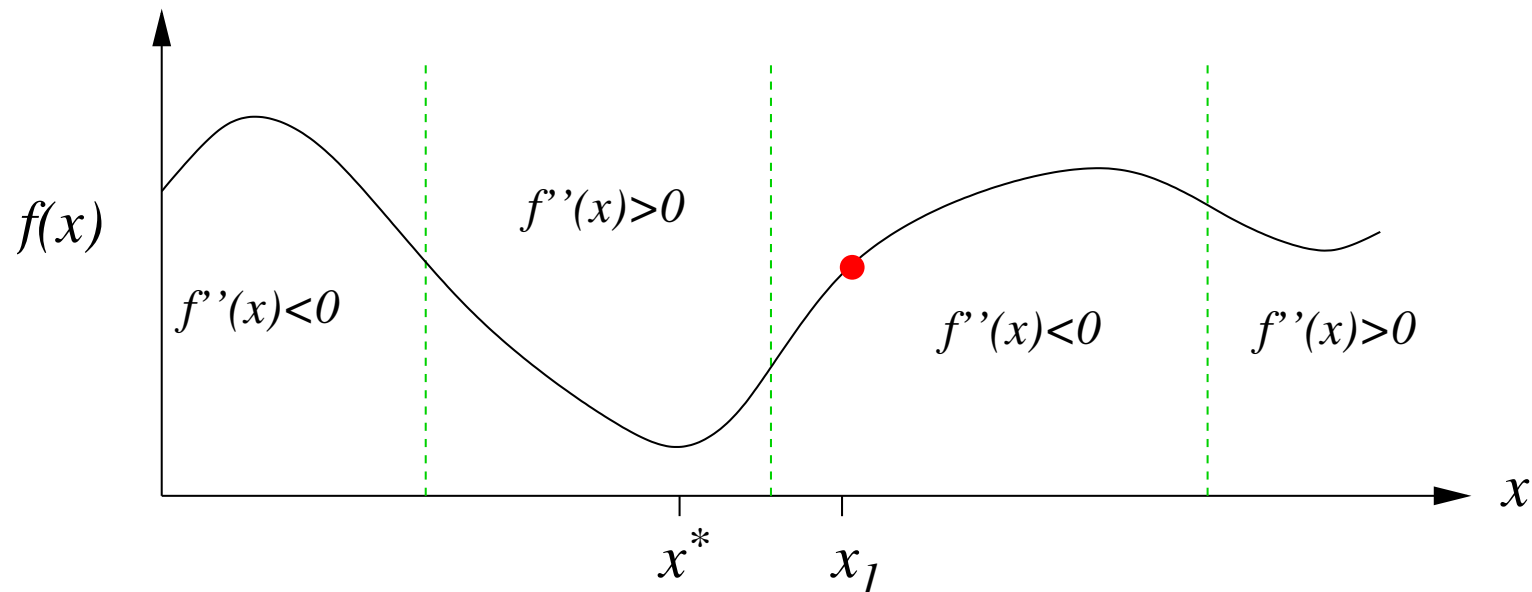
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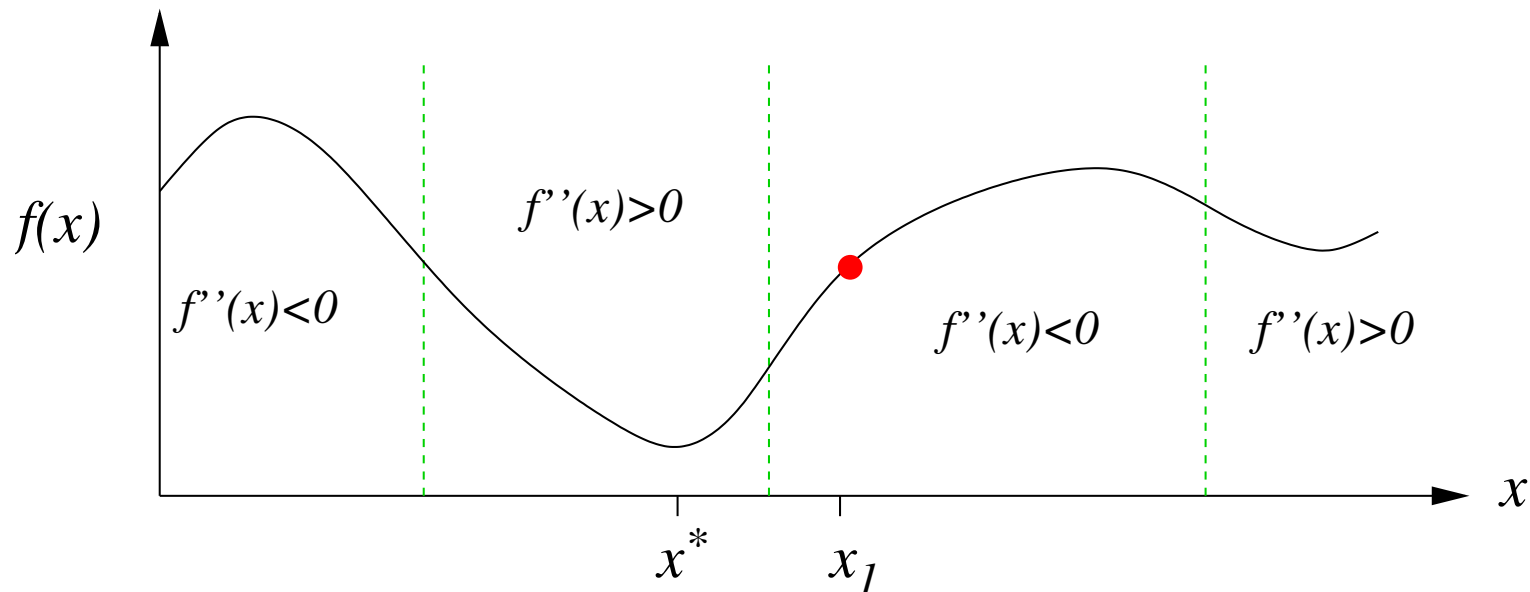
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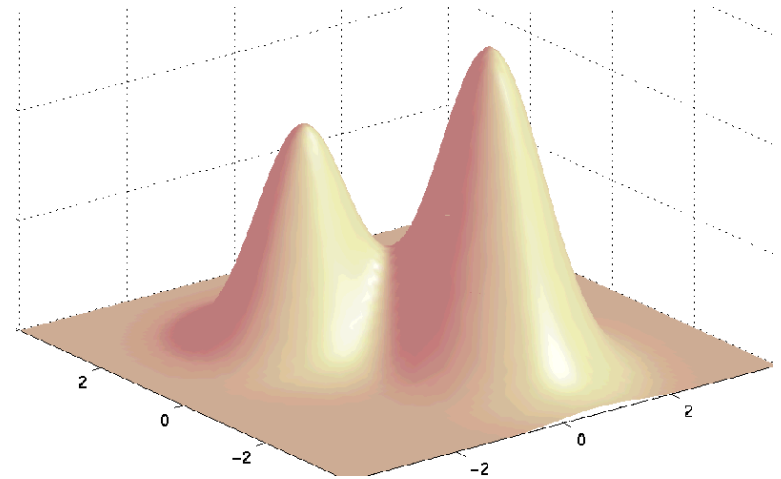
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Outline

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



Step Size

- Gradient descent

$$x' = x - r \nabla f(x)$$

- Need to choose the learning rate of step size, r
- Too small steps takes lots of time
- Too large steps takes you away from a minimum

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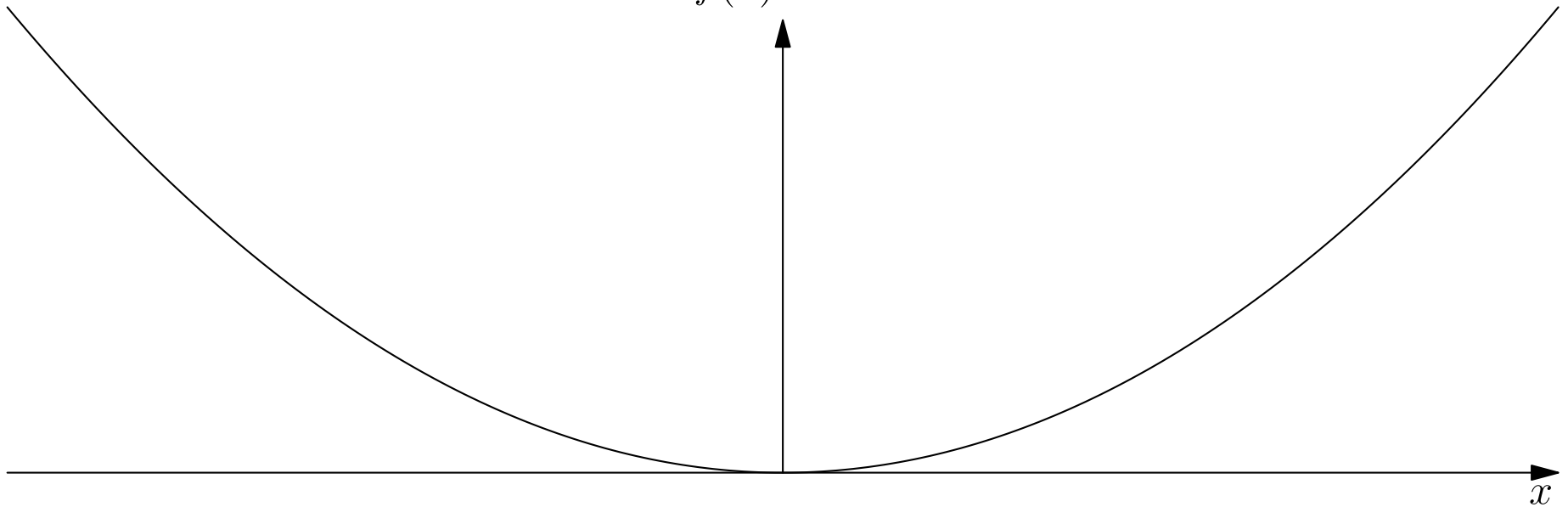
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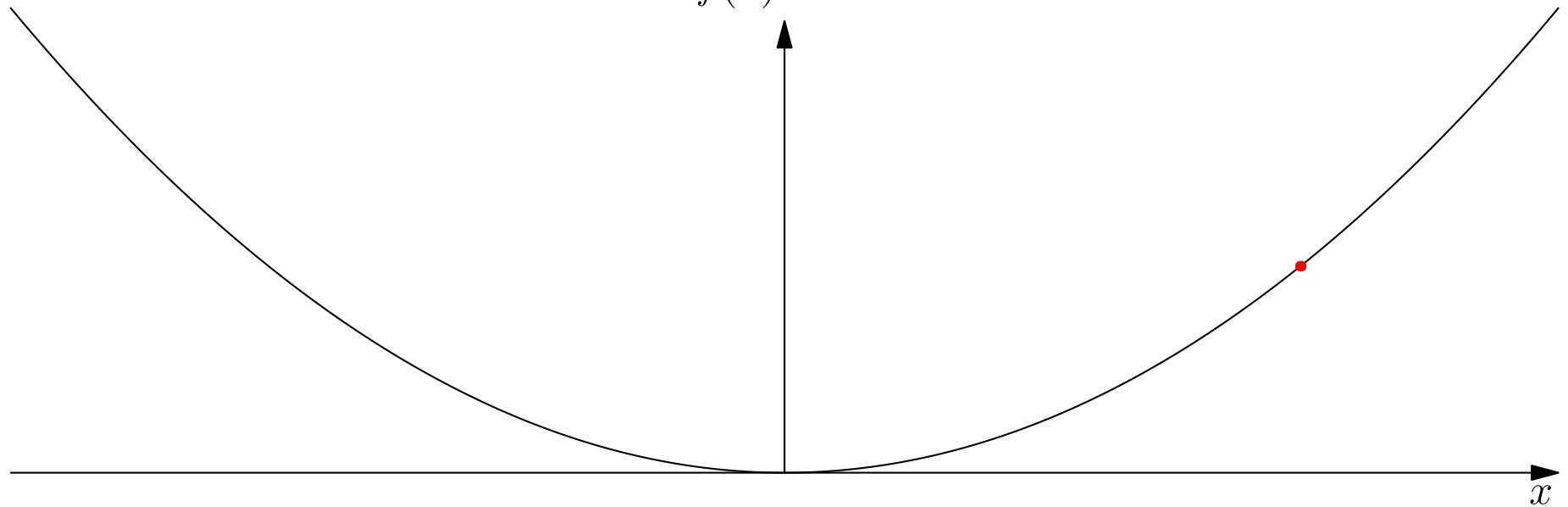
$$f(x) = x^2$$



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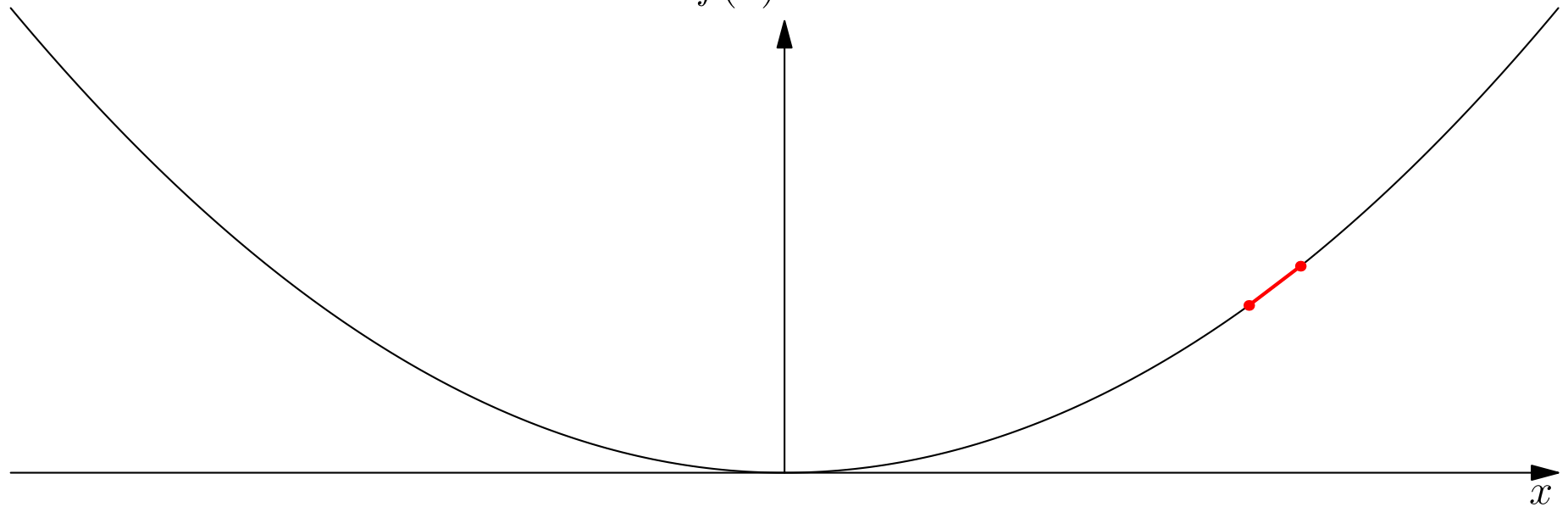


$$r = 0.05$$

Step Size

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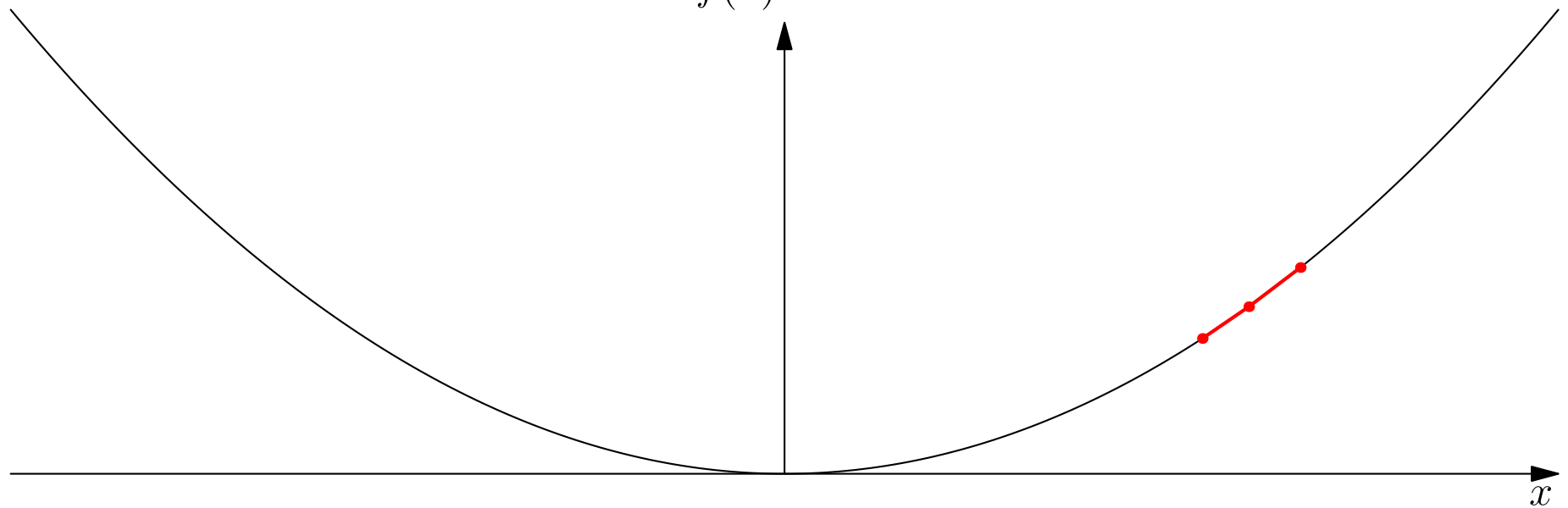


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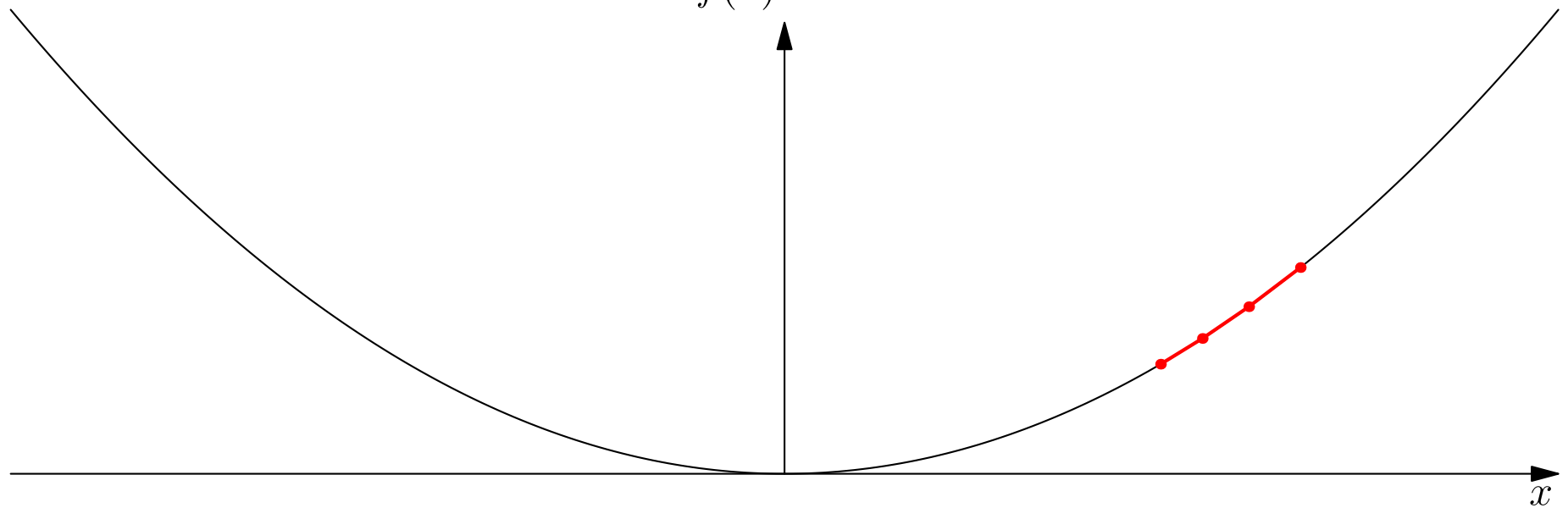


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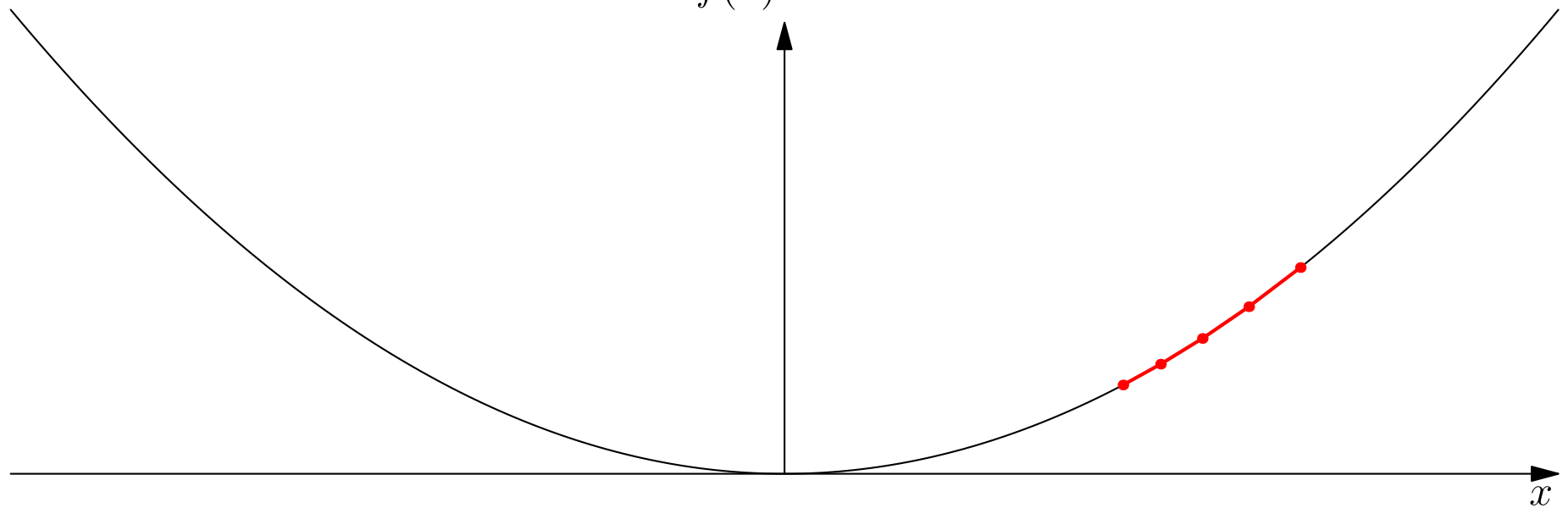


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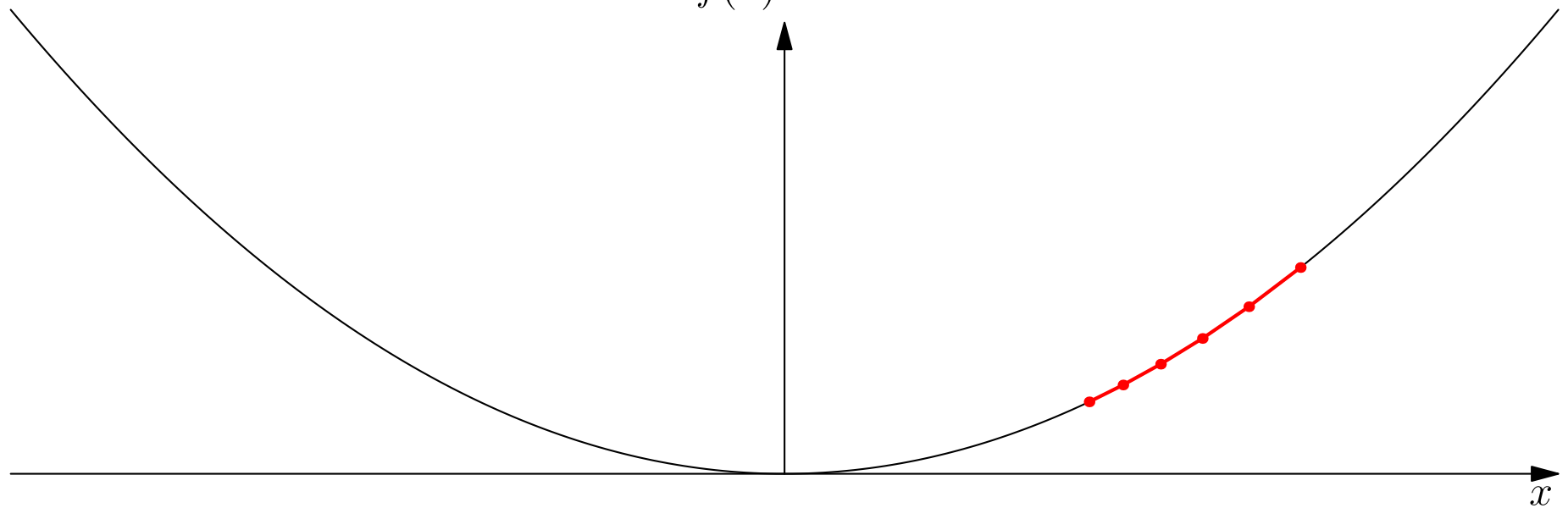


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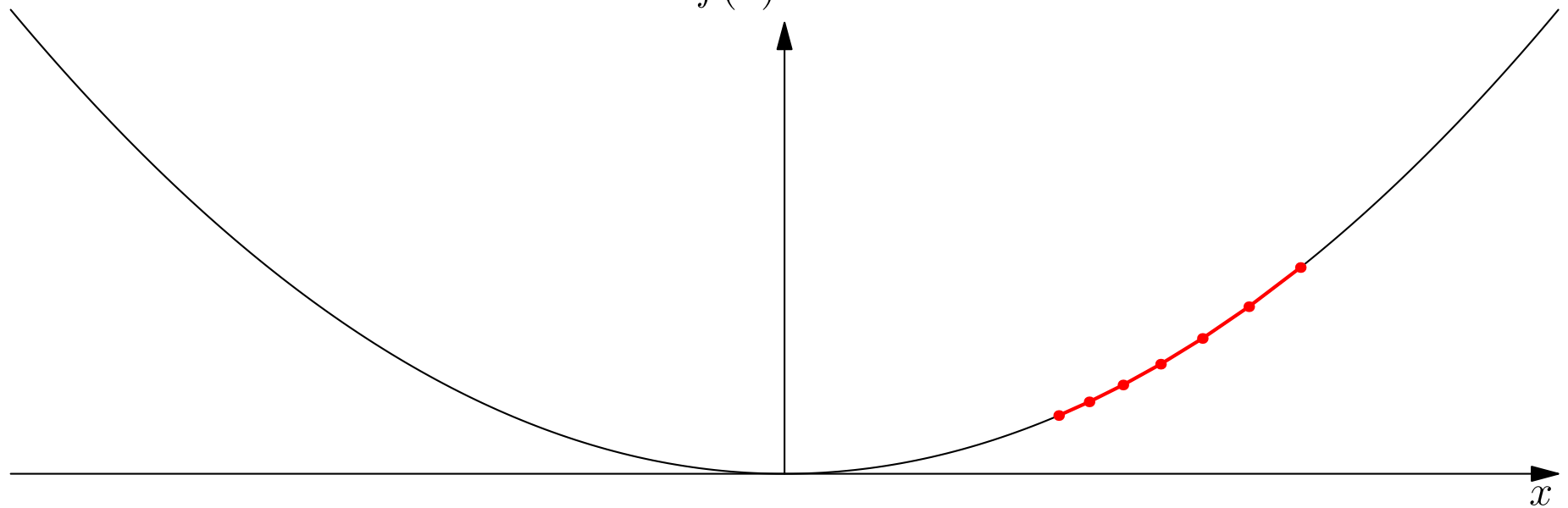


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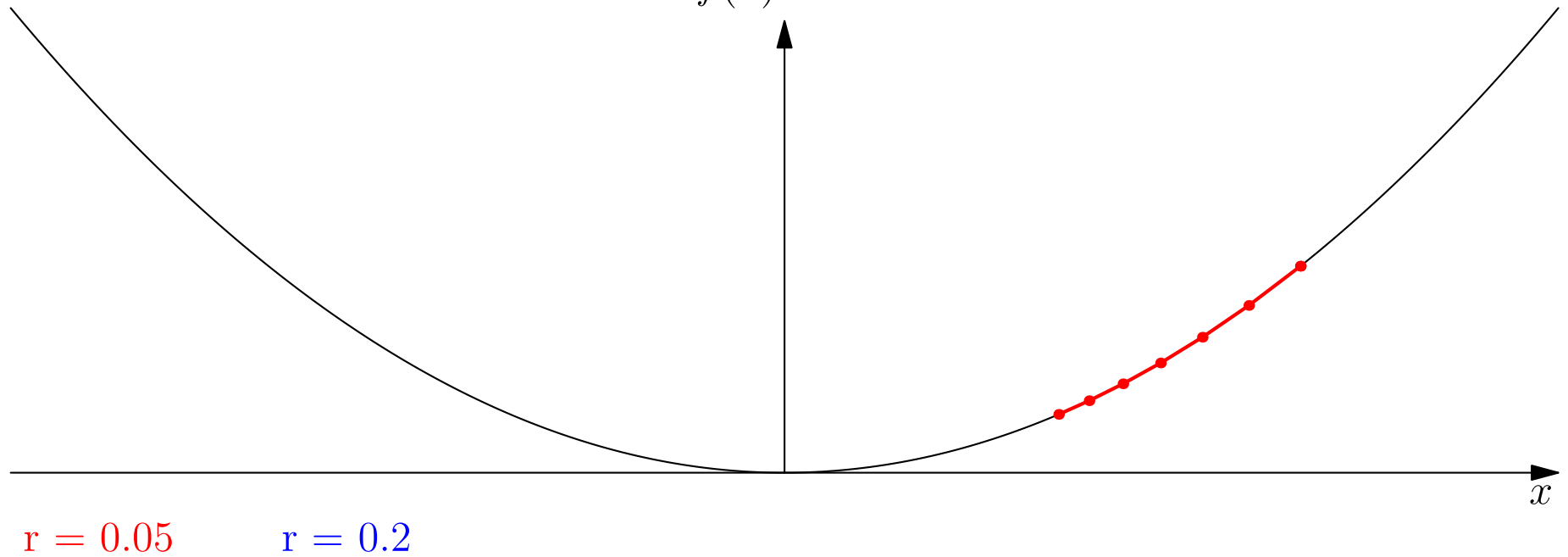


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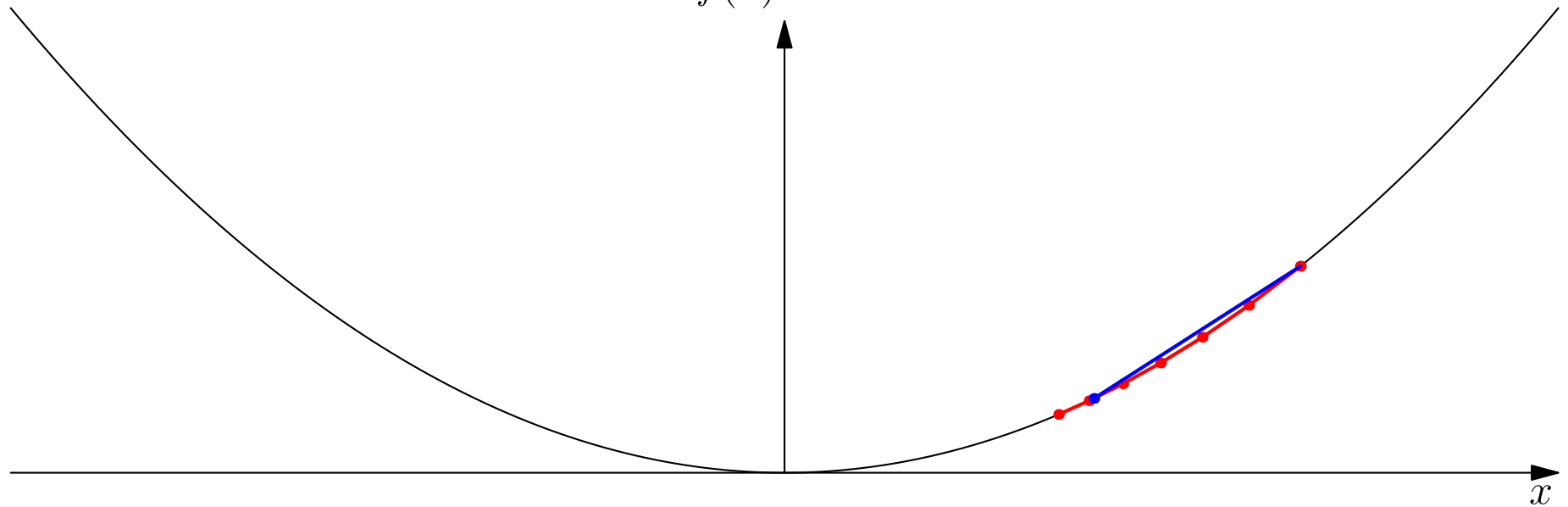
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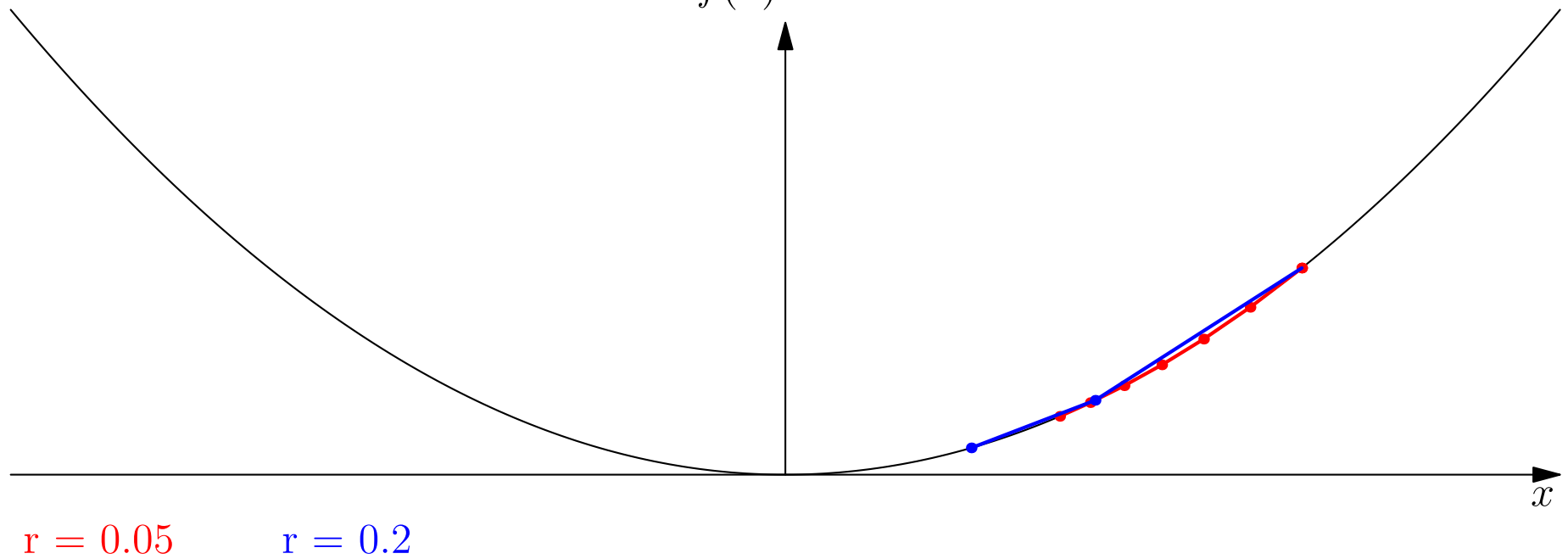
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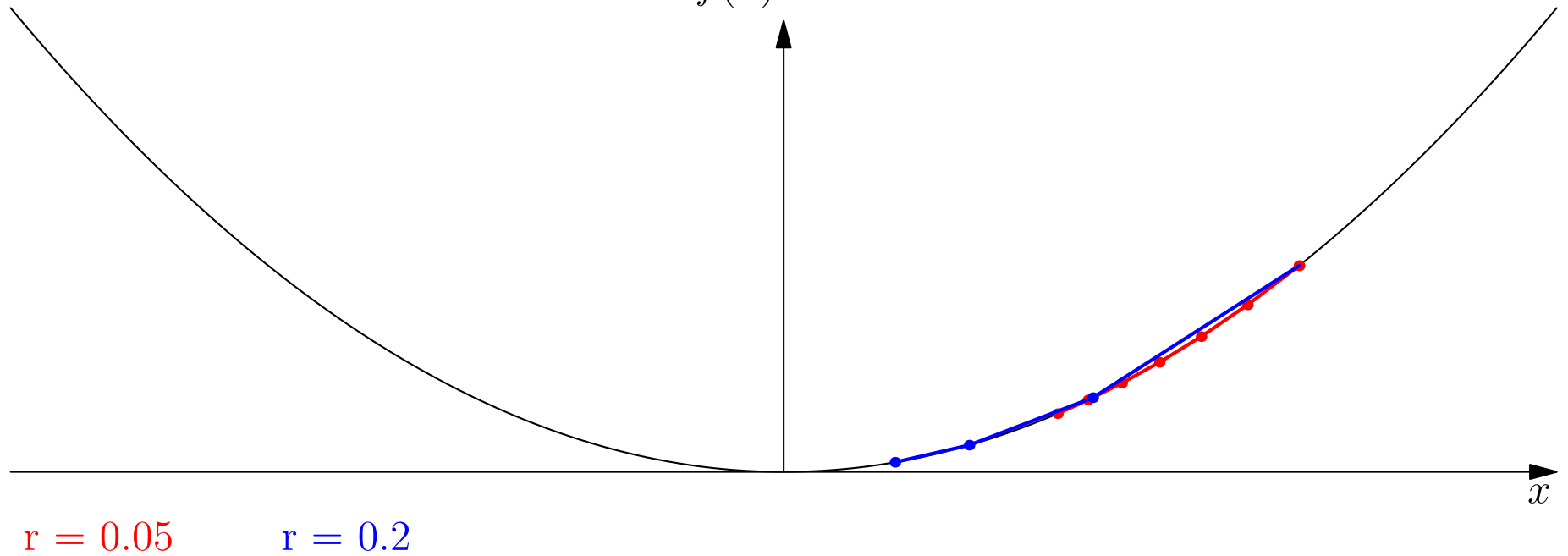
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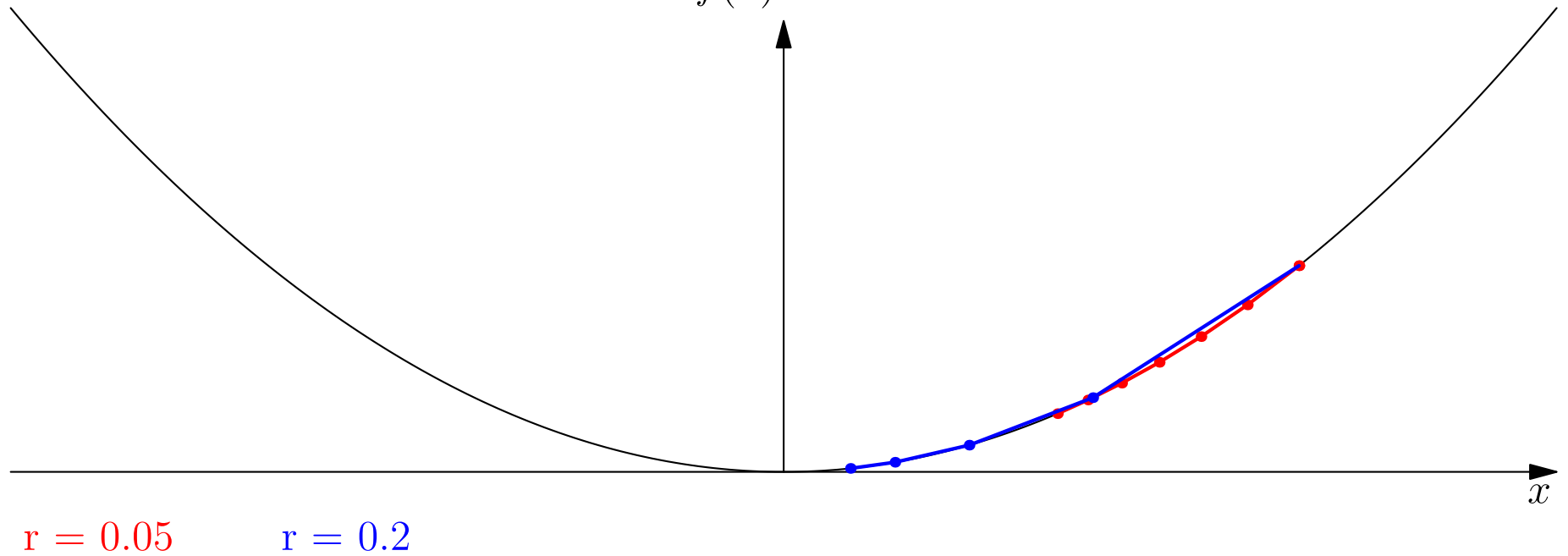
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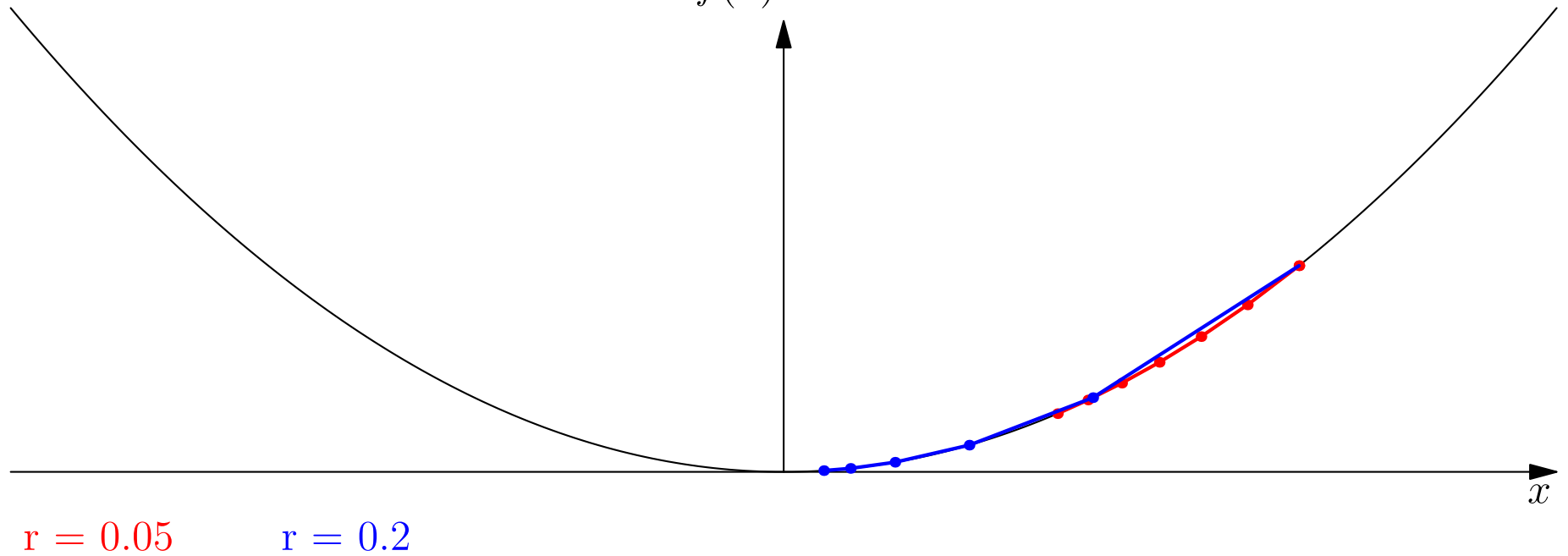
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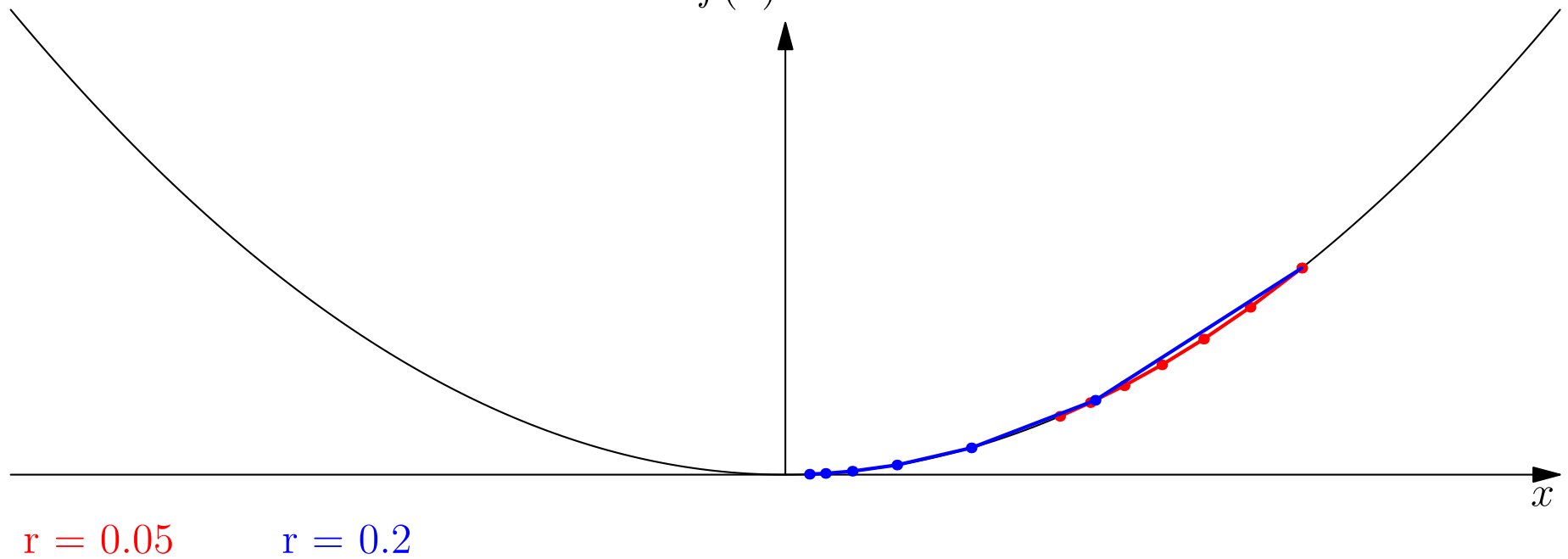
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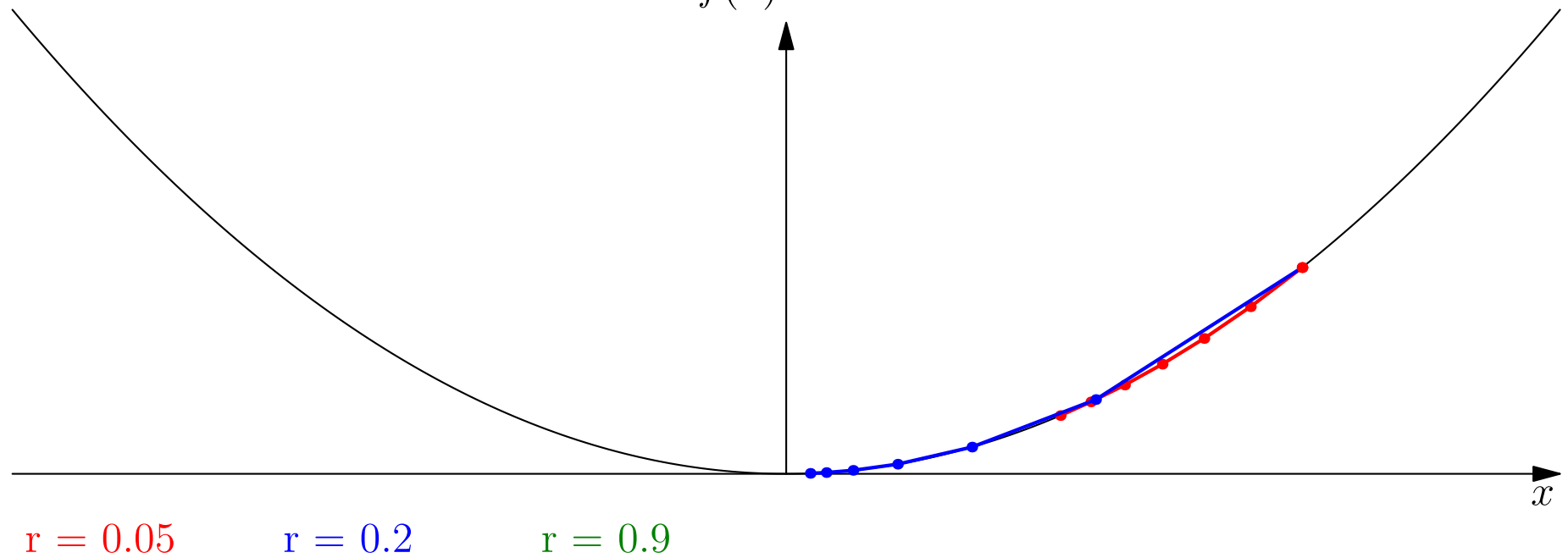
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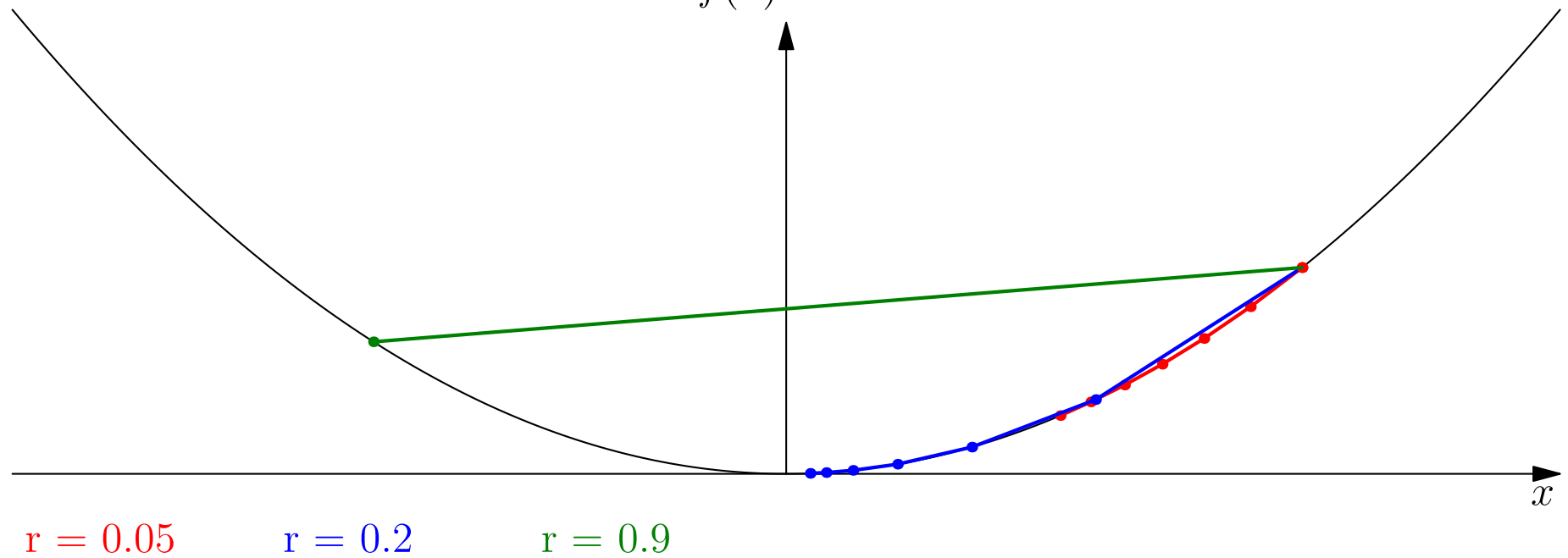
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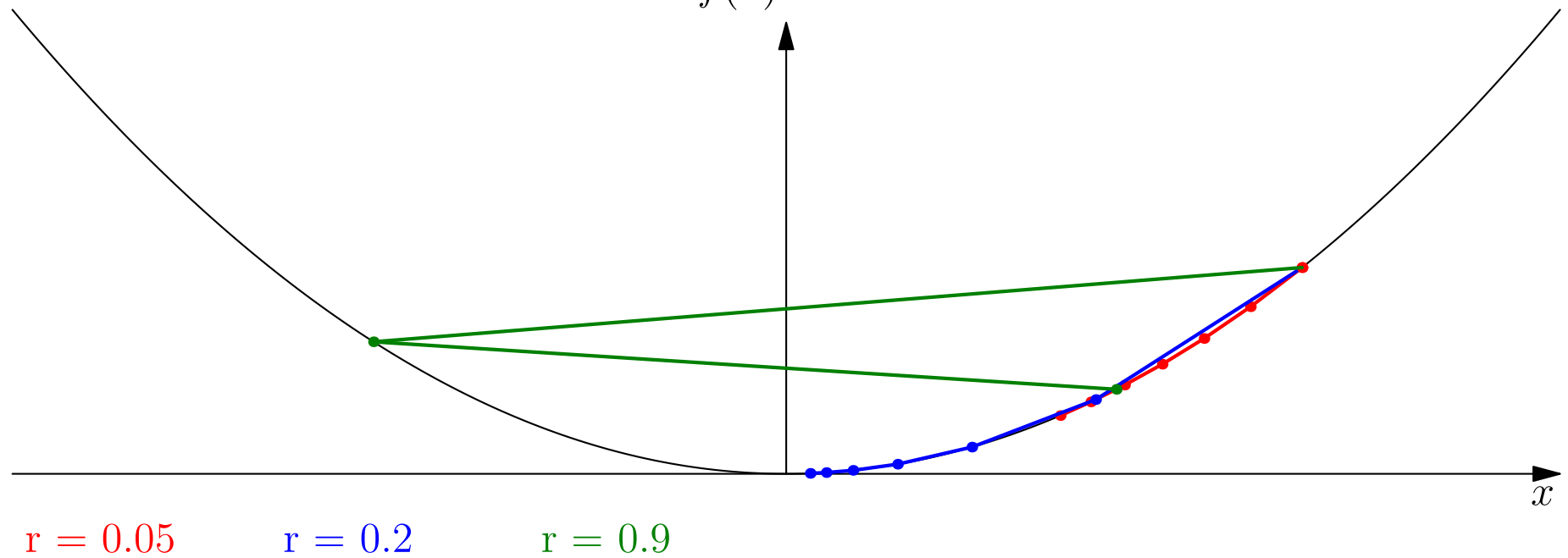
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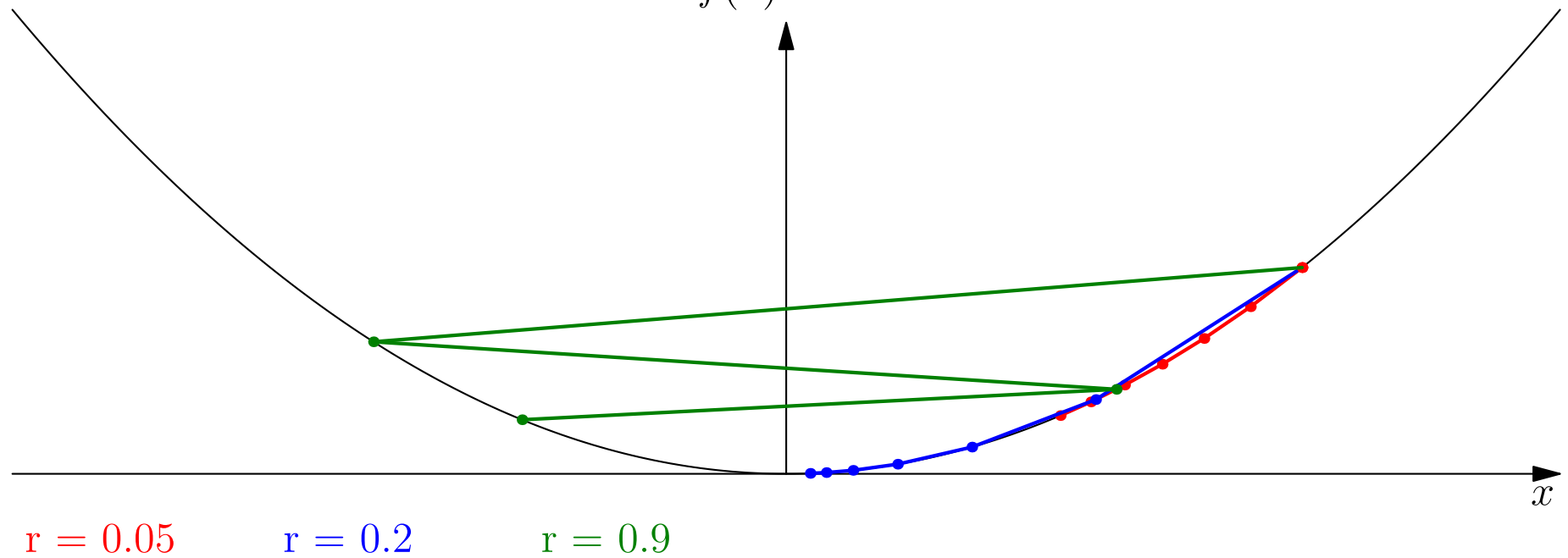
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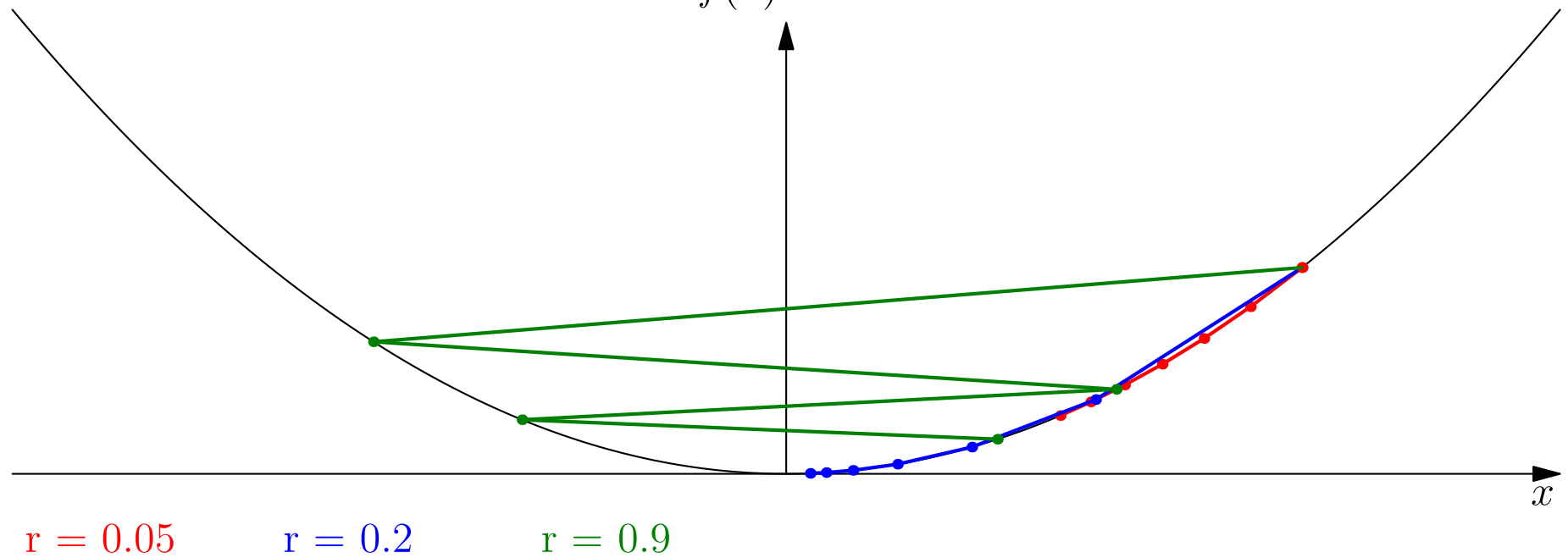
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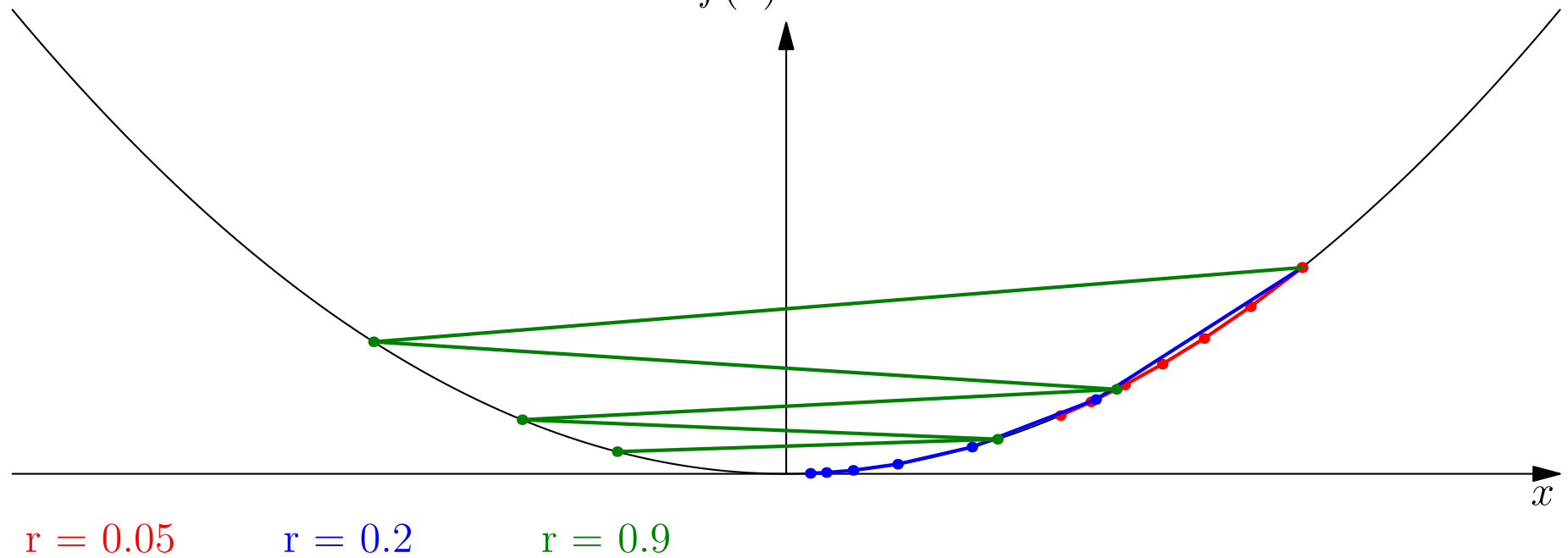
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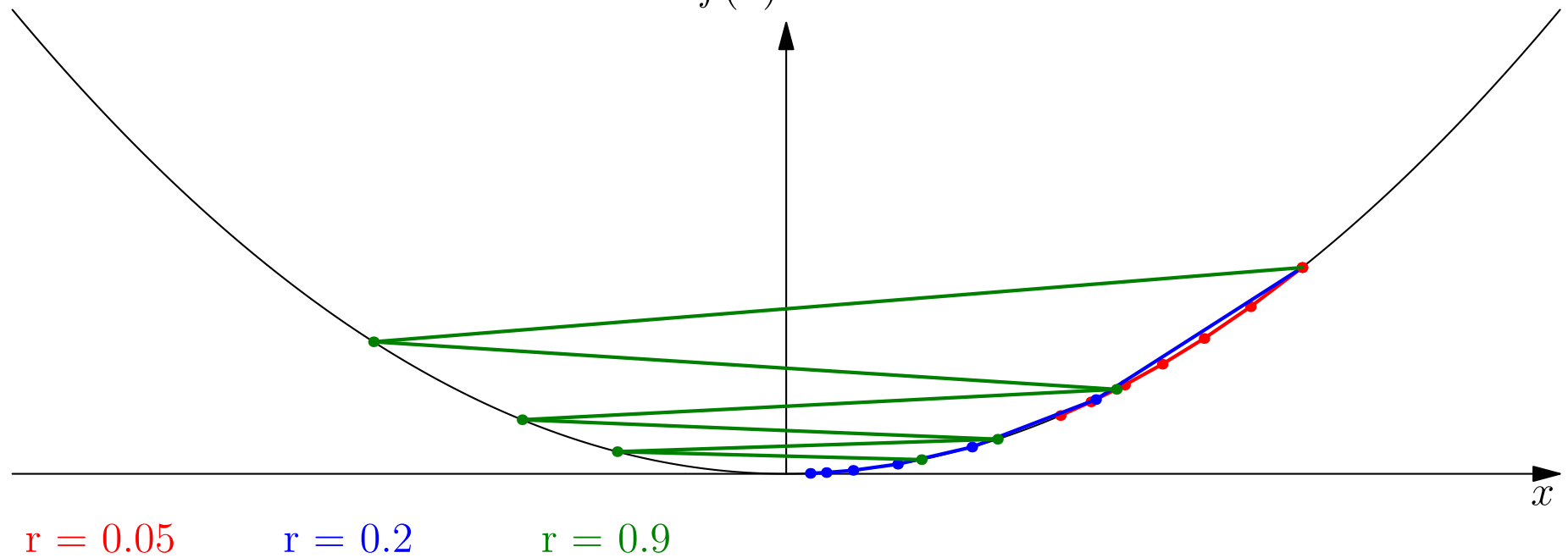
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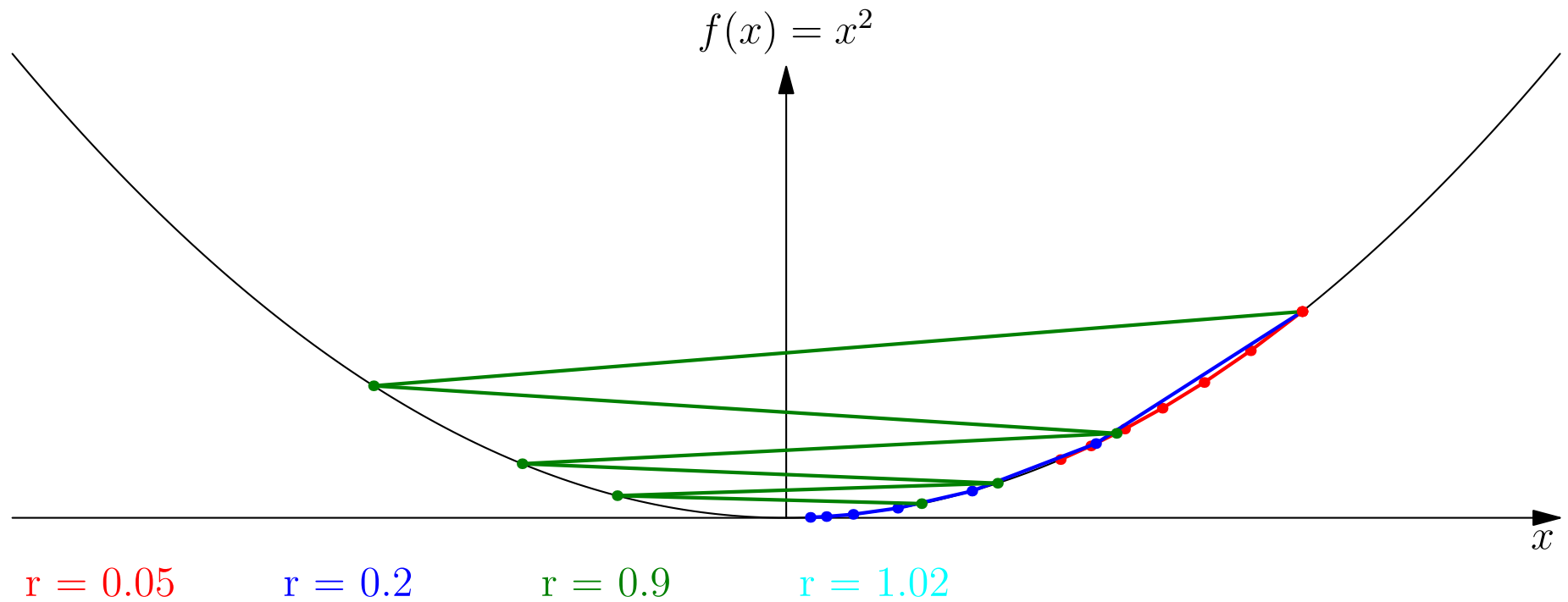
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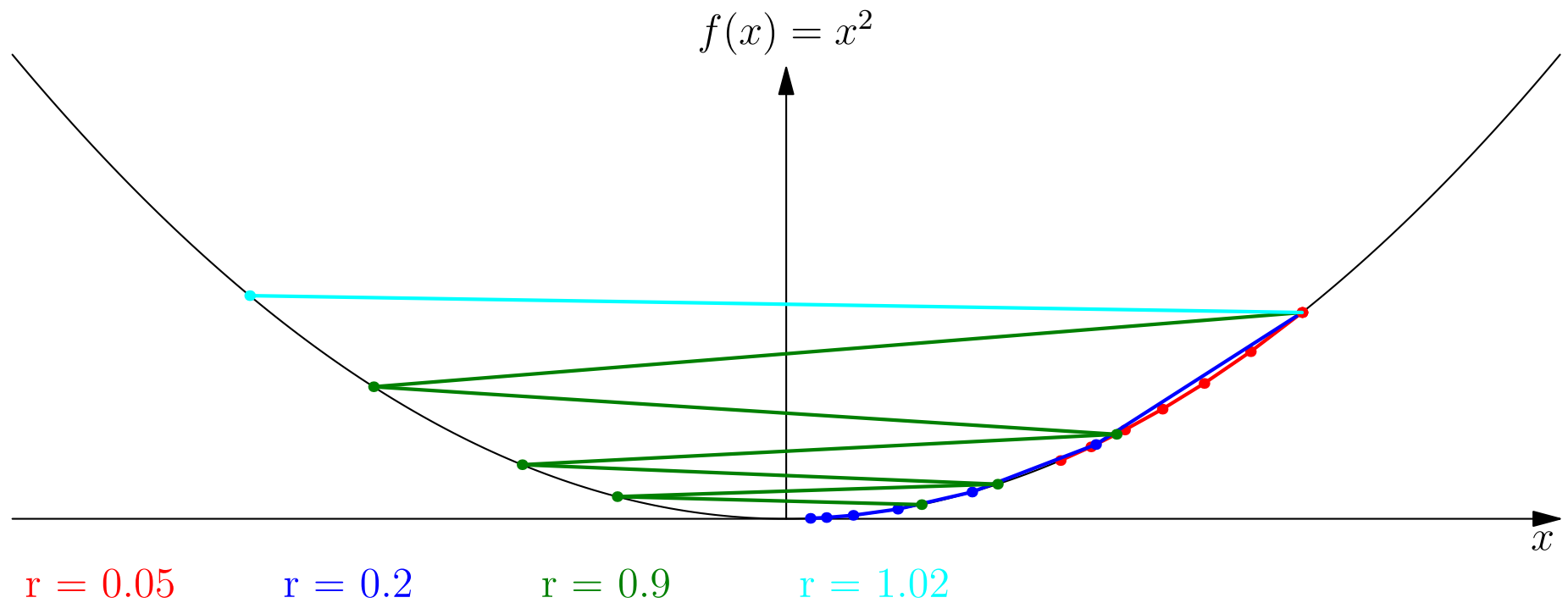
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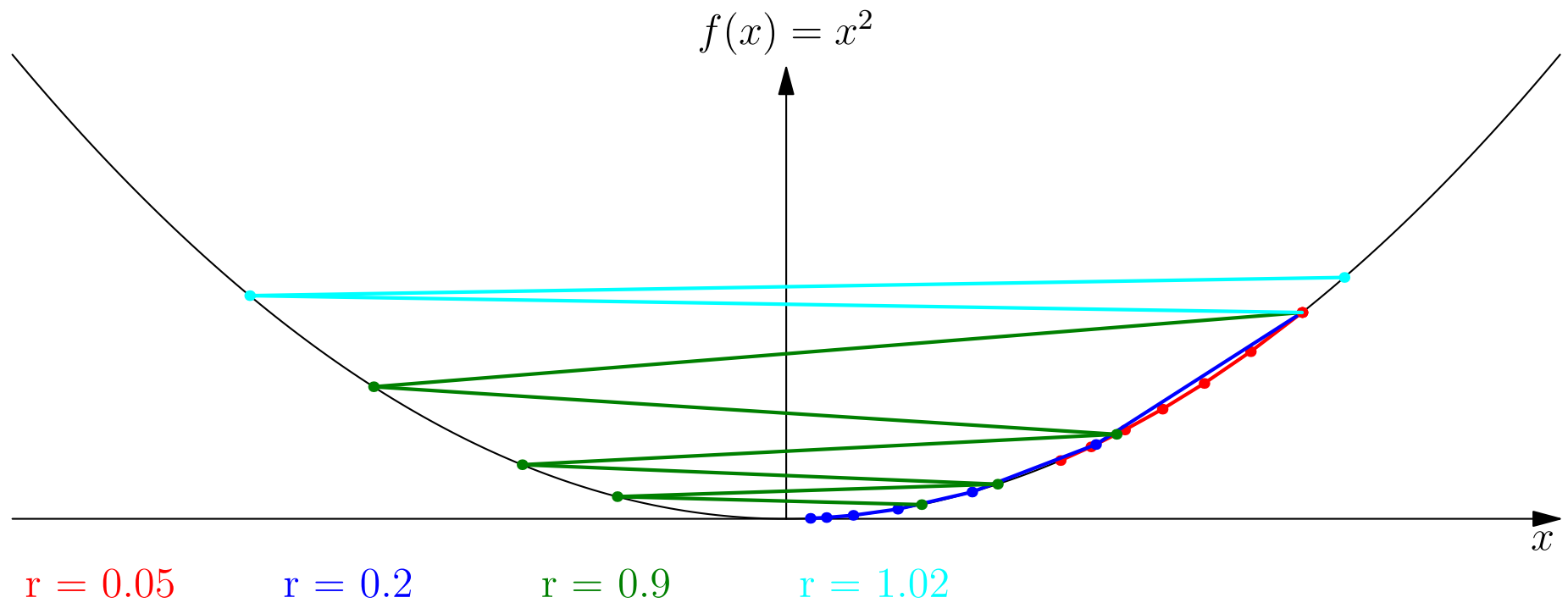
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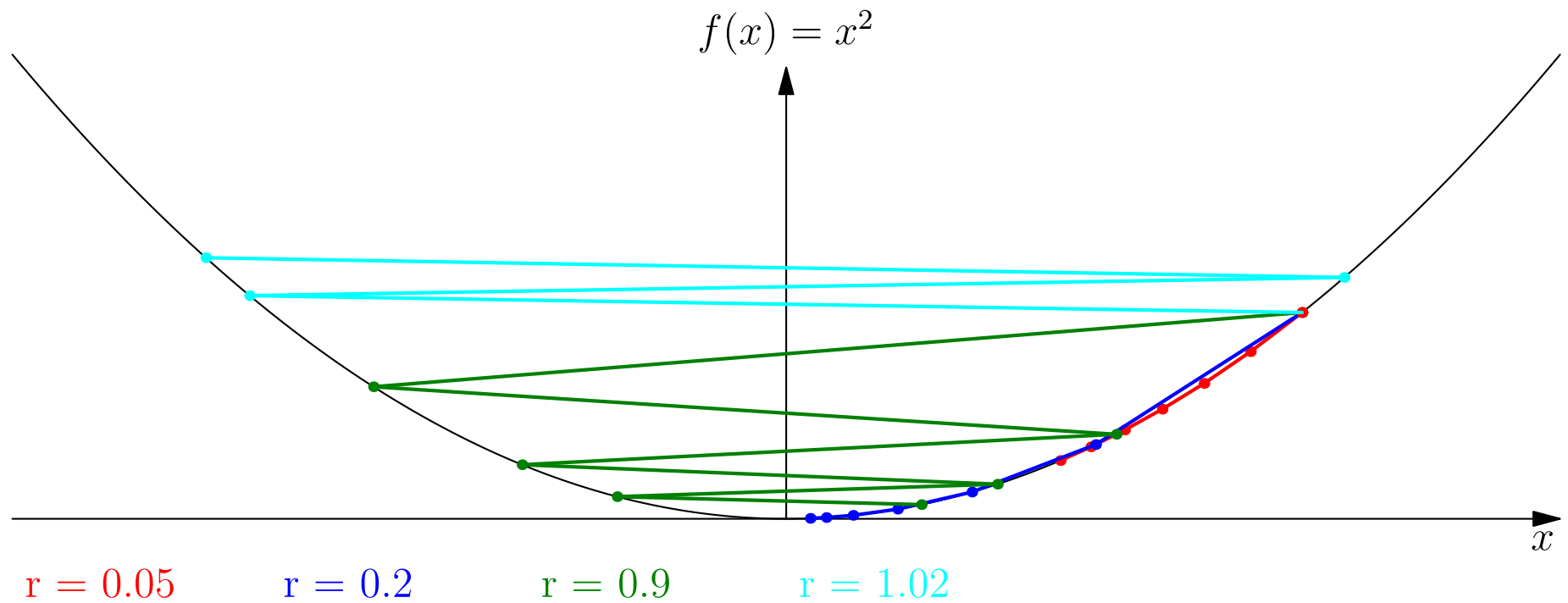
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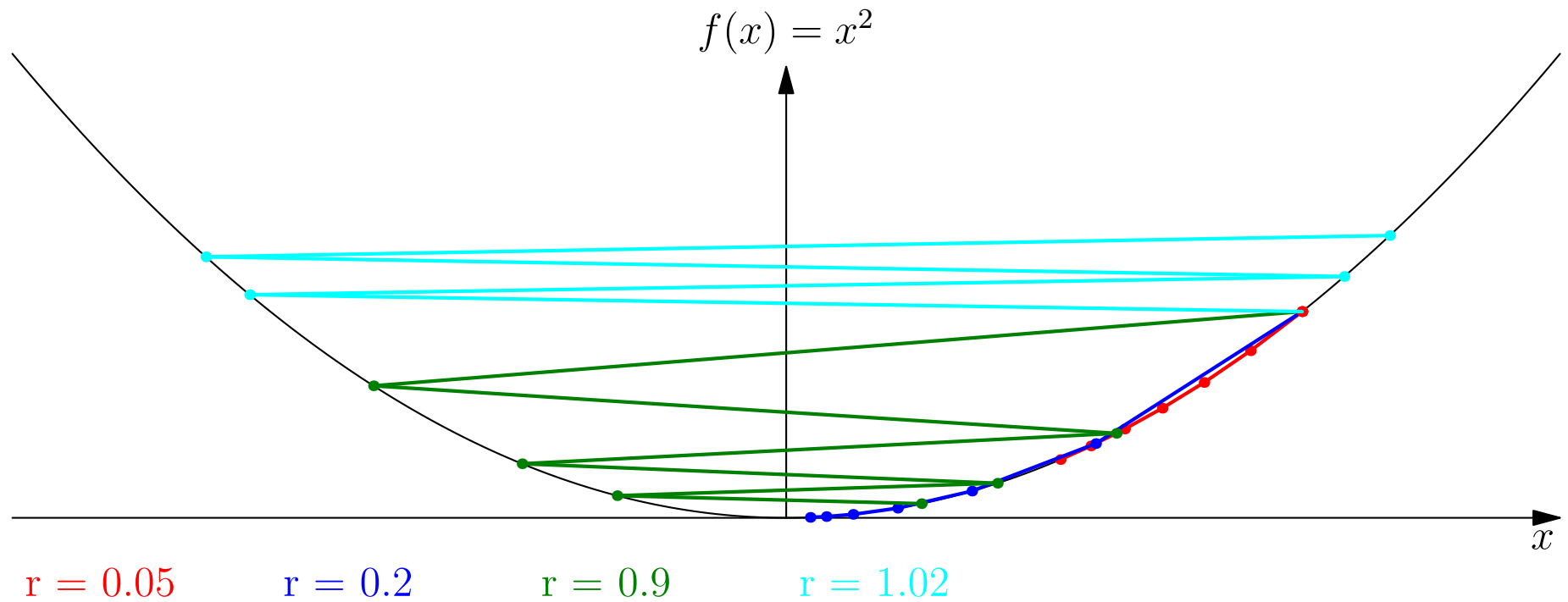
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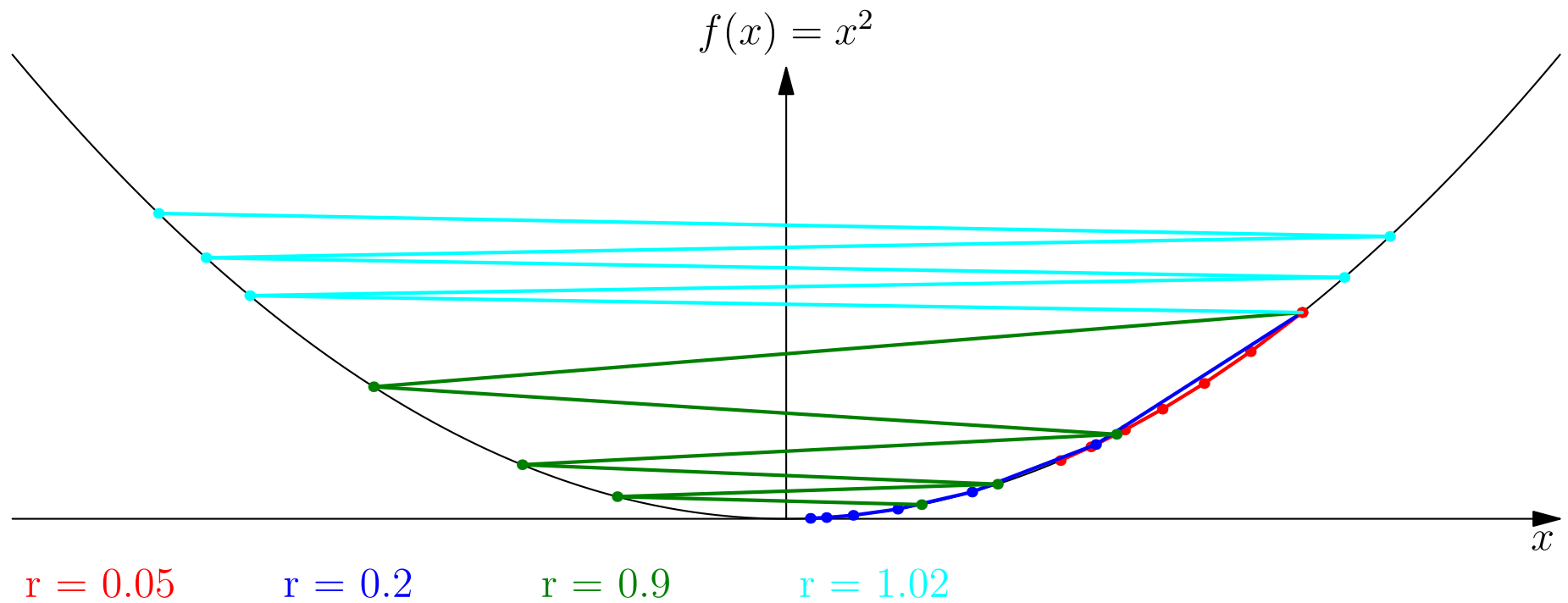
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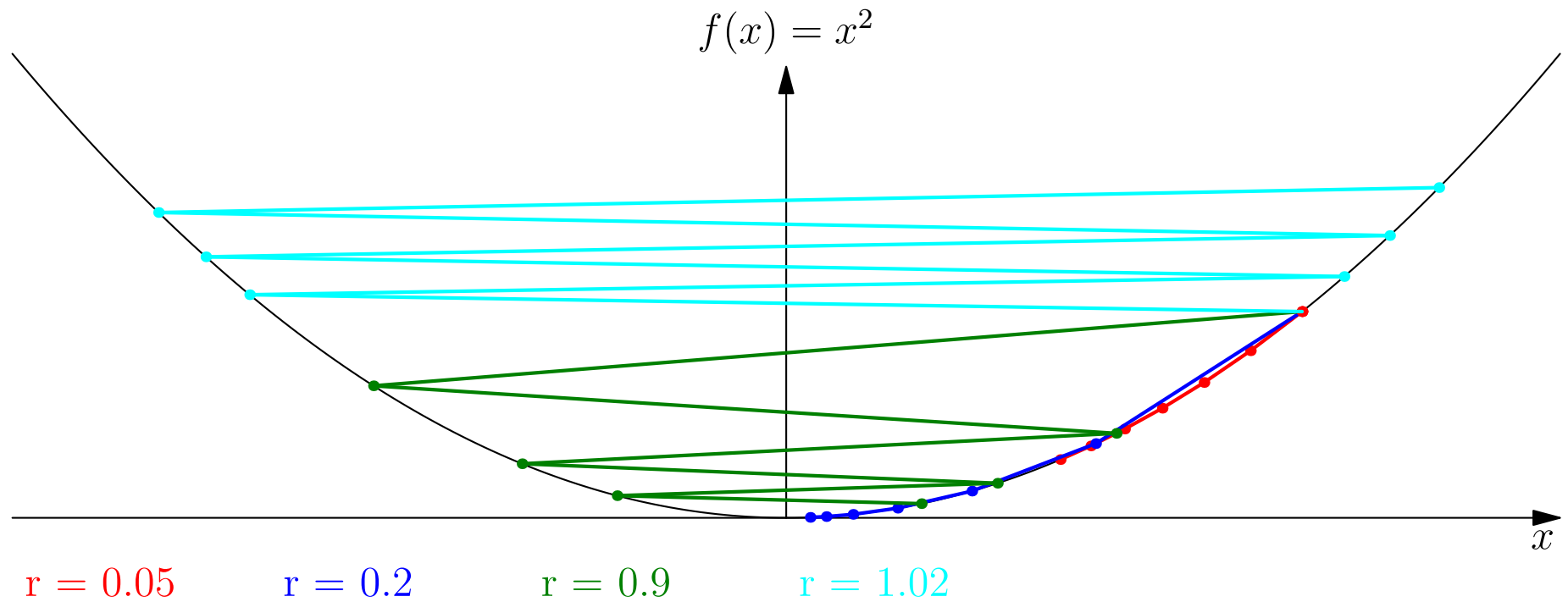
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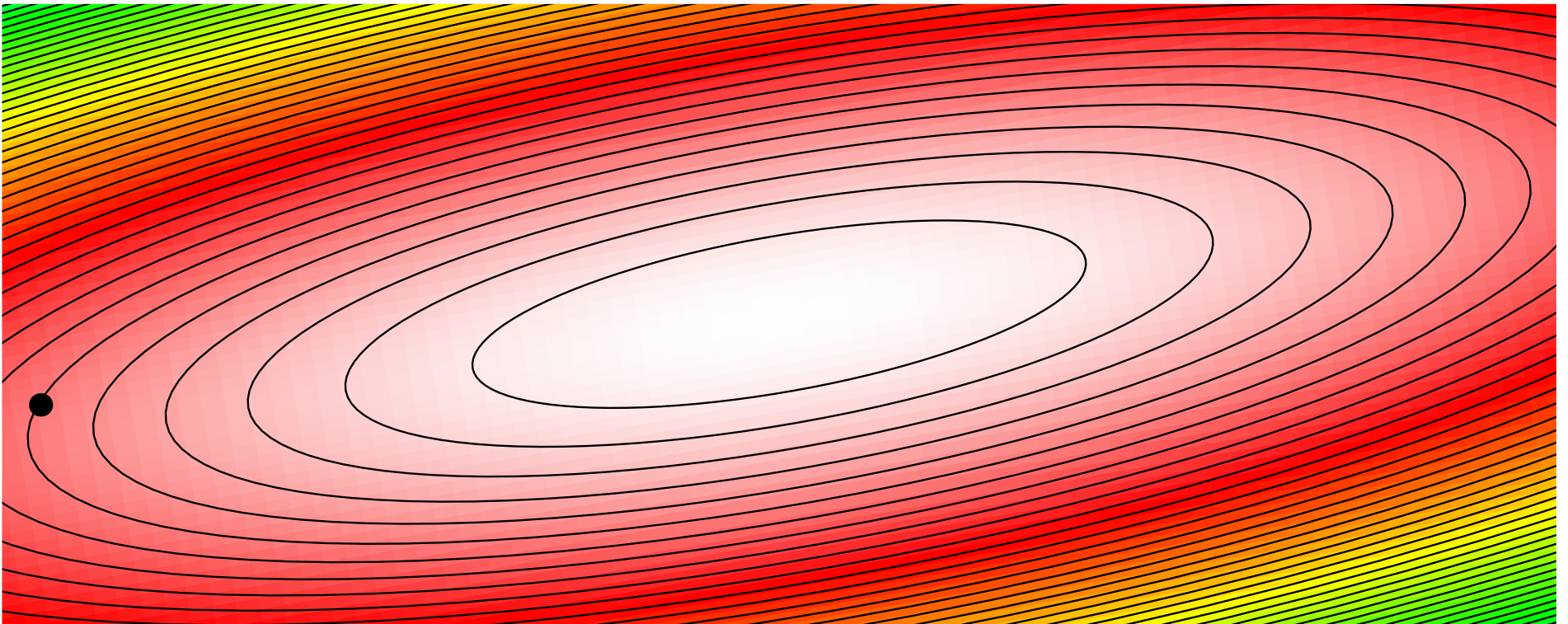


Higher Dimensions

- In higher dimensions the problem is that there are some directions you need to move a long way

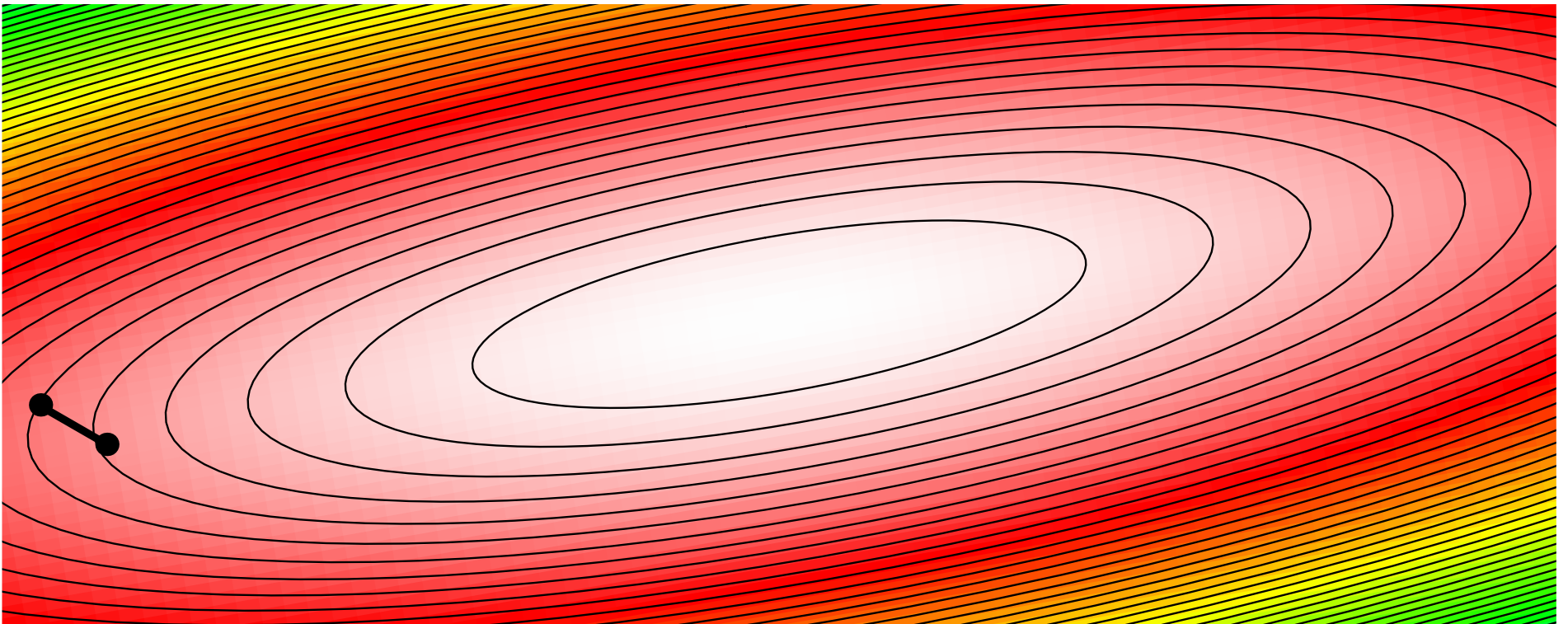
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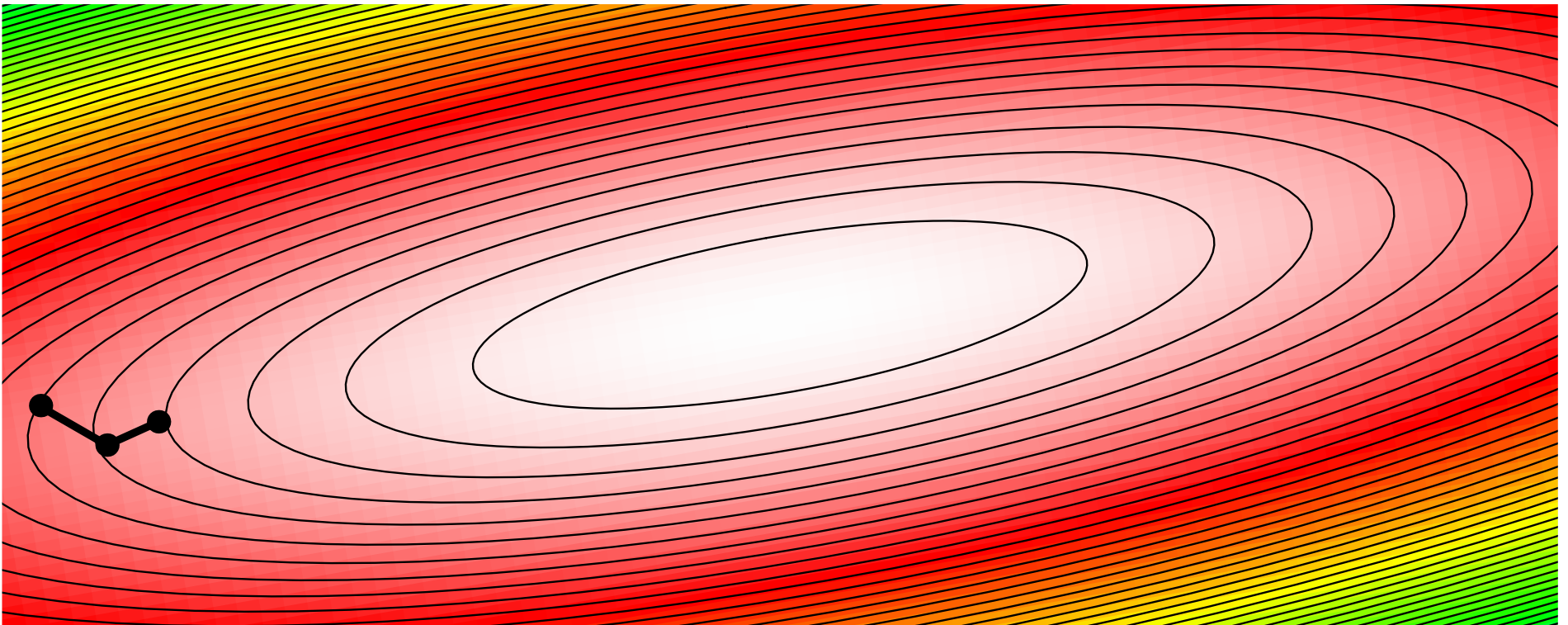
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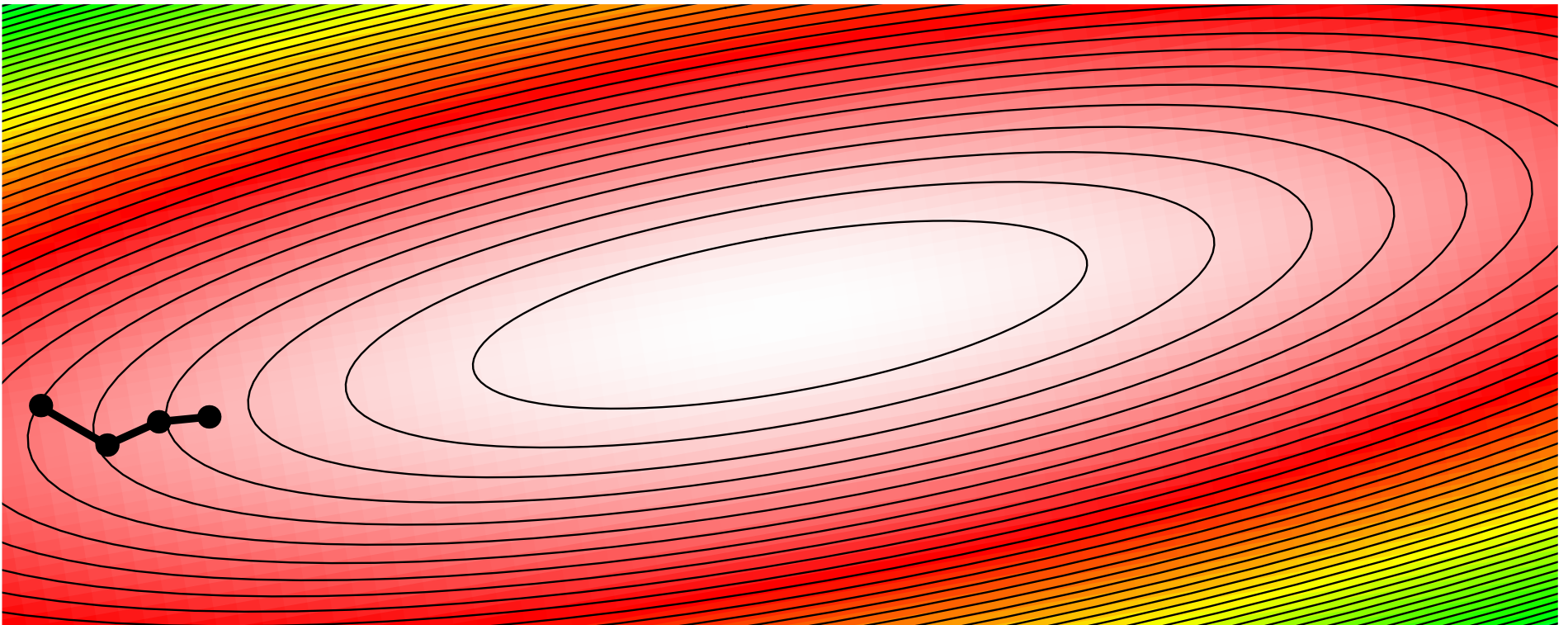
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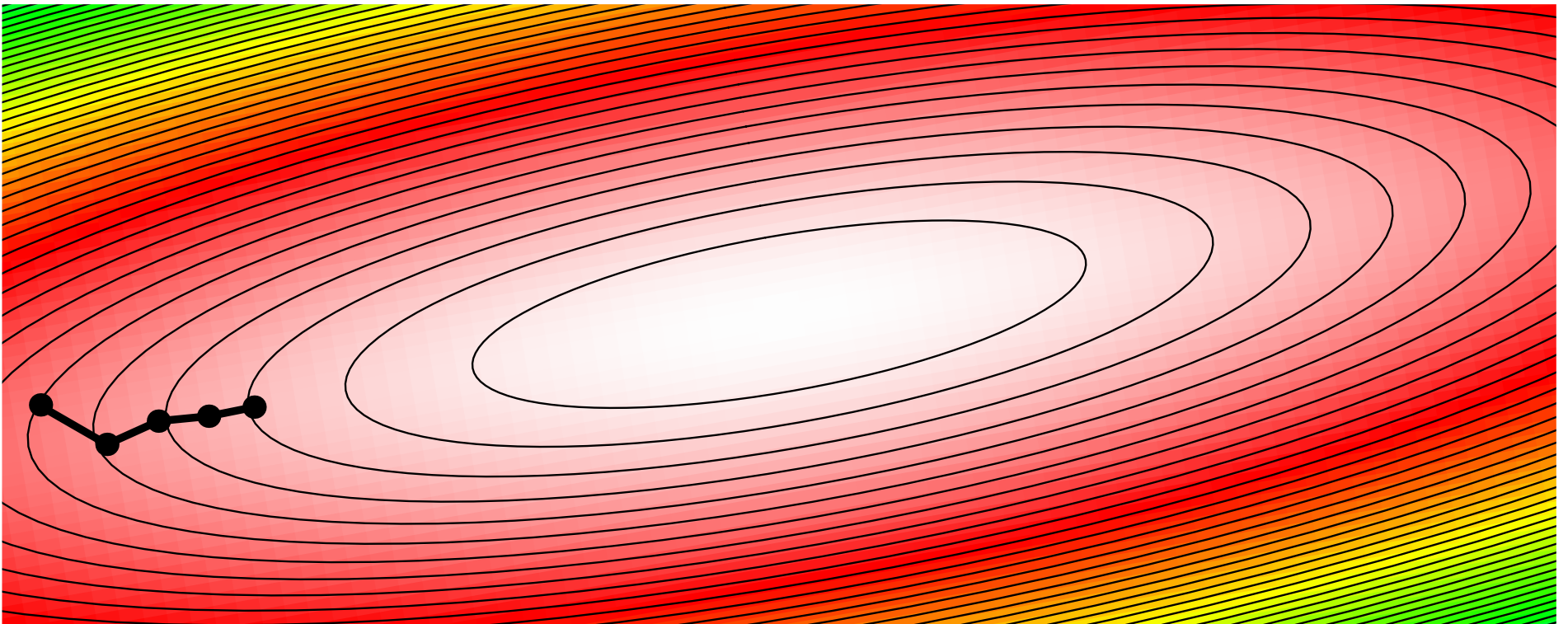
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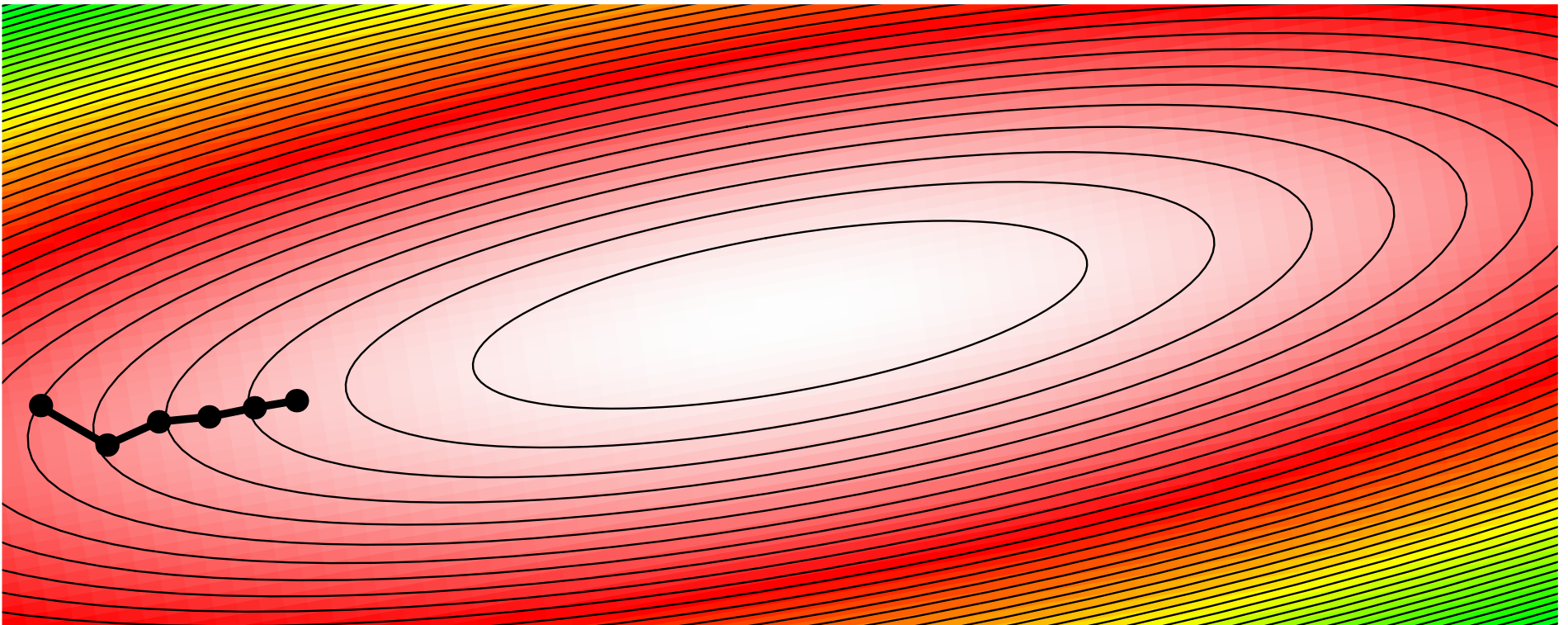
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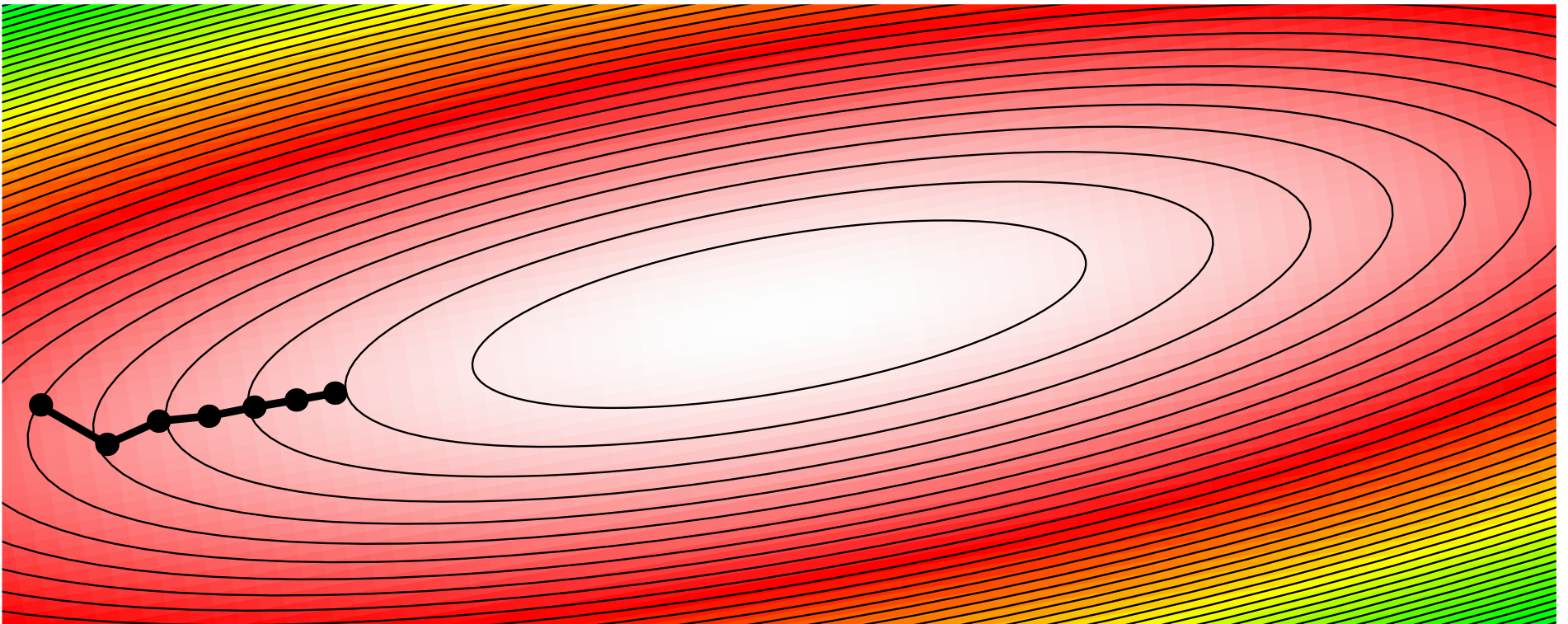
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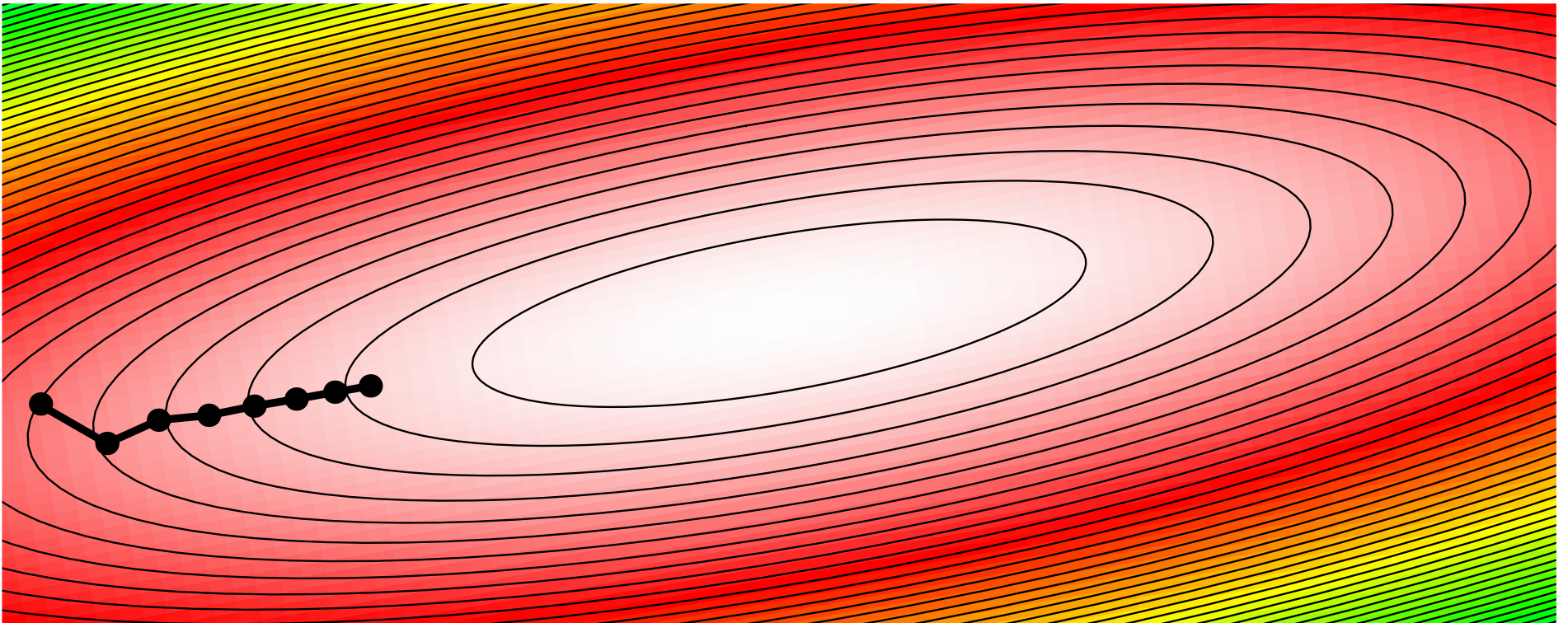
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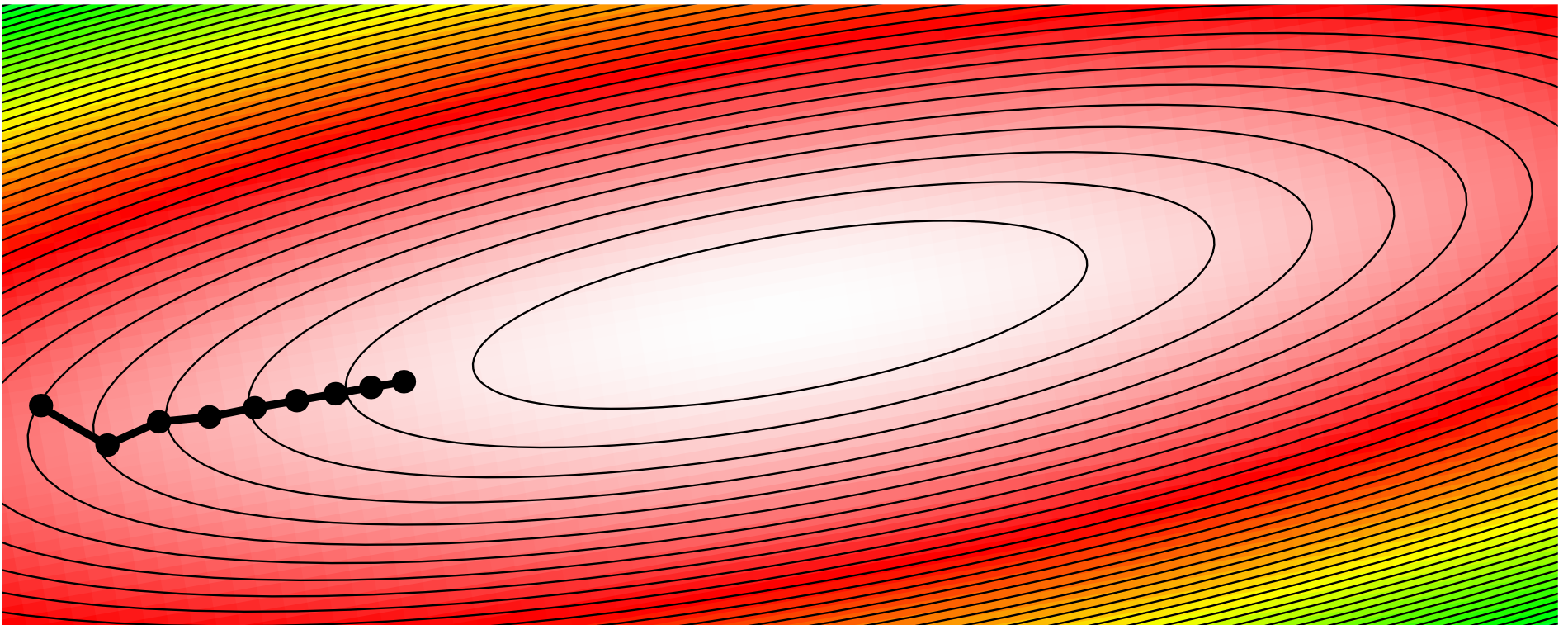
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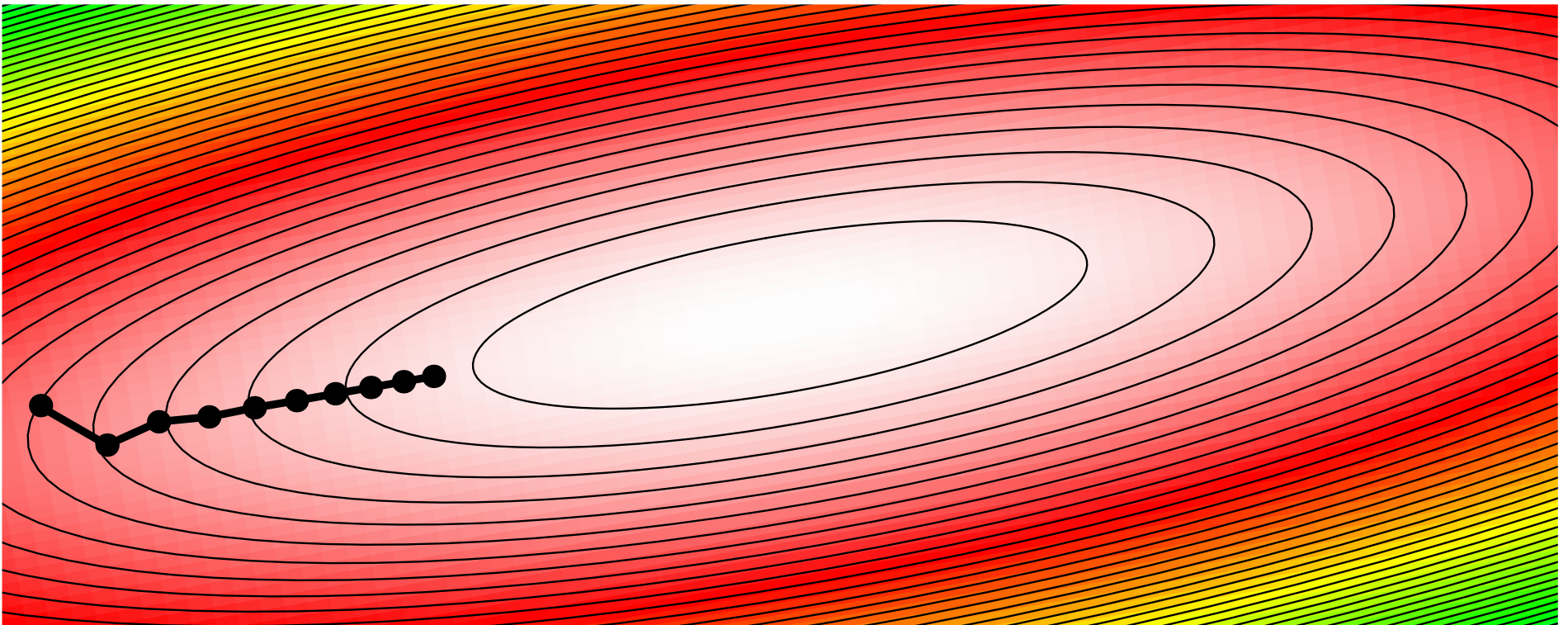
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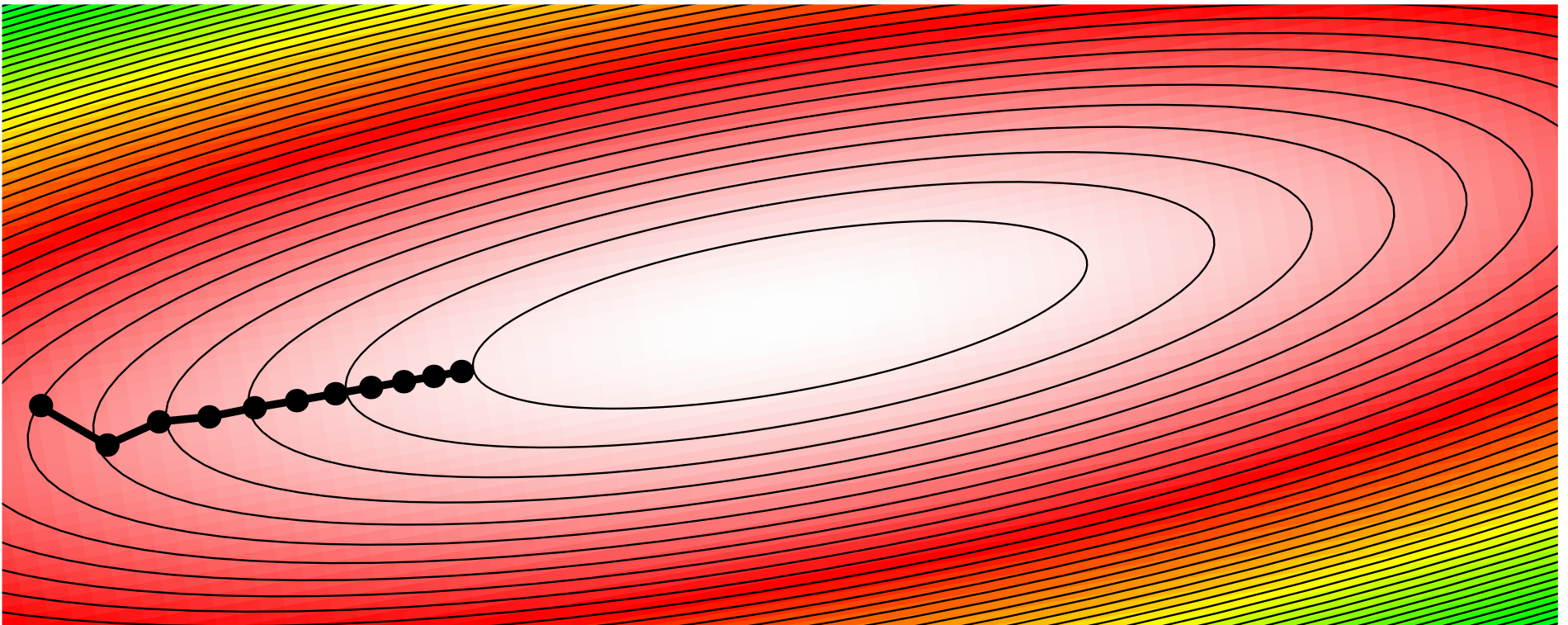
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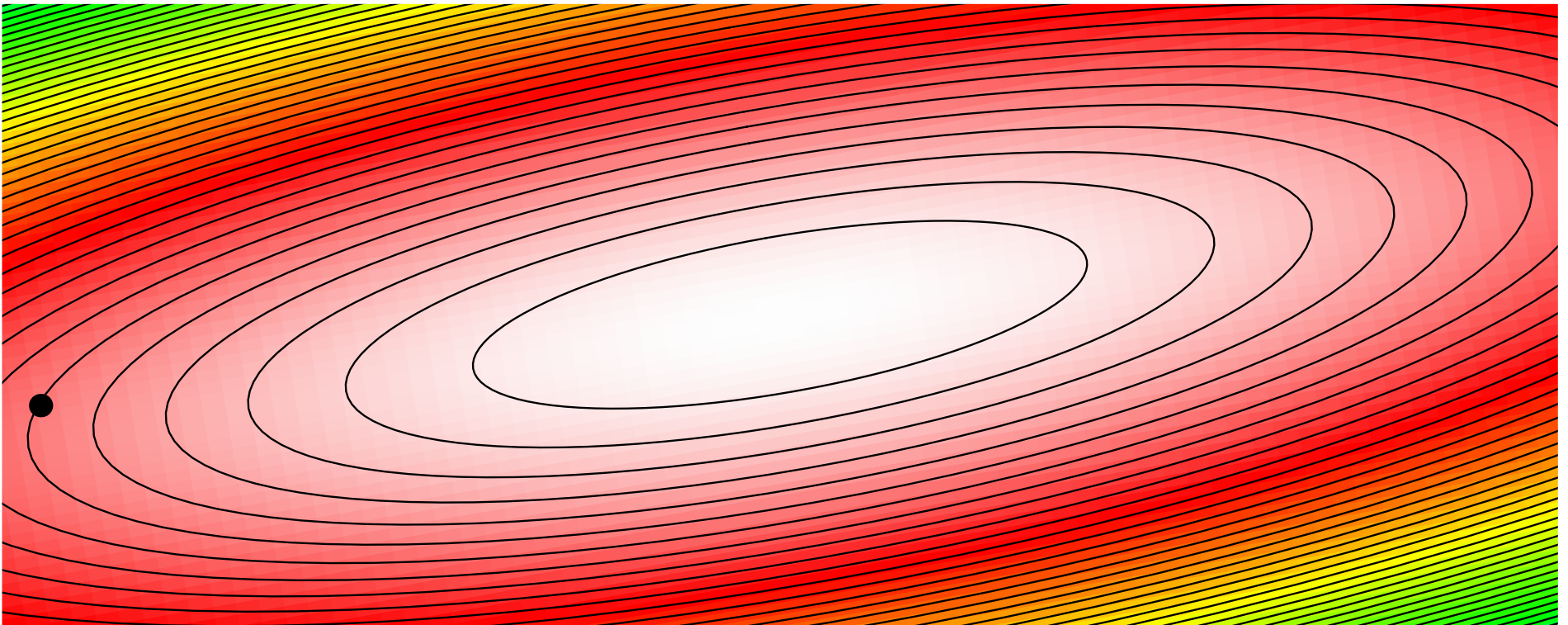


Getting There Quicker

- Increasing the step size speeds up convergence, but the direction of steepest descent doesn't point to the minimum

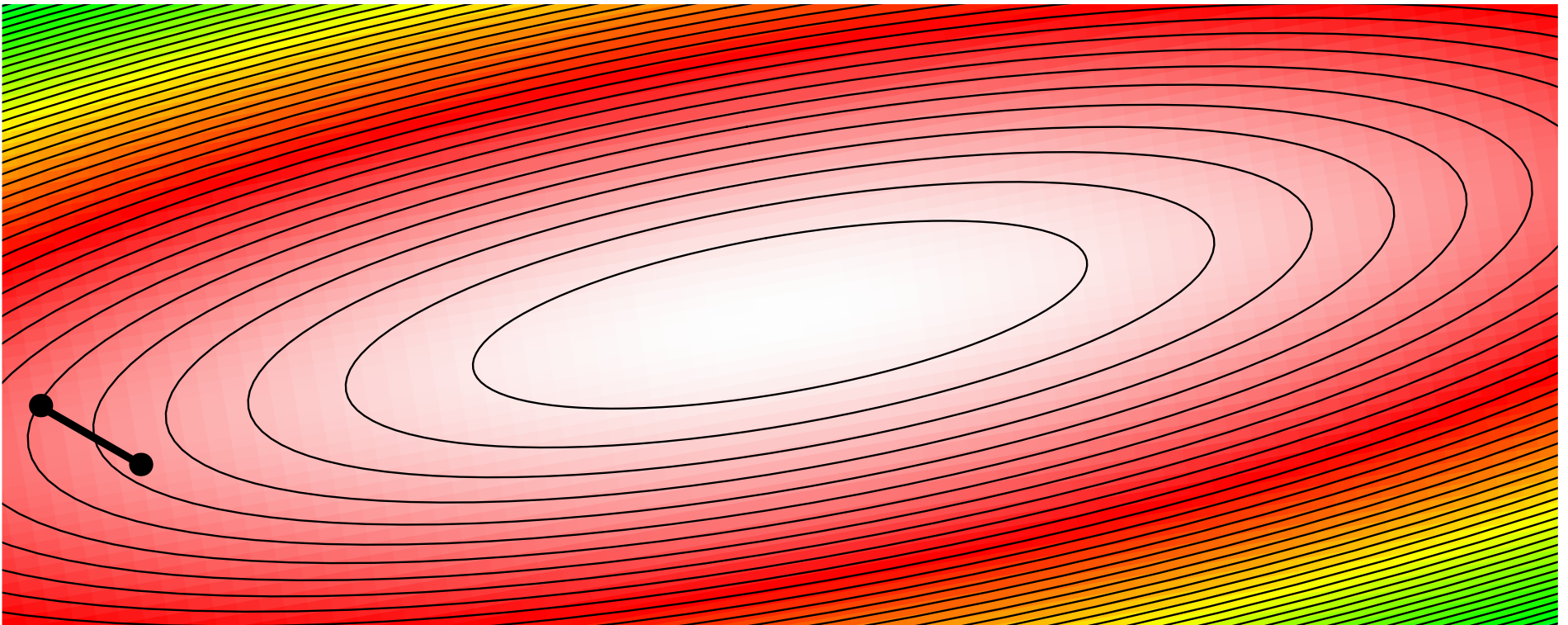
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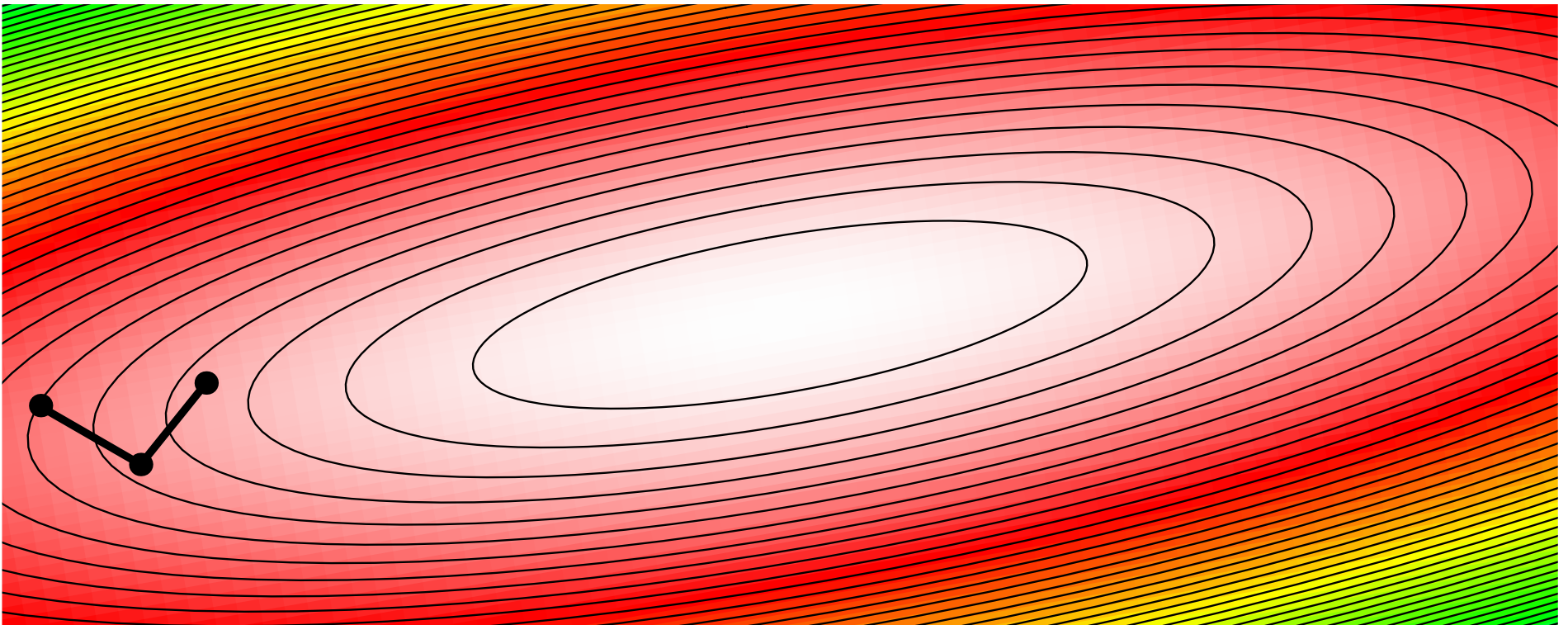
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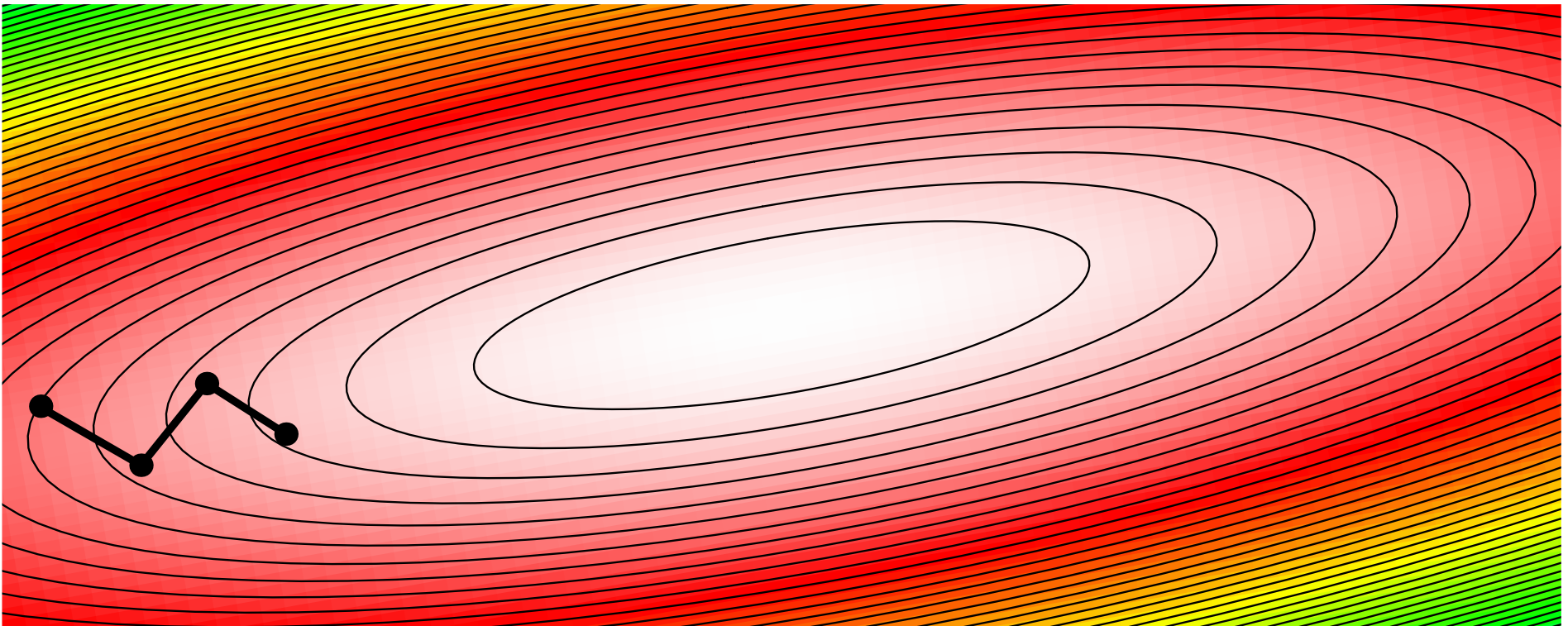
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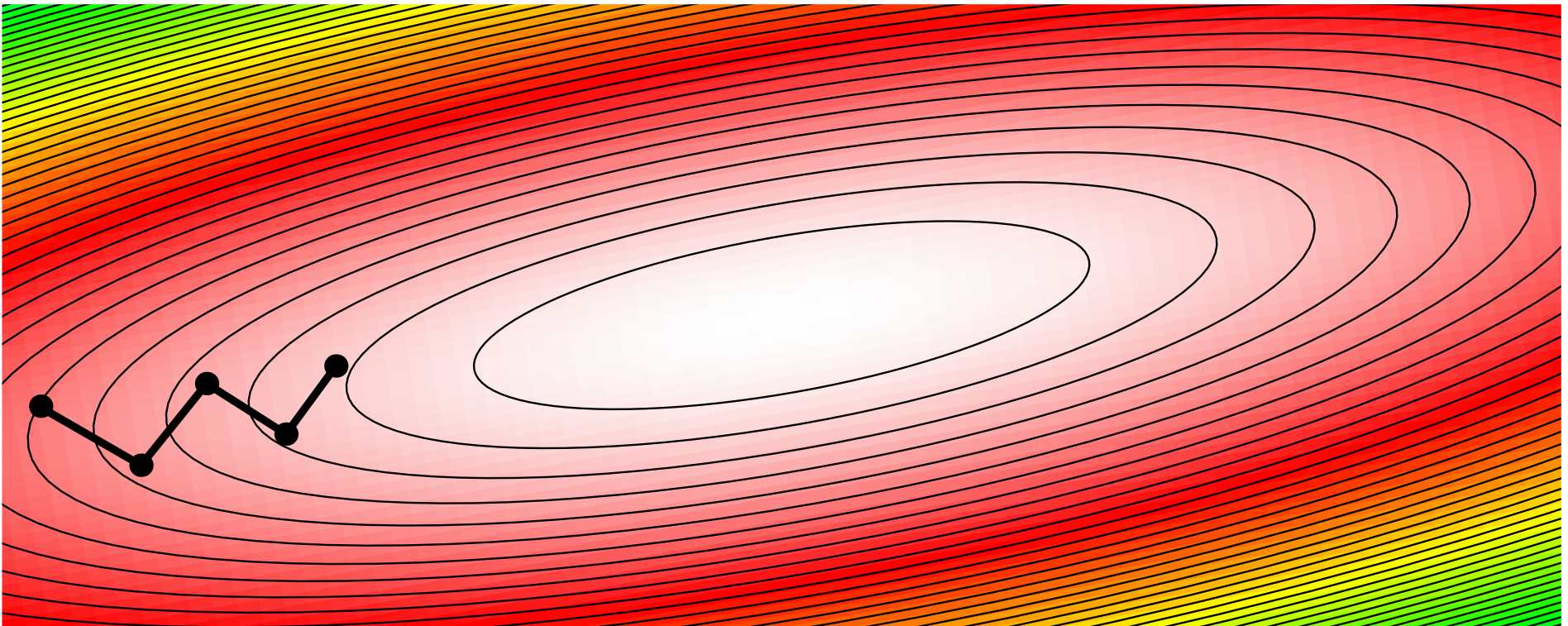
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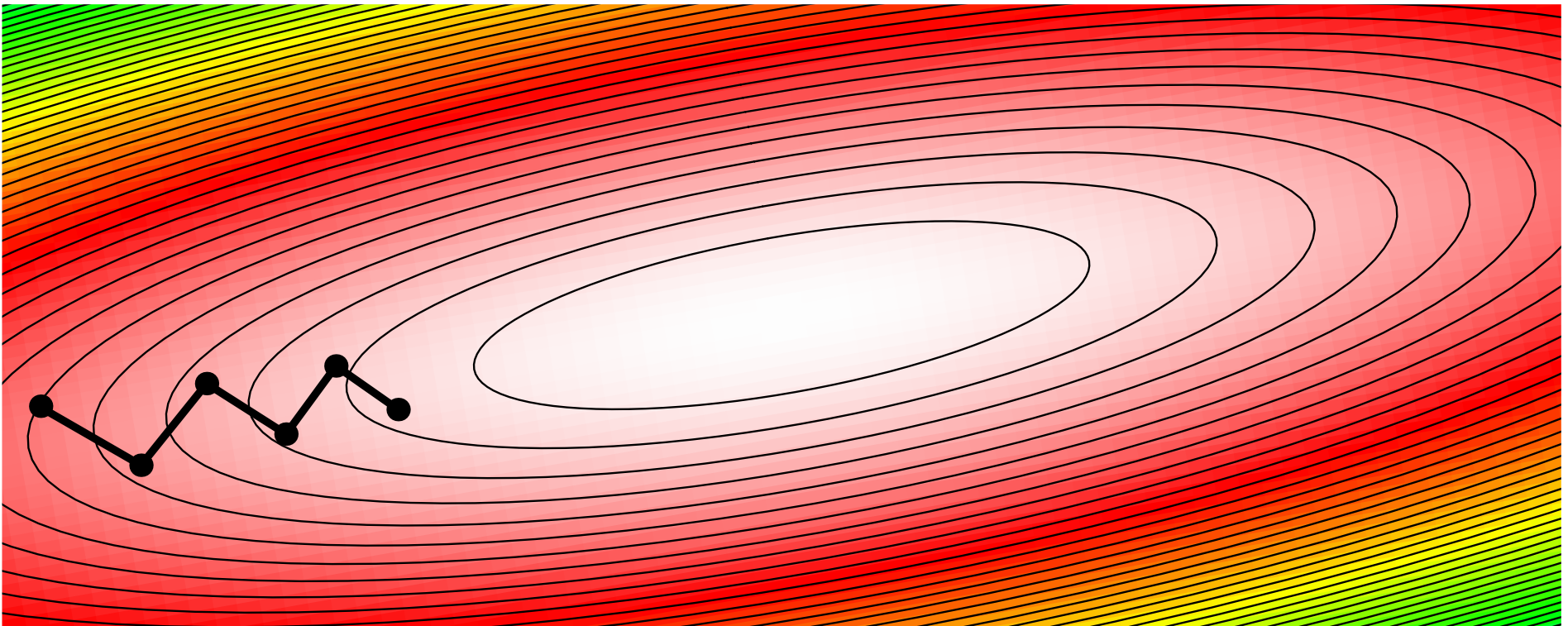
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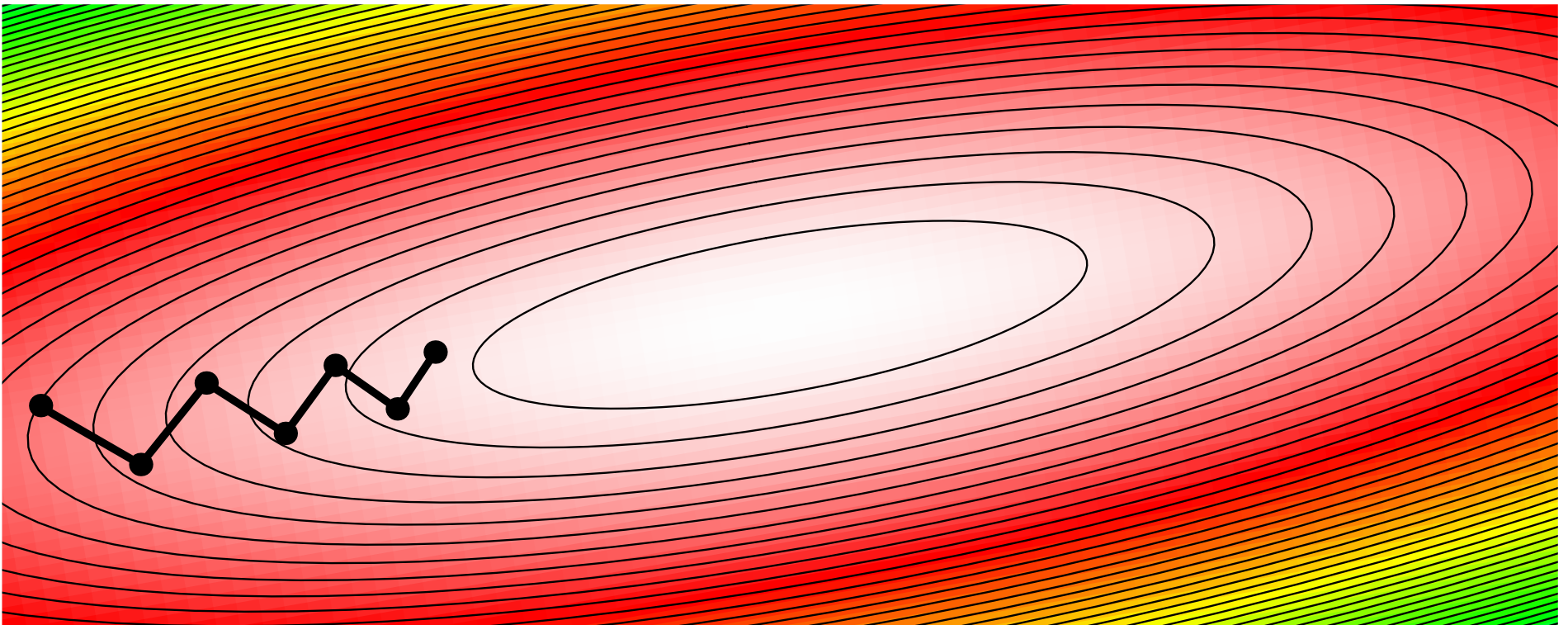
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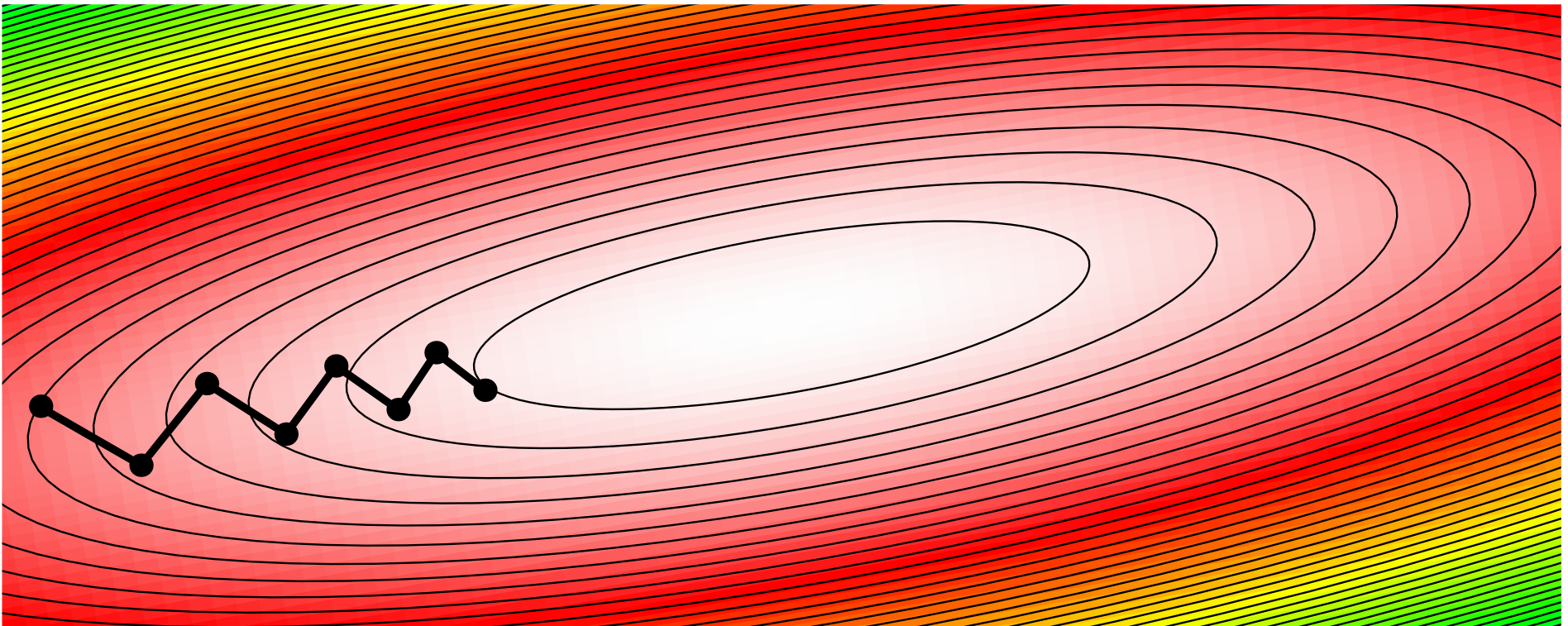
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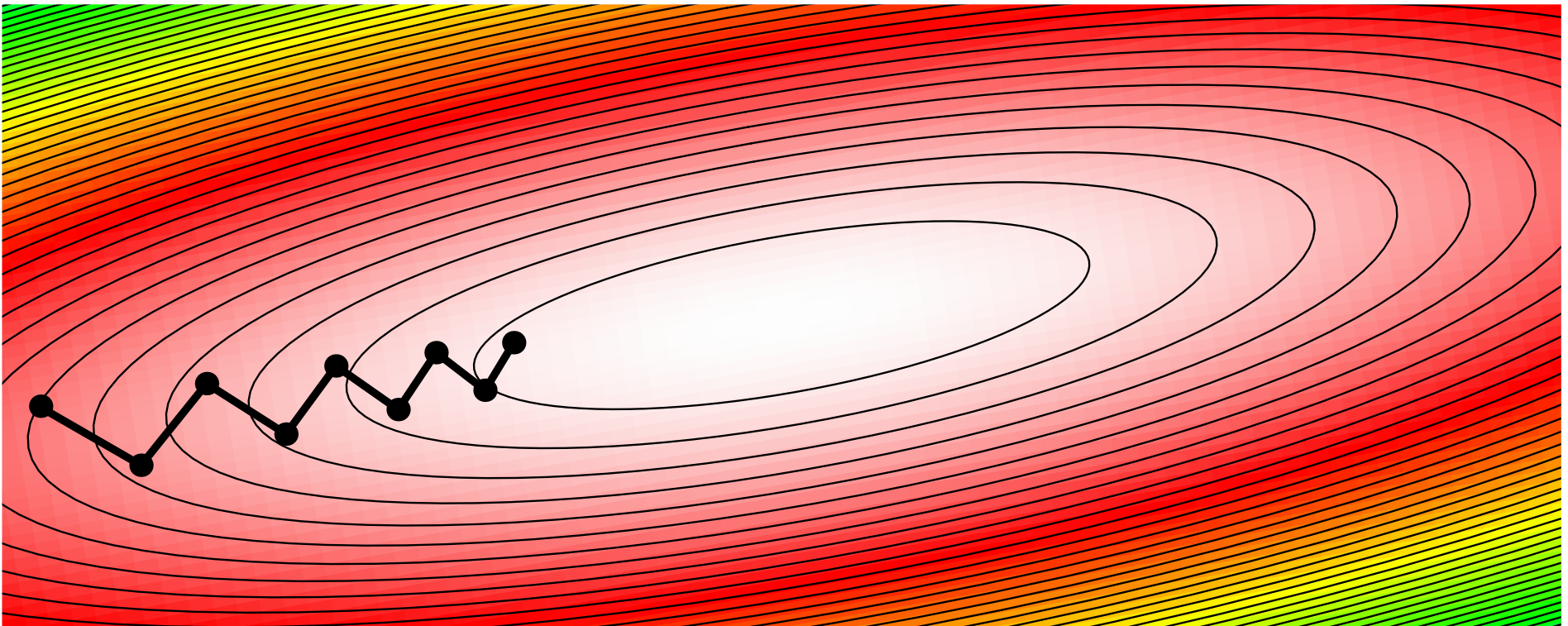
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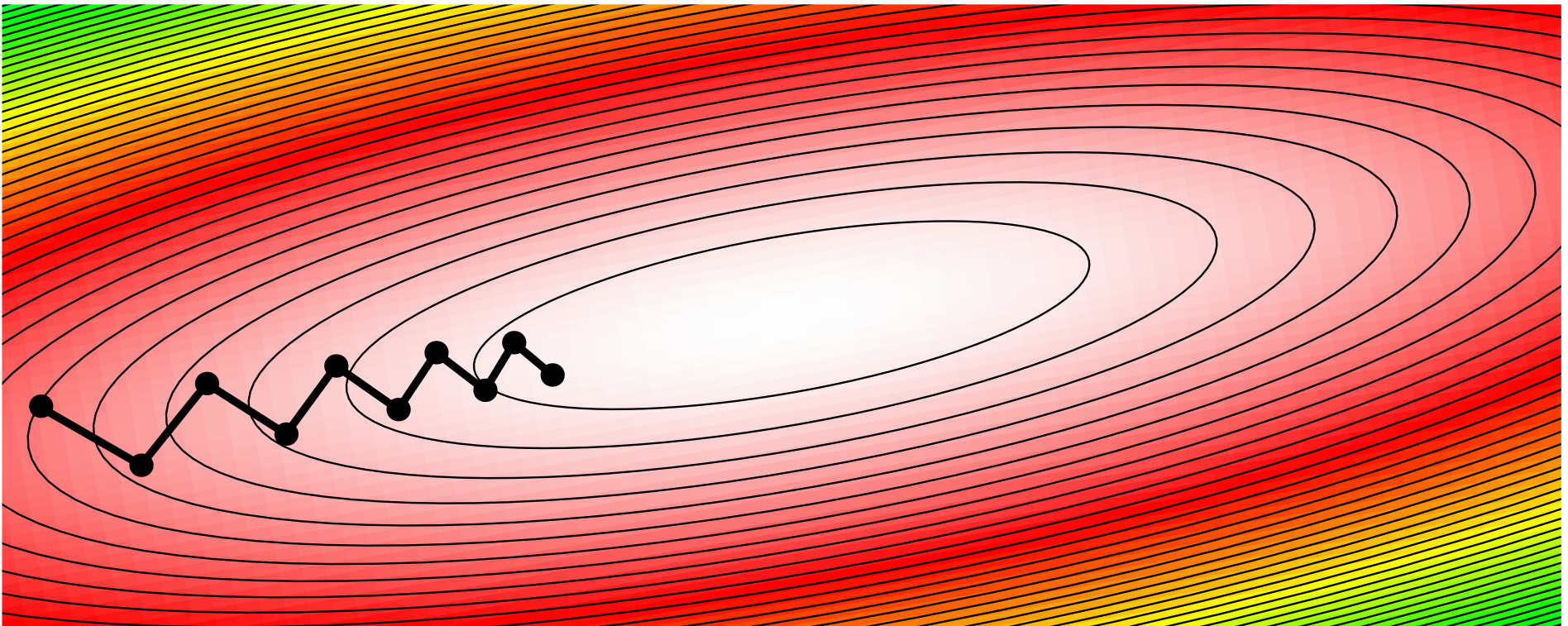
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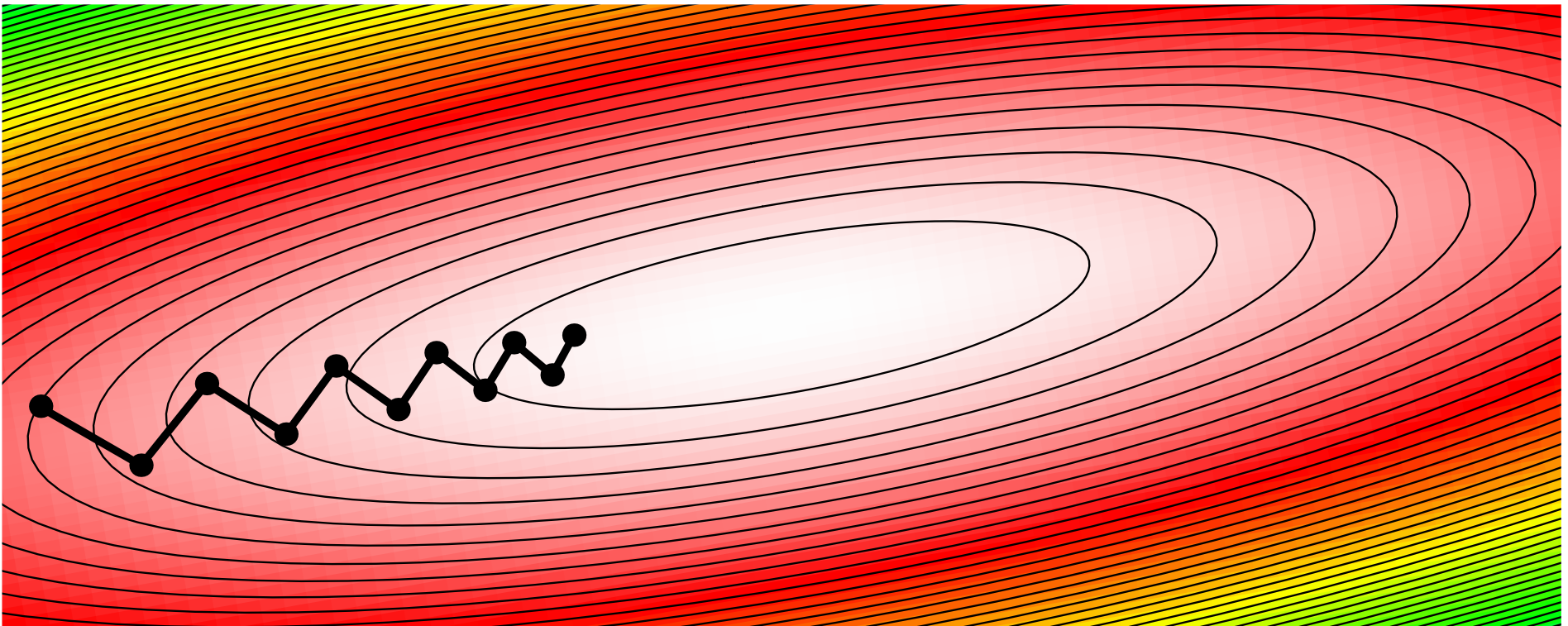
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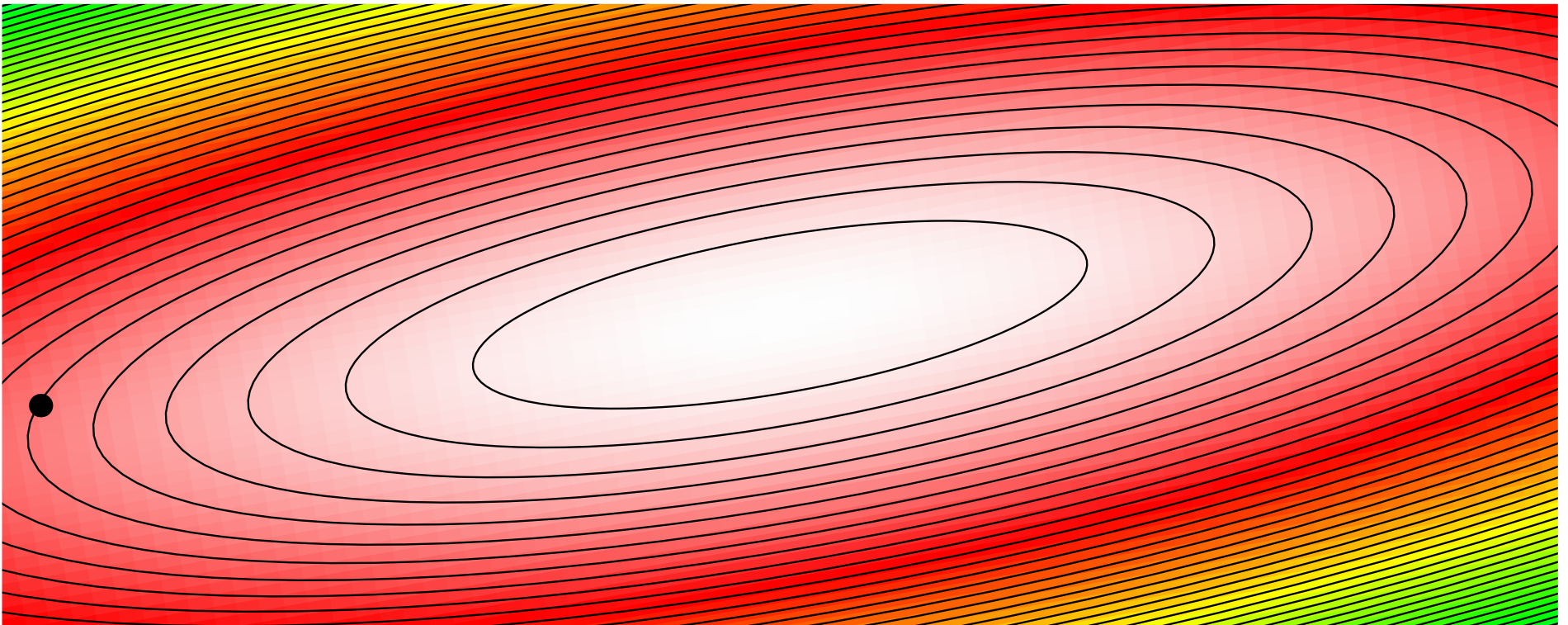


More Haste Less Speed

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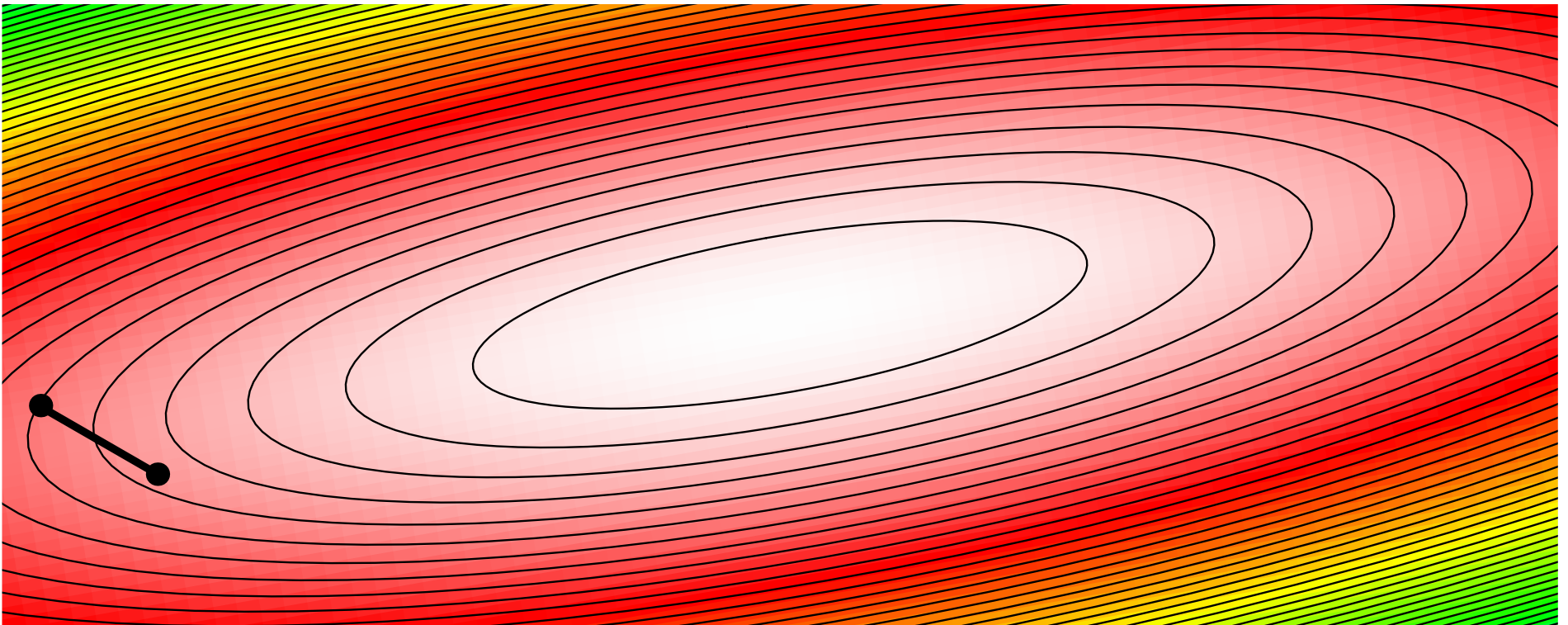
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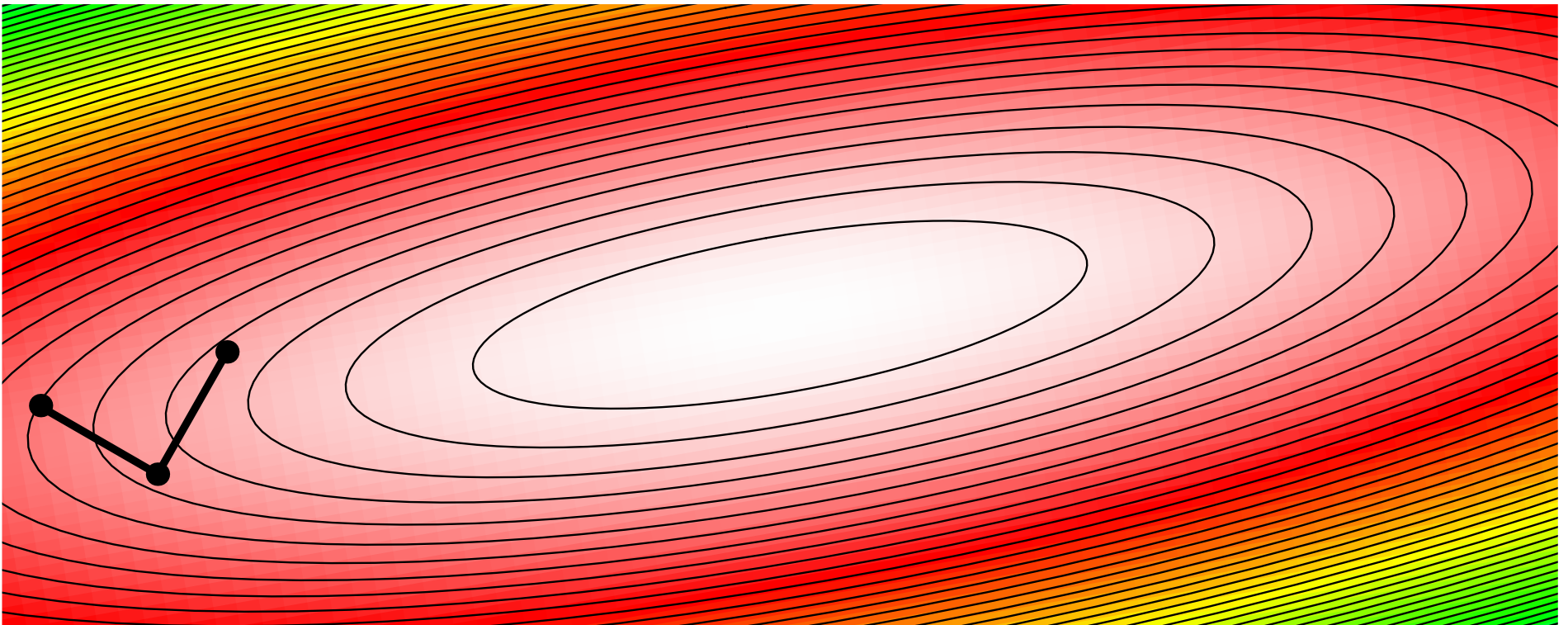
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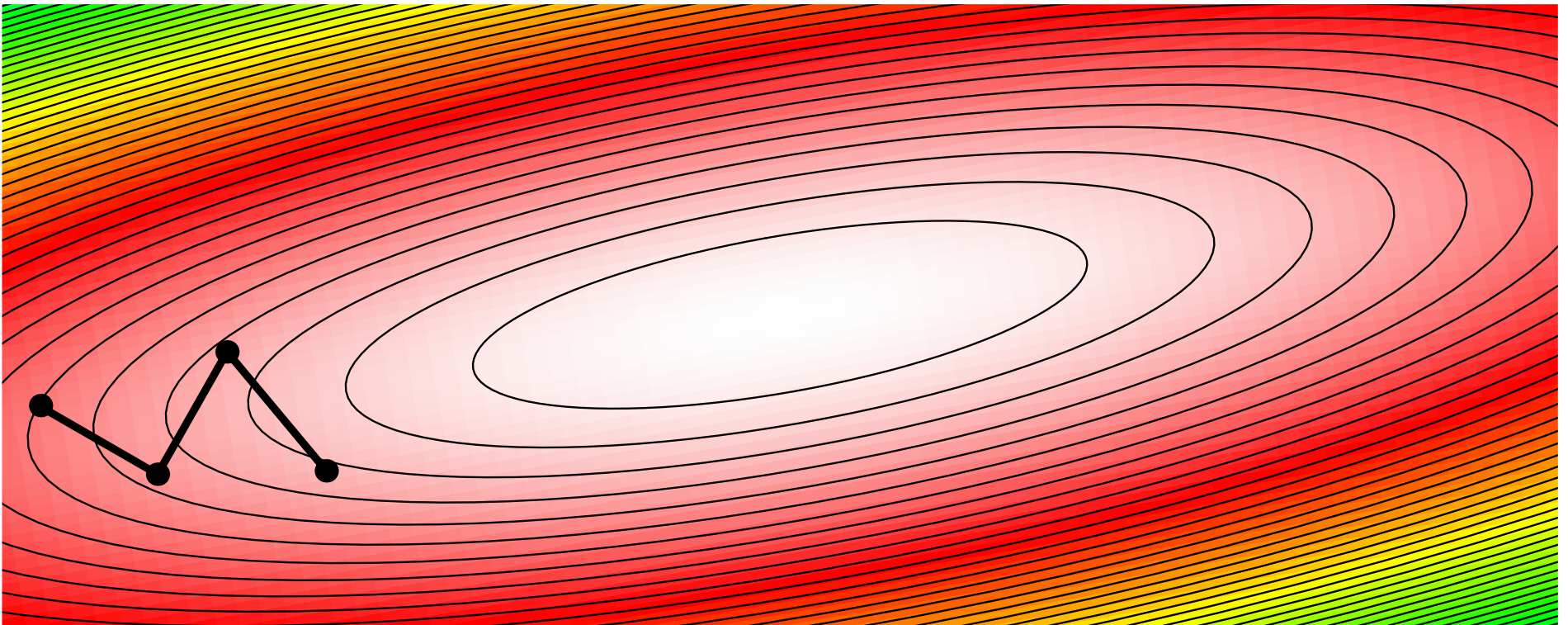
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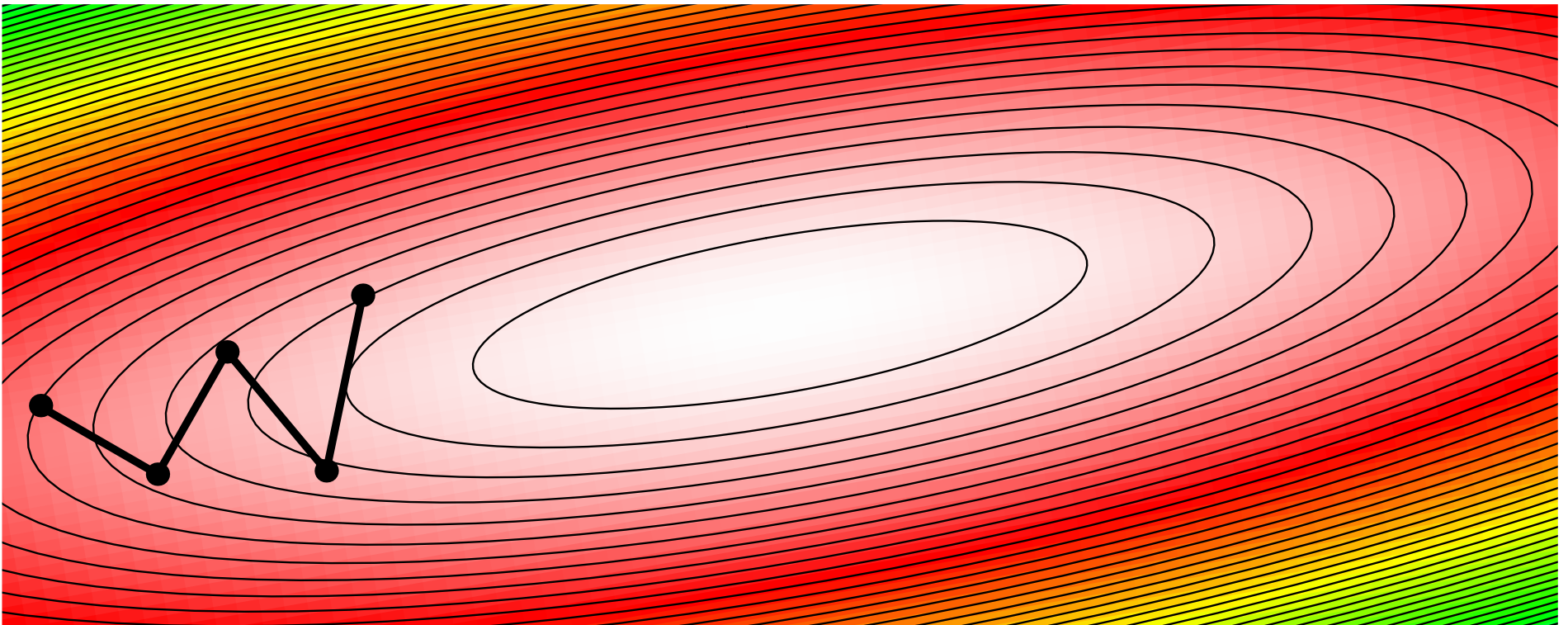
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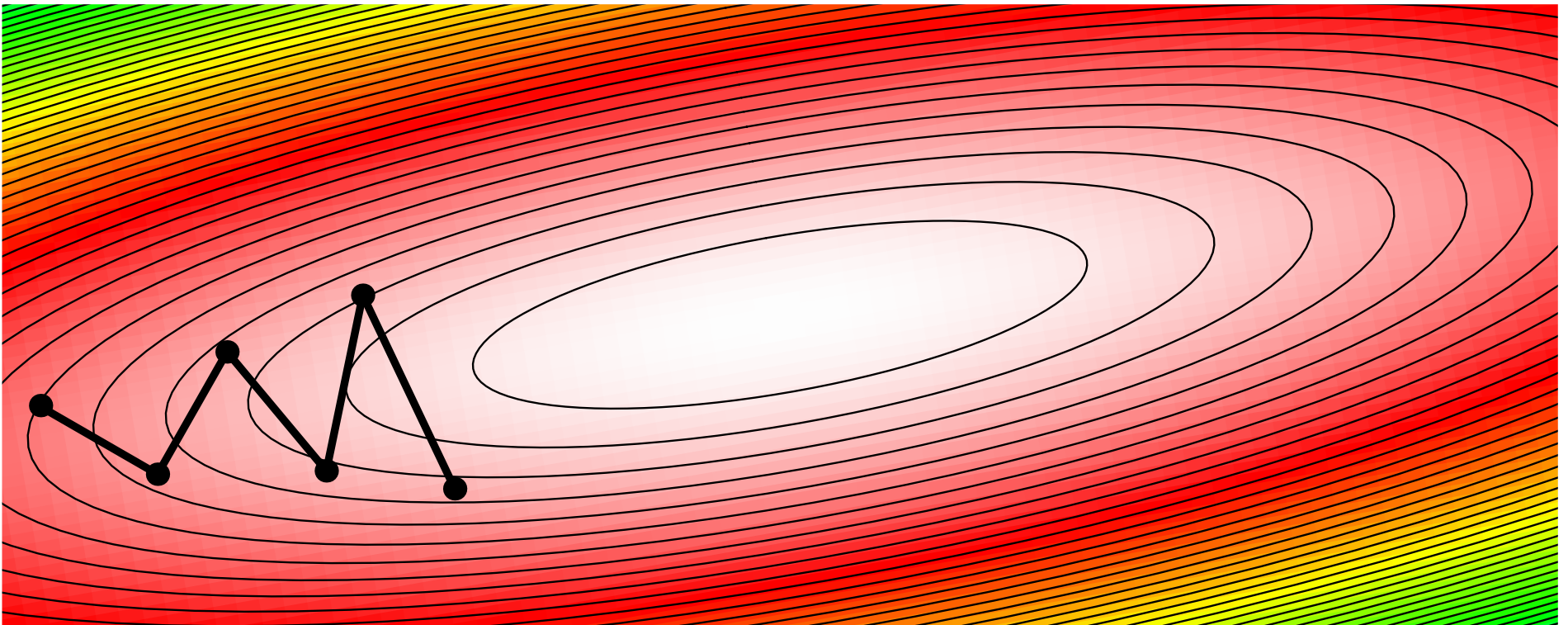
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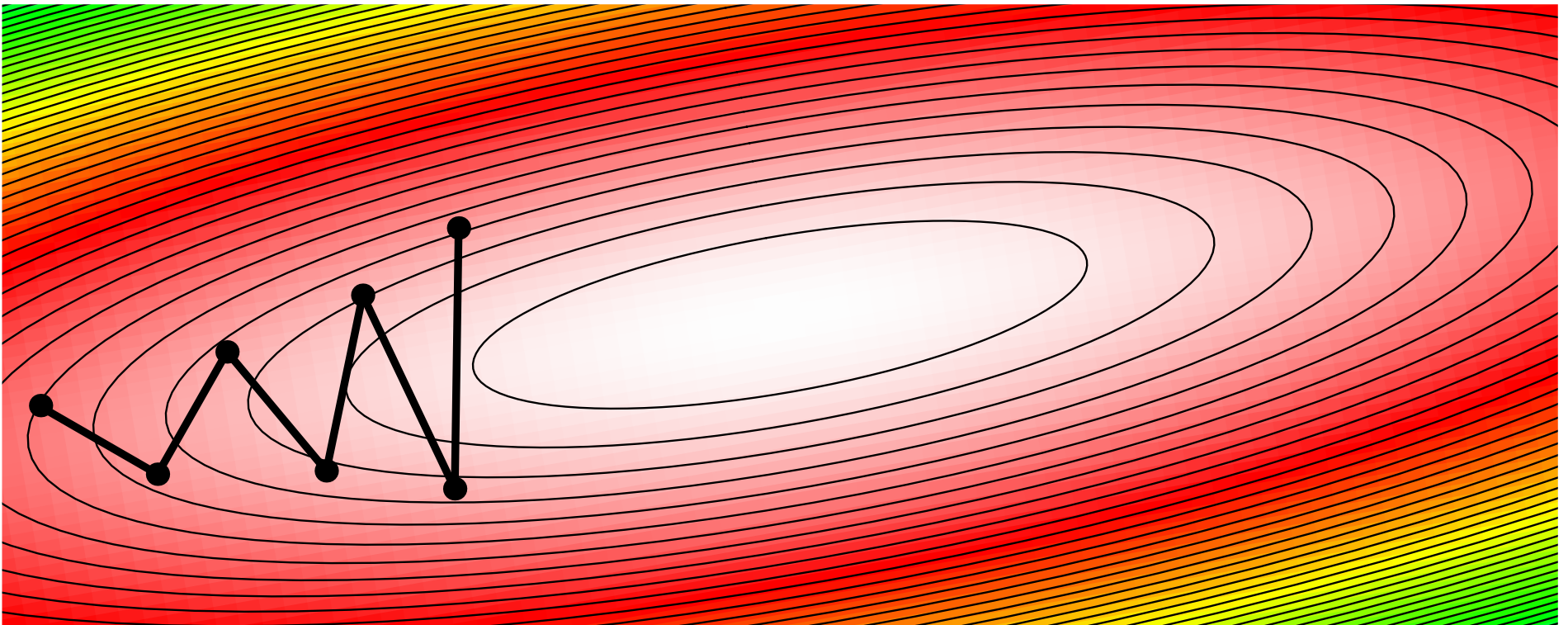
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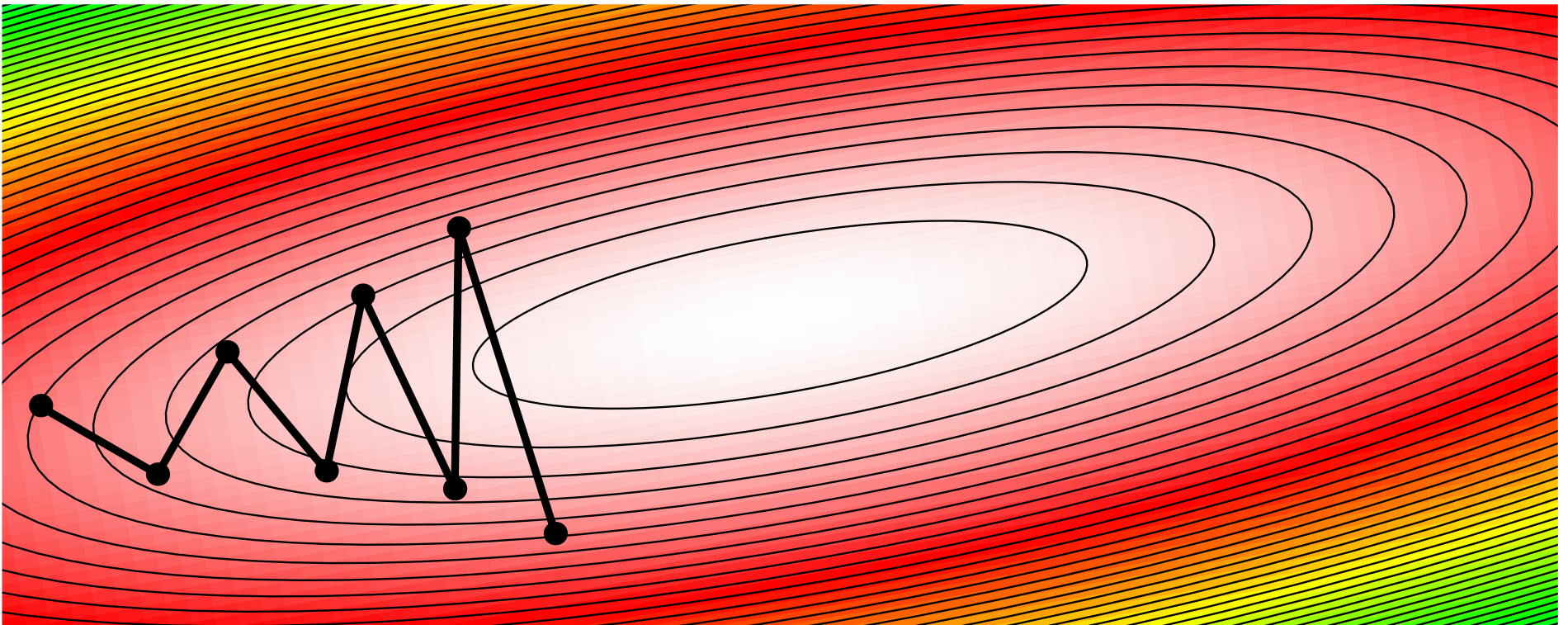
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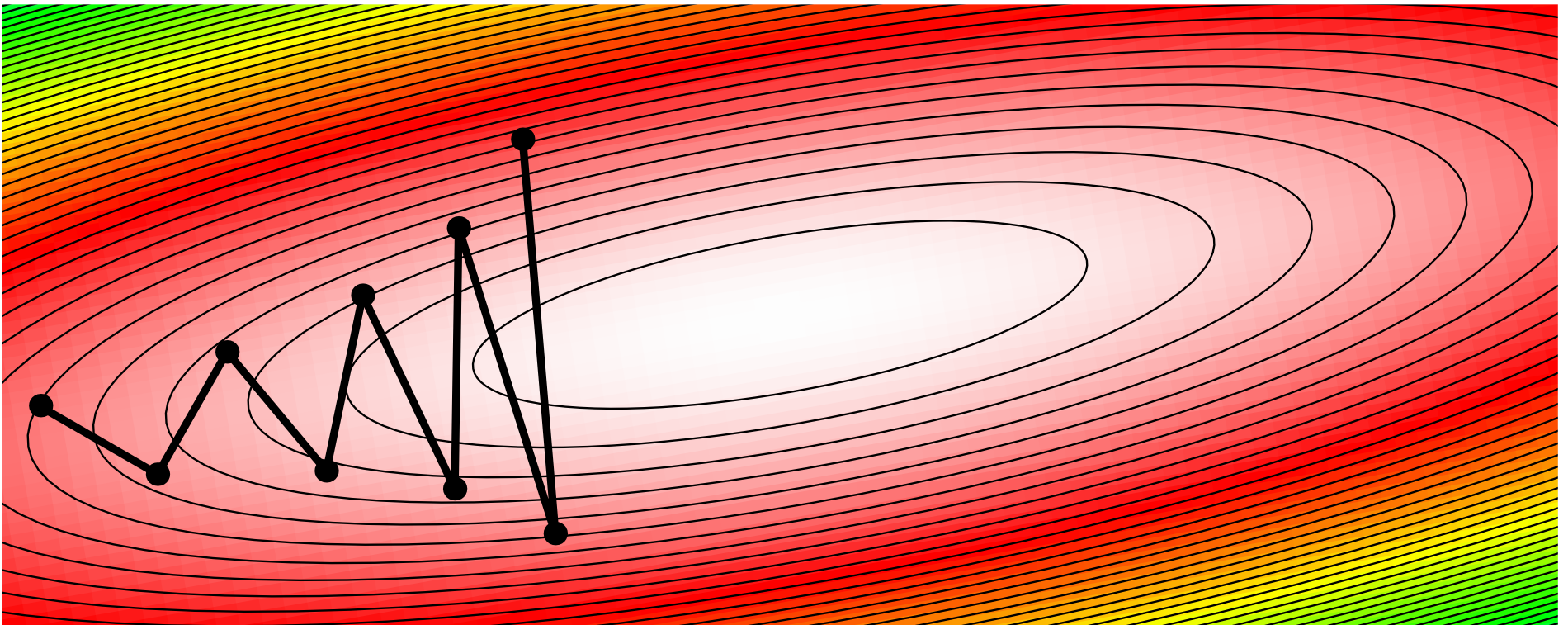
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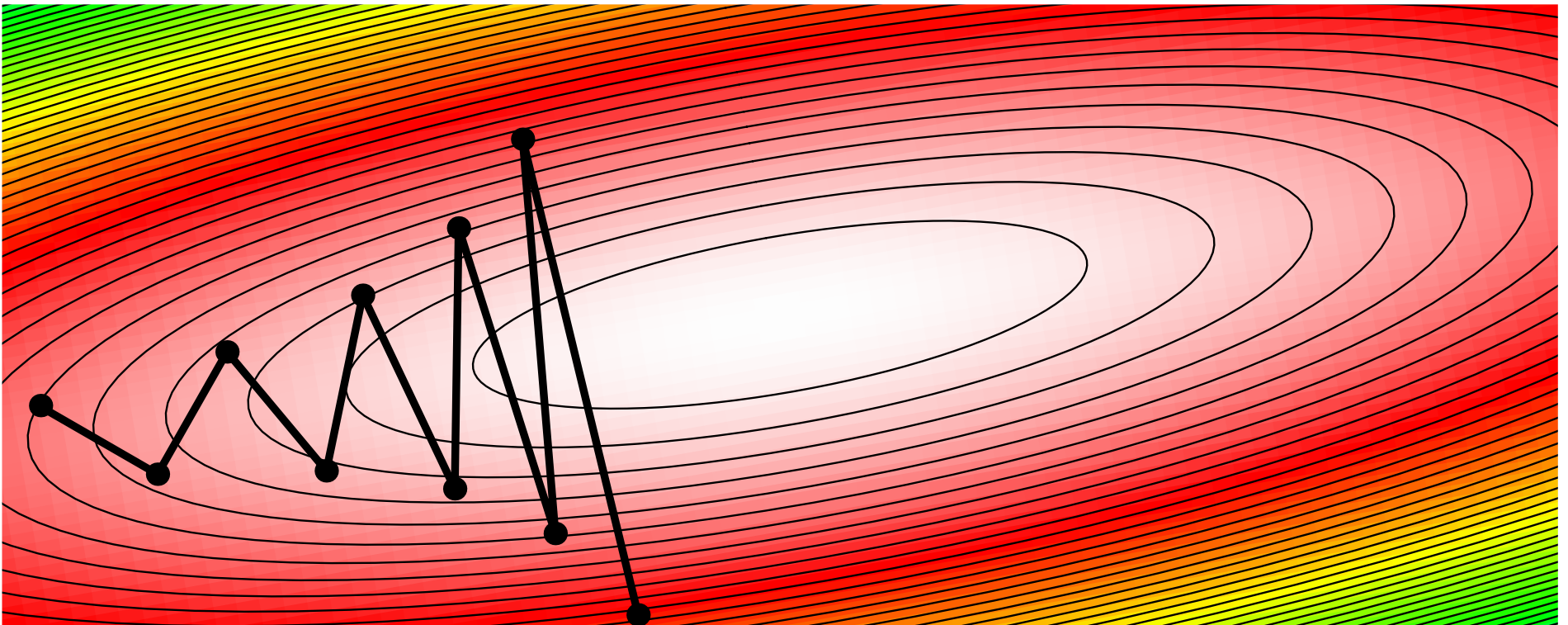
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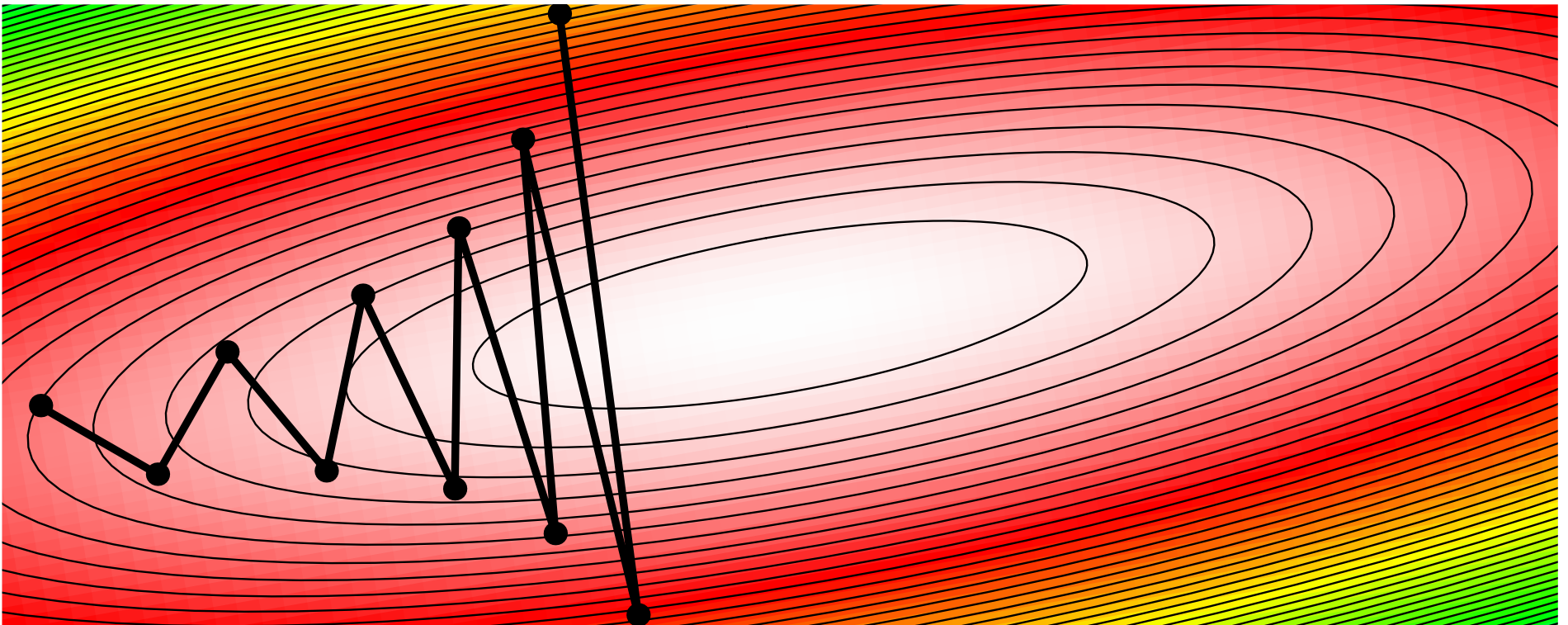
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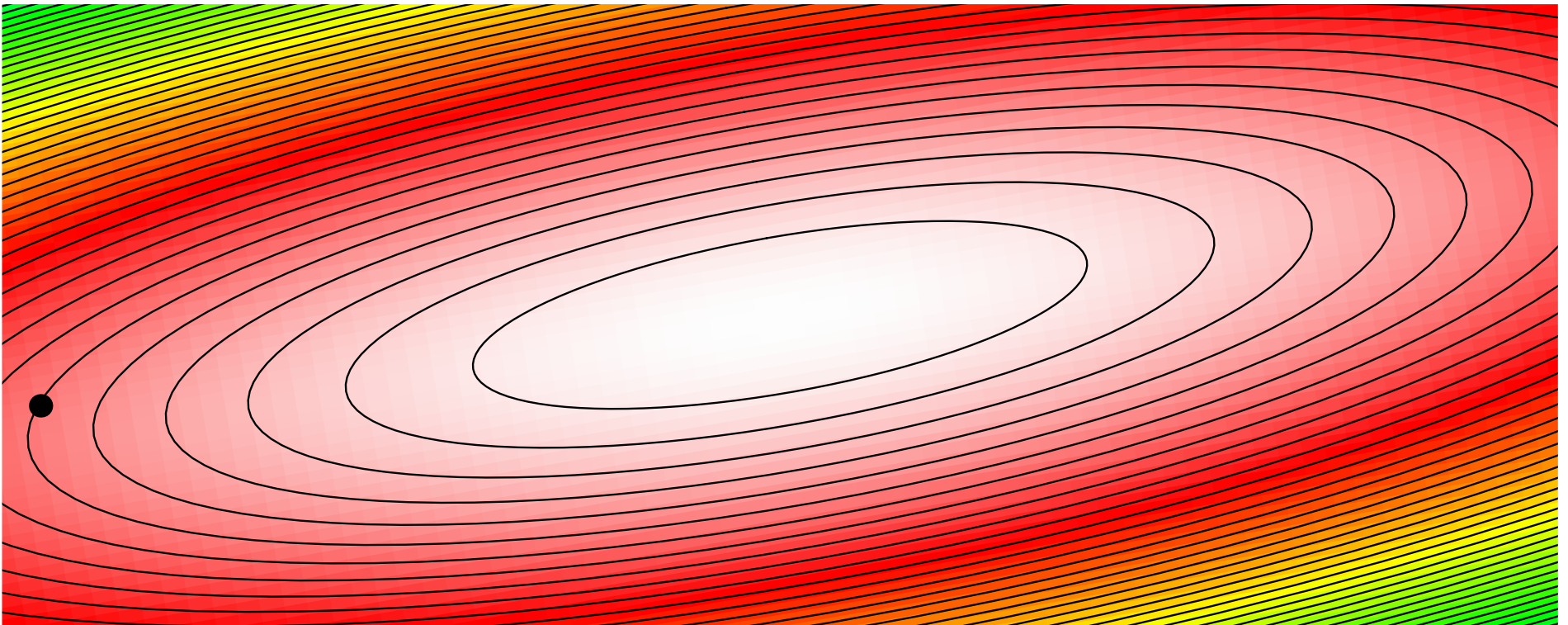


Line Minimisation

- We can systematically seek the minimum along a line of the gradient

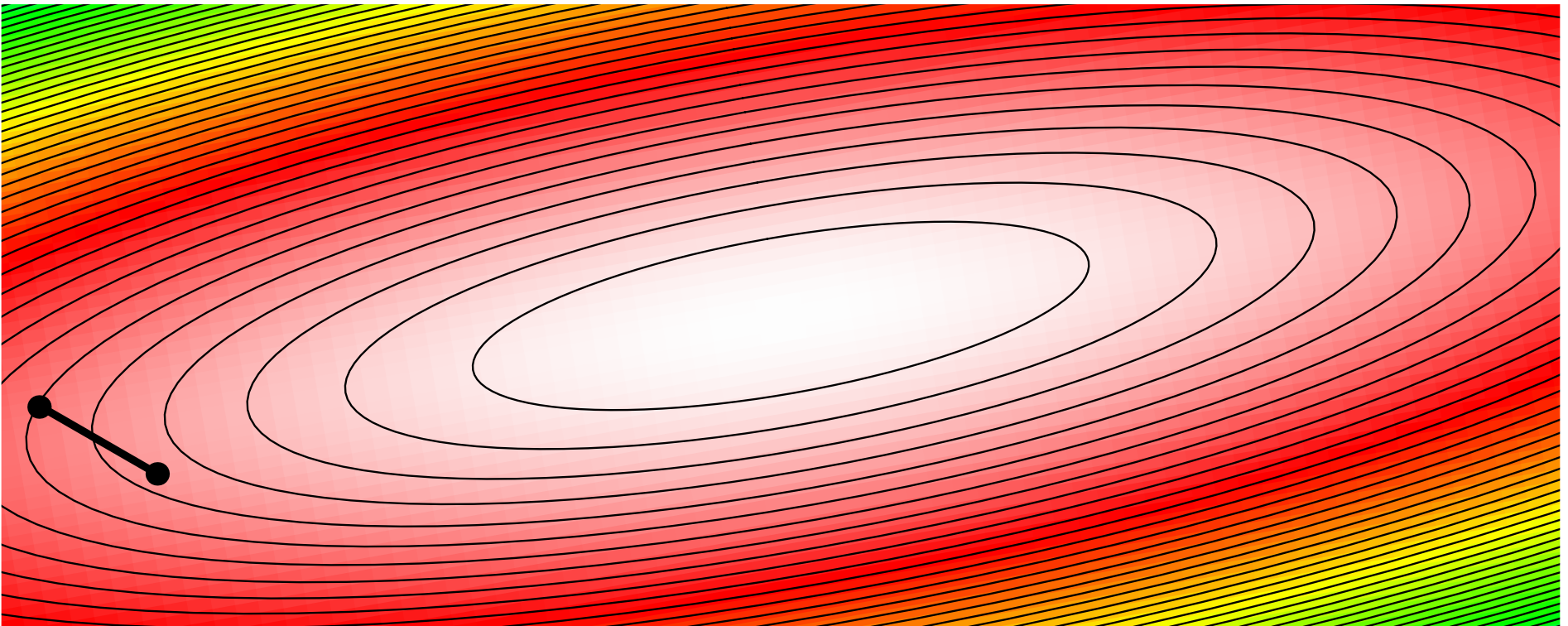
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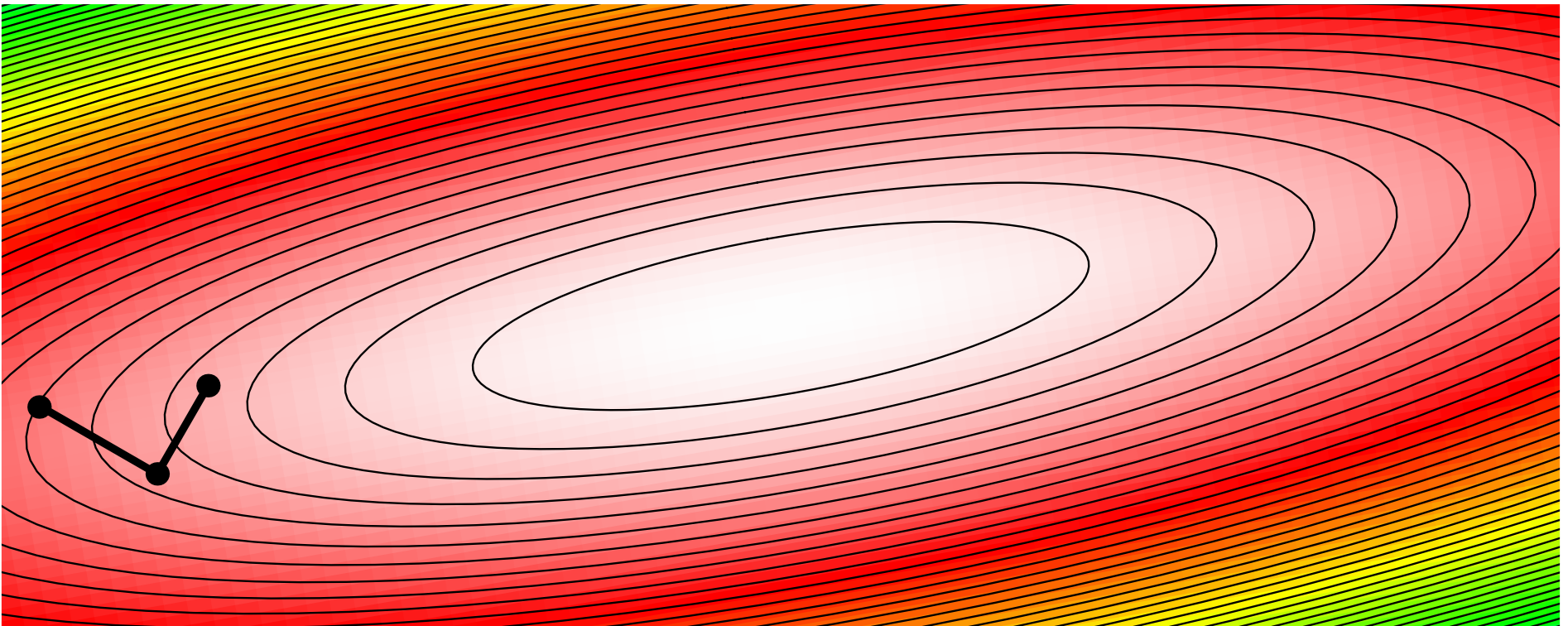
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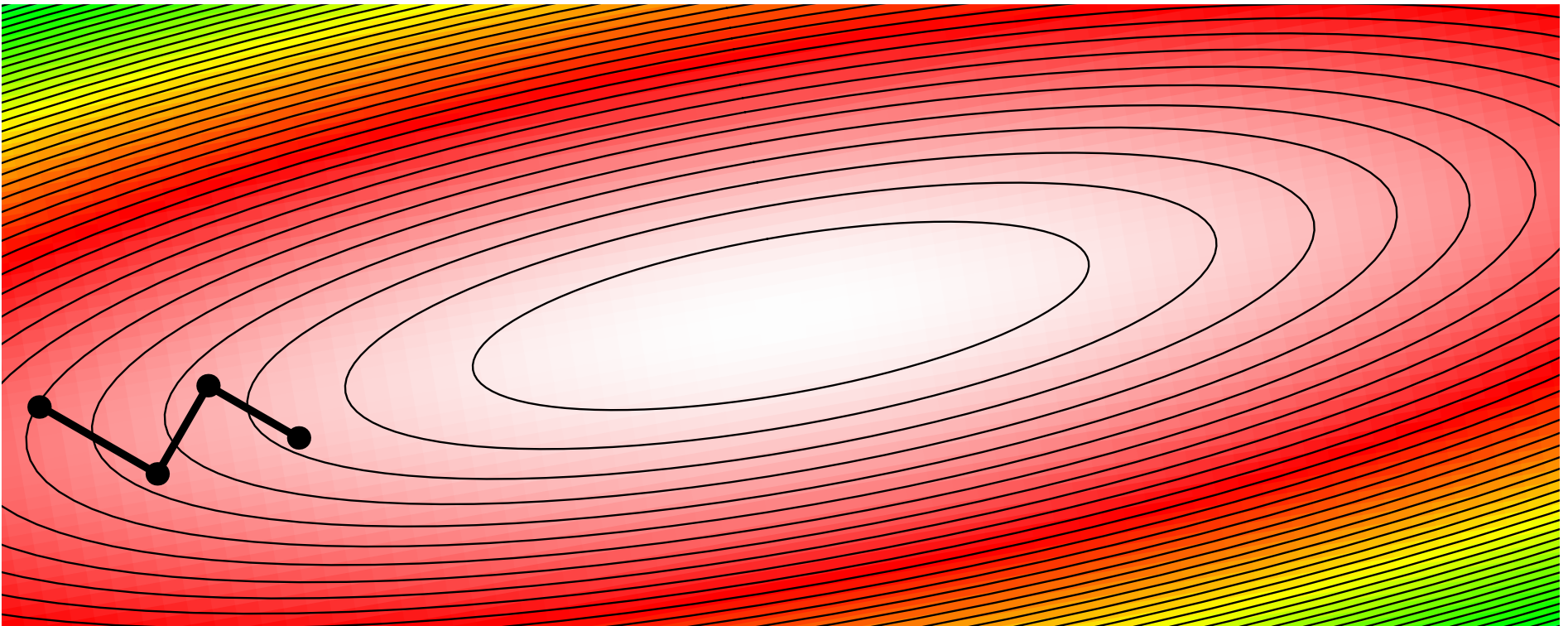
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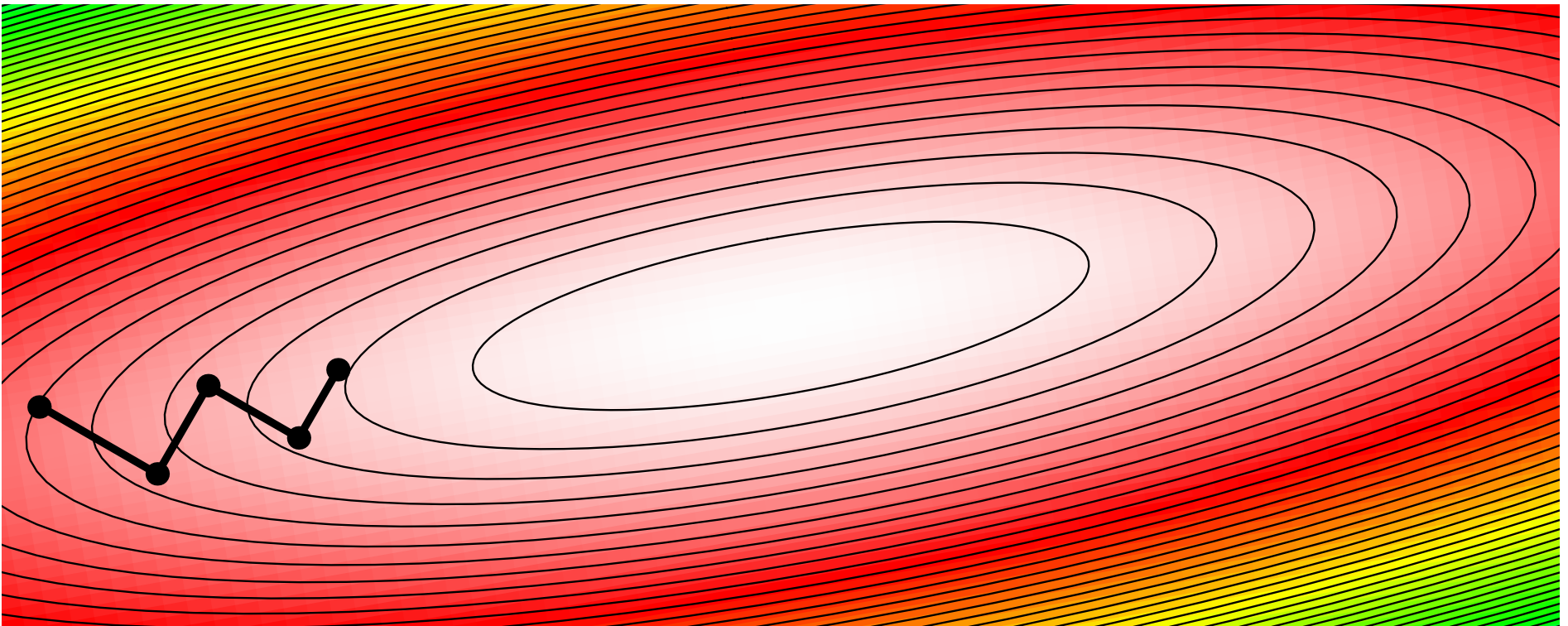
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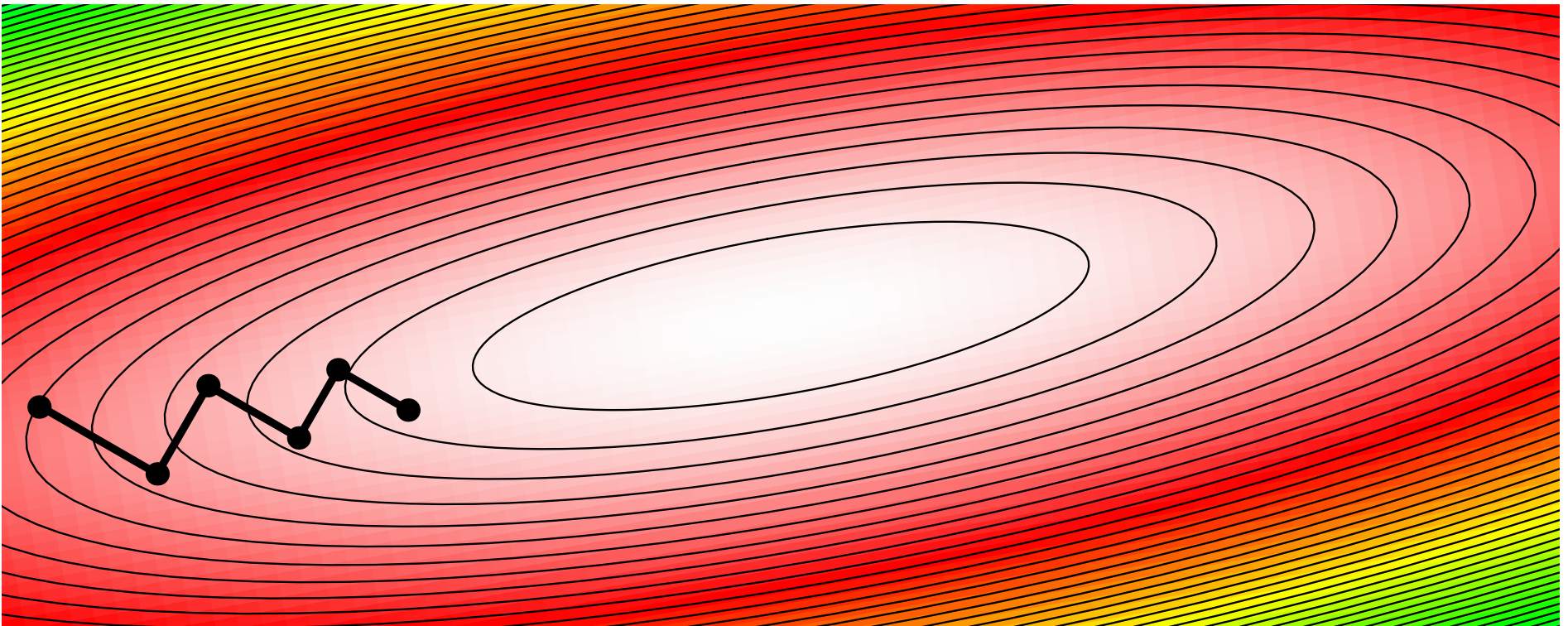
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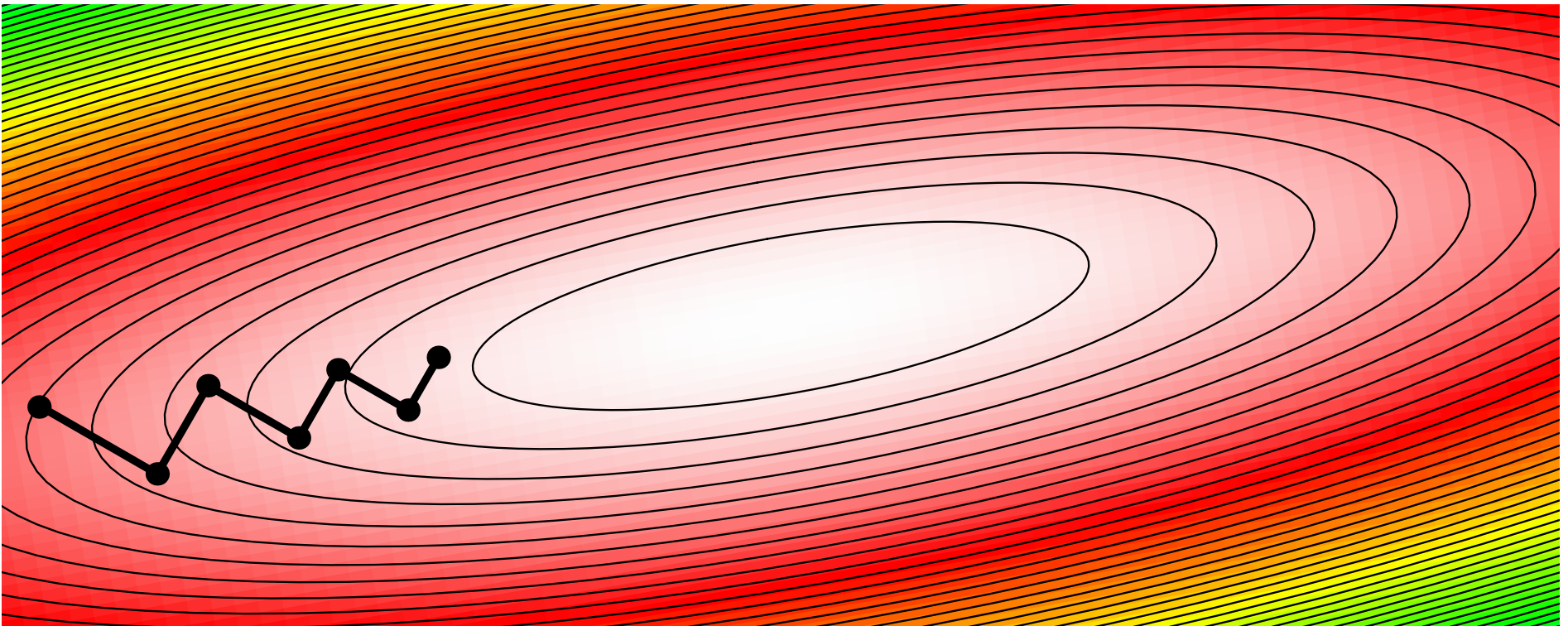
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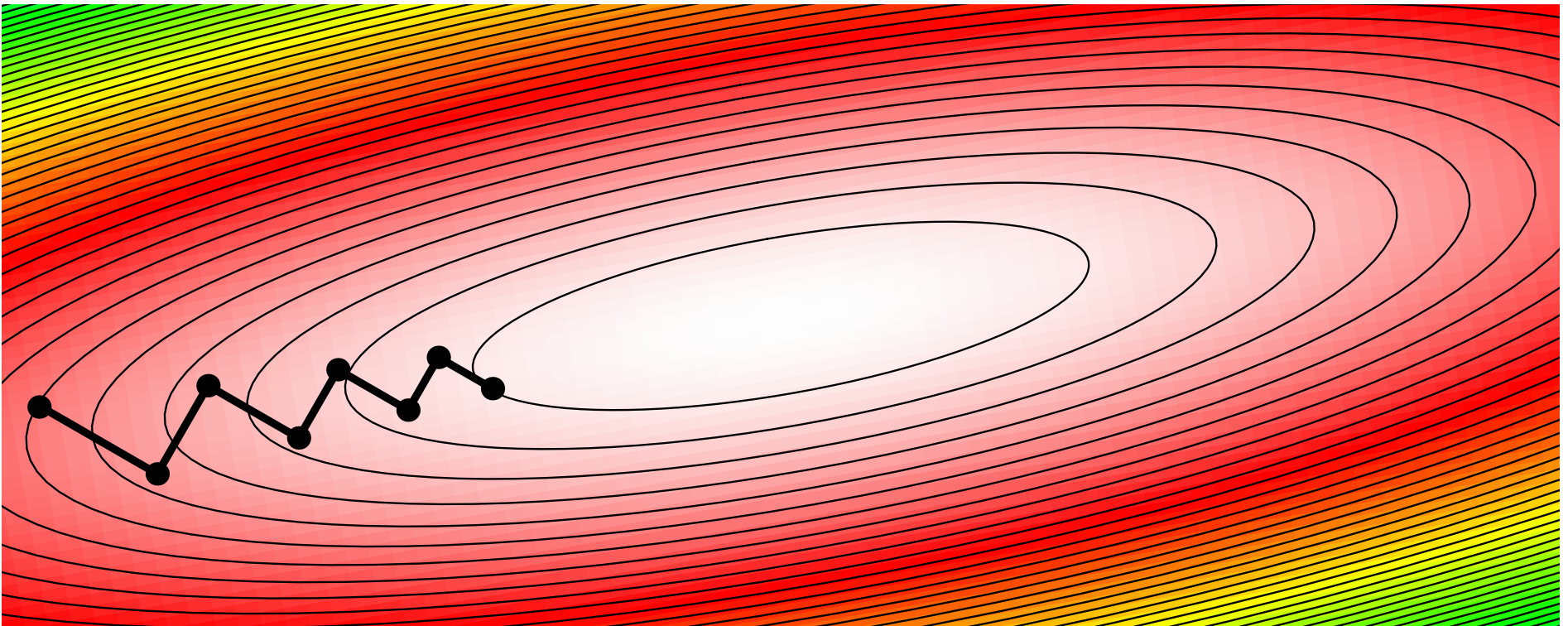
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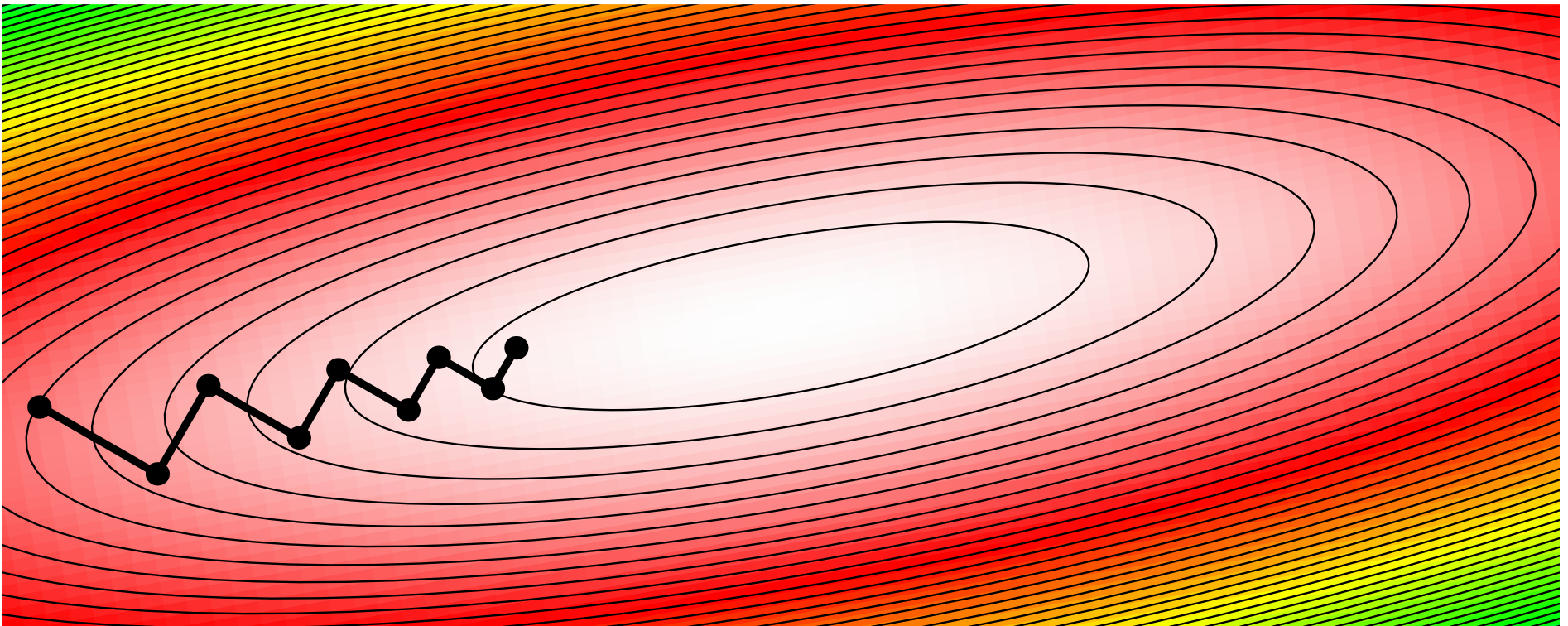
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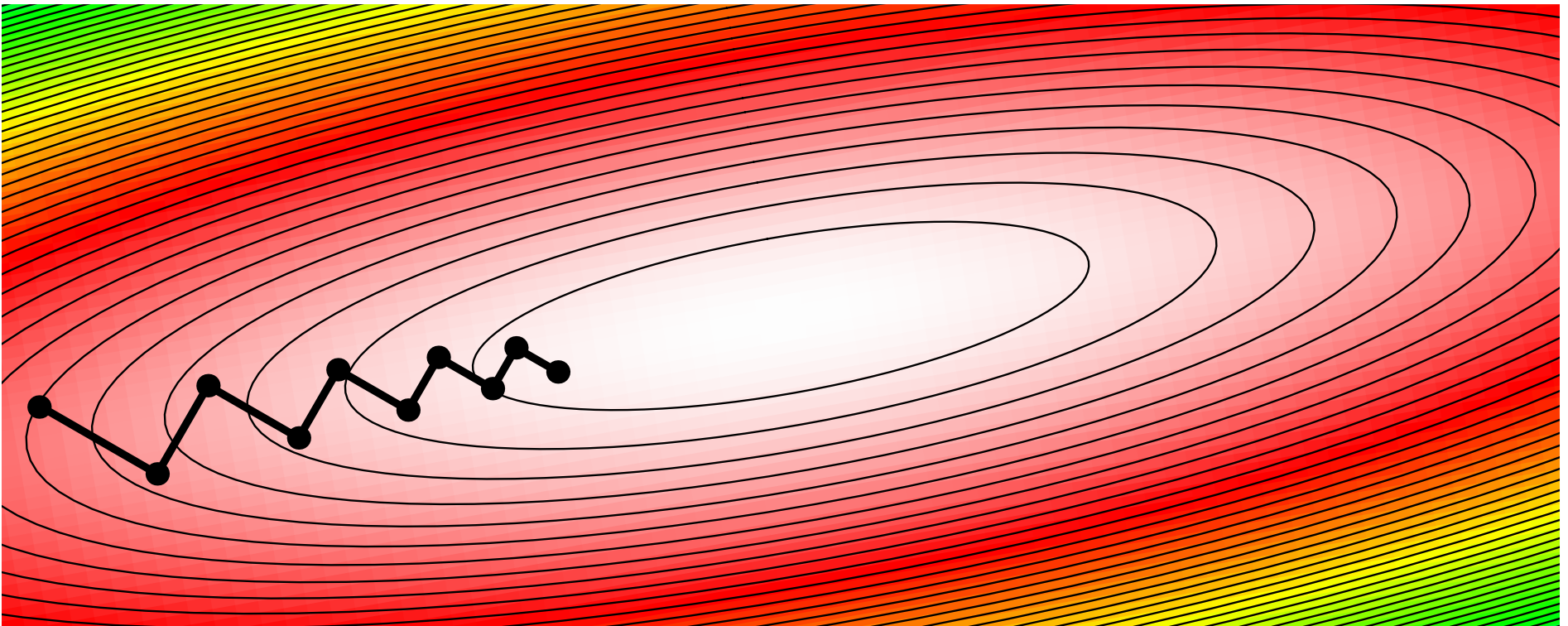
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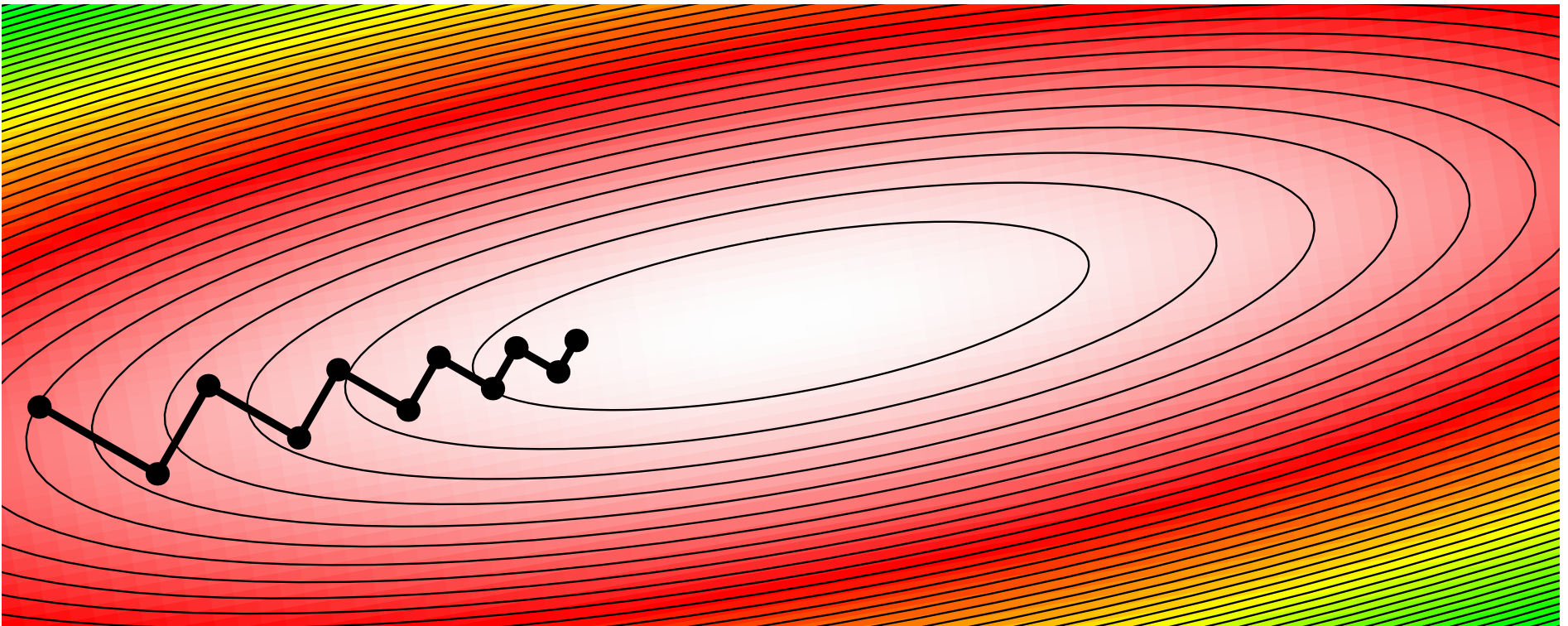
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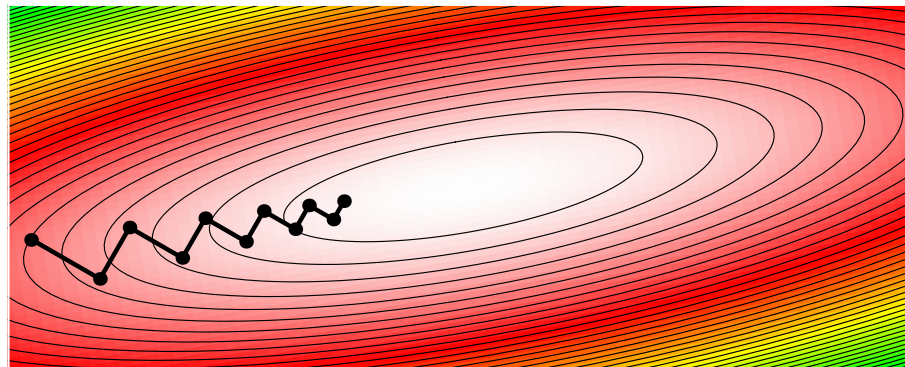
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Zig-Zag

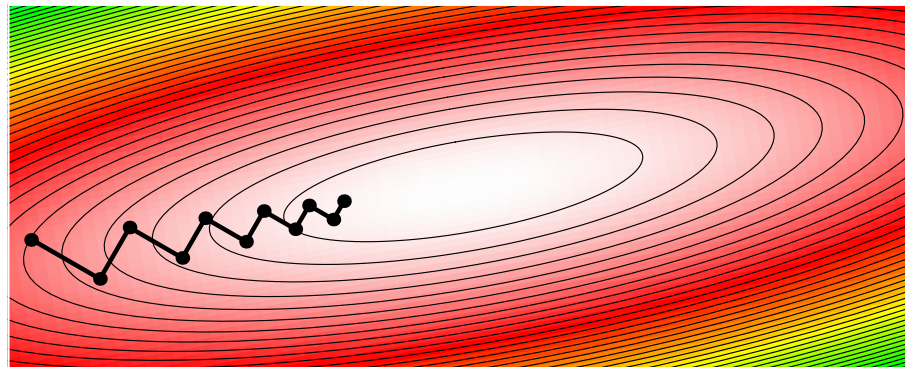
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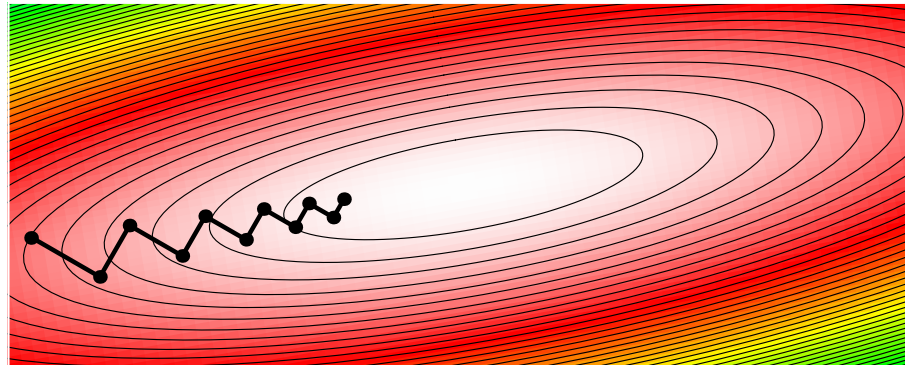
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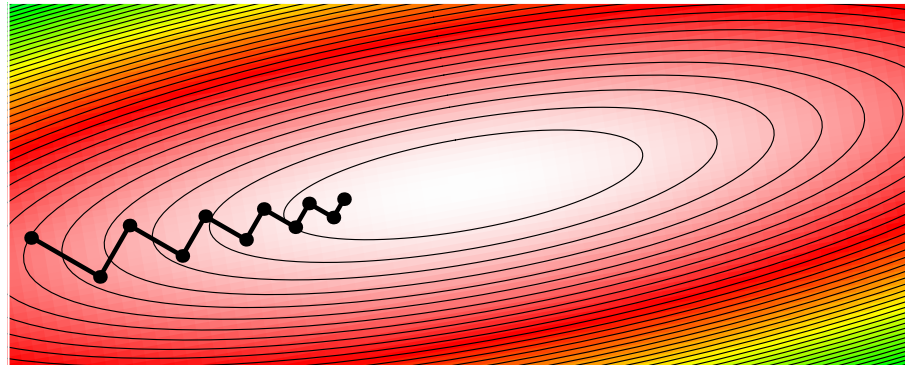
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Better Optimisation Algorithms

- Good optimisation algorithms often compute an approximation of the Hessian
- E.g. Conjugate gradient
 - ★ Performs Line Minimisation
 - ★ 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
 - ★ Used on least squares problem only
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Levenberg-Marquardt

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

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

with $\nabla \epsilon_i(\mathbf{w}^{(k)}) = \nabla f(\mathbf{x}_i|\mathbf{w}^{(k)})$

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

$$L_{\text{approx}}(\mathbf{w}) = \|\epsilon(\mathbf{w}^{(k)}) + \mathbf{J}(\mathbf{w} - \mathbf{w}^{(k)})\|^2$$

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$$\begin{aligned} L_{\text{approx}}(\mathbf{w}) &= \|\epsilon(\mathbf{w}^{(k)}) + \mathbf{J}(\mathbf{w} - \mathbf{w}^{(k)})\|^2 \\ &= \epsilon(\mathbf{w}^{(k)})^\top \epsilon(\mathbf{w}^{(k)}) + 2(\mathbf{w} - \mathbf{w}^{(k)})^\top \mathbf{J}^\top \epsilon(\mathbf{w}^{(k)}) \\ &\quad + (\mathbf{w} - \mathbf{w}^{(k)})^\top \mathbf{J}^\top \mathbf{J} (\mathbf{w} - \mathbf{w}^{(k)}) \end{aligned}$$

Trust Region

- Solution given by $\nabla_{\mathbf{w}} L_{approx}(\mathbf{w}) = 0$ gives

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - (\mathbf{J}^T \mathbf{J})^{-1} \mathbf{J}^T \boldsymbol{\epsilon}(\mathbf{w}^{(k)})$$

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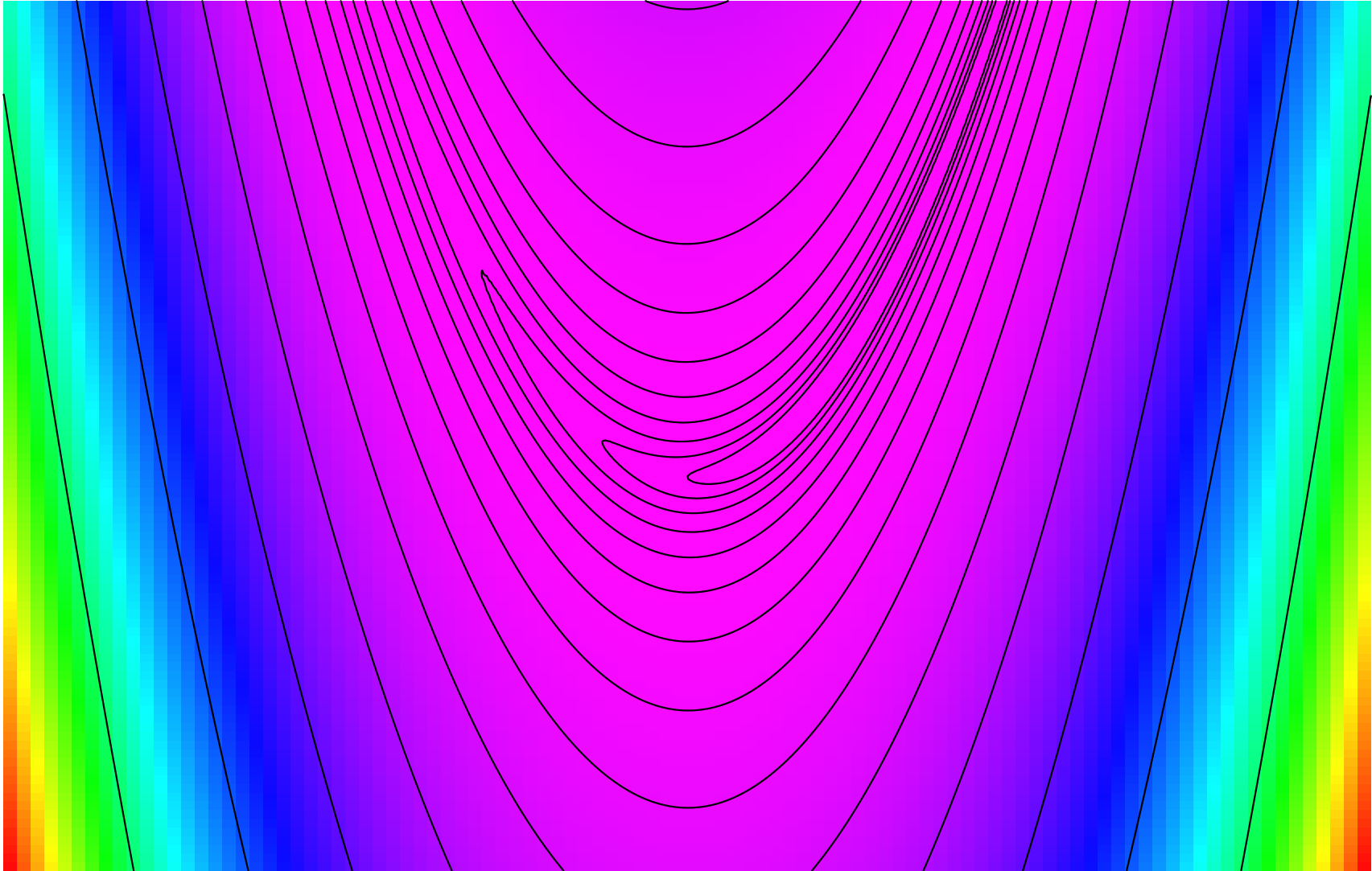
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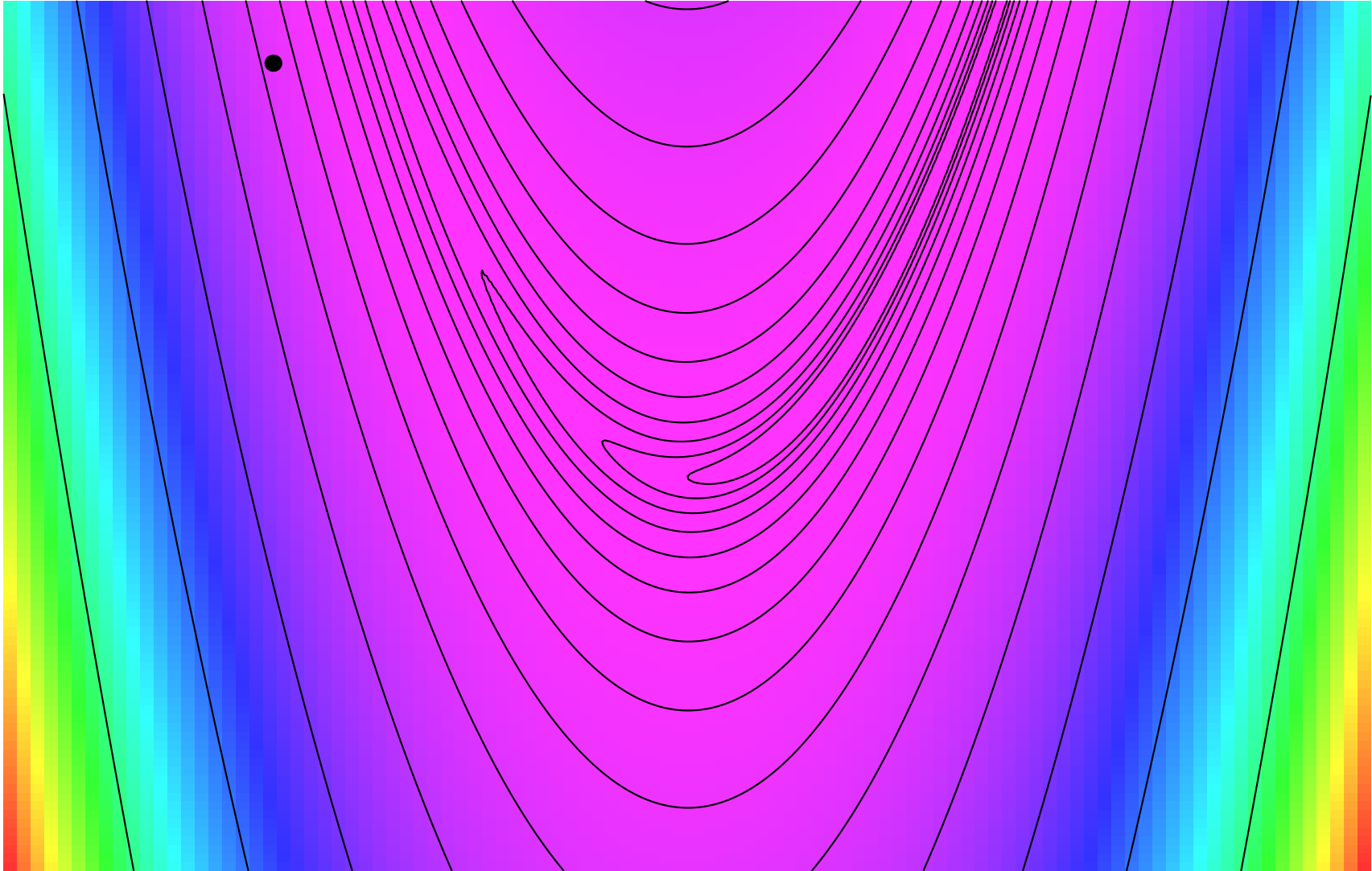
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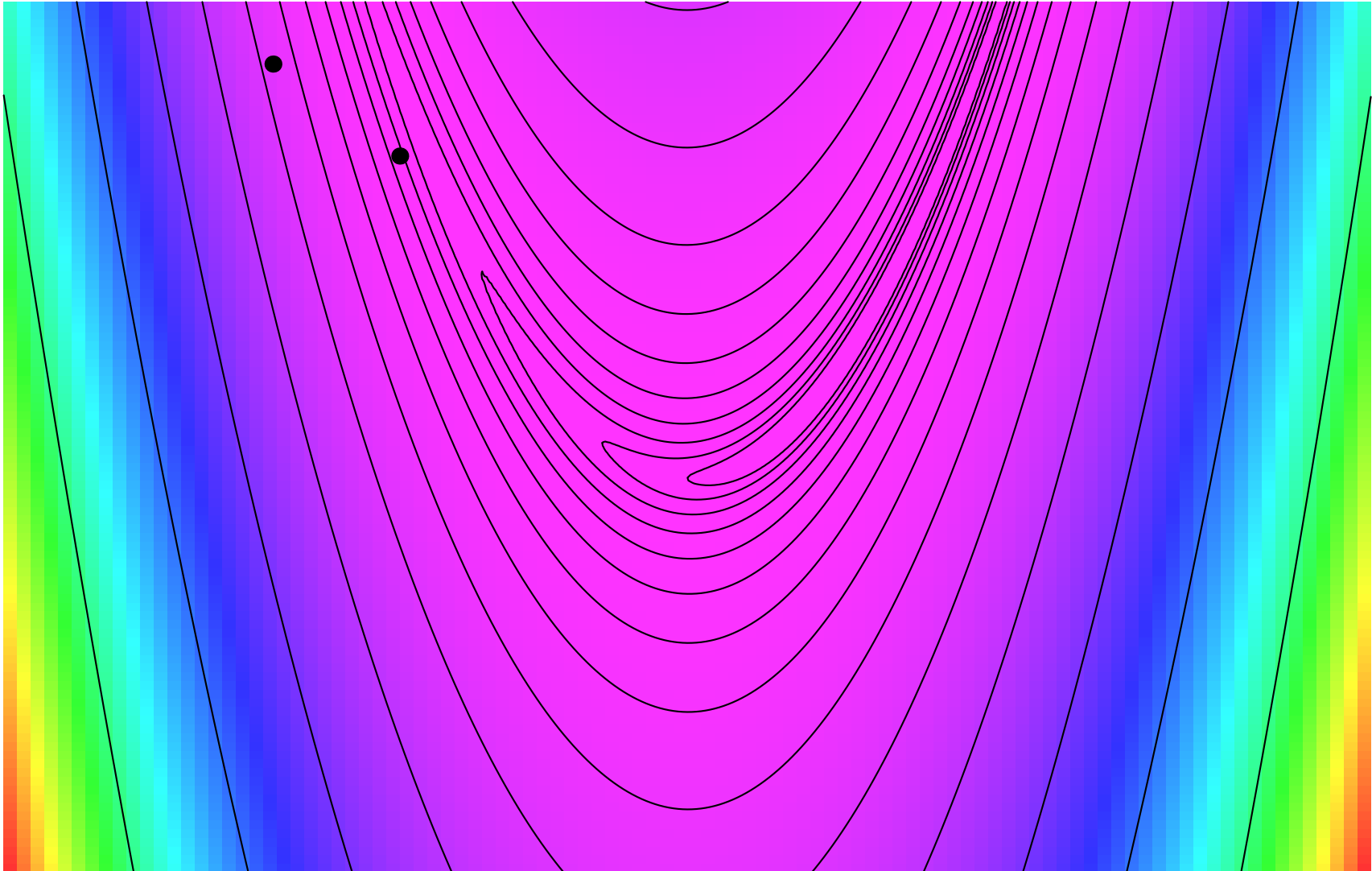
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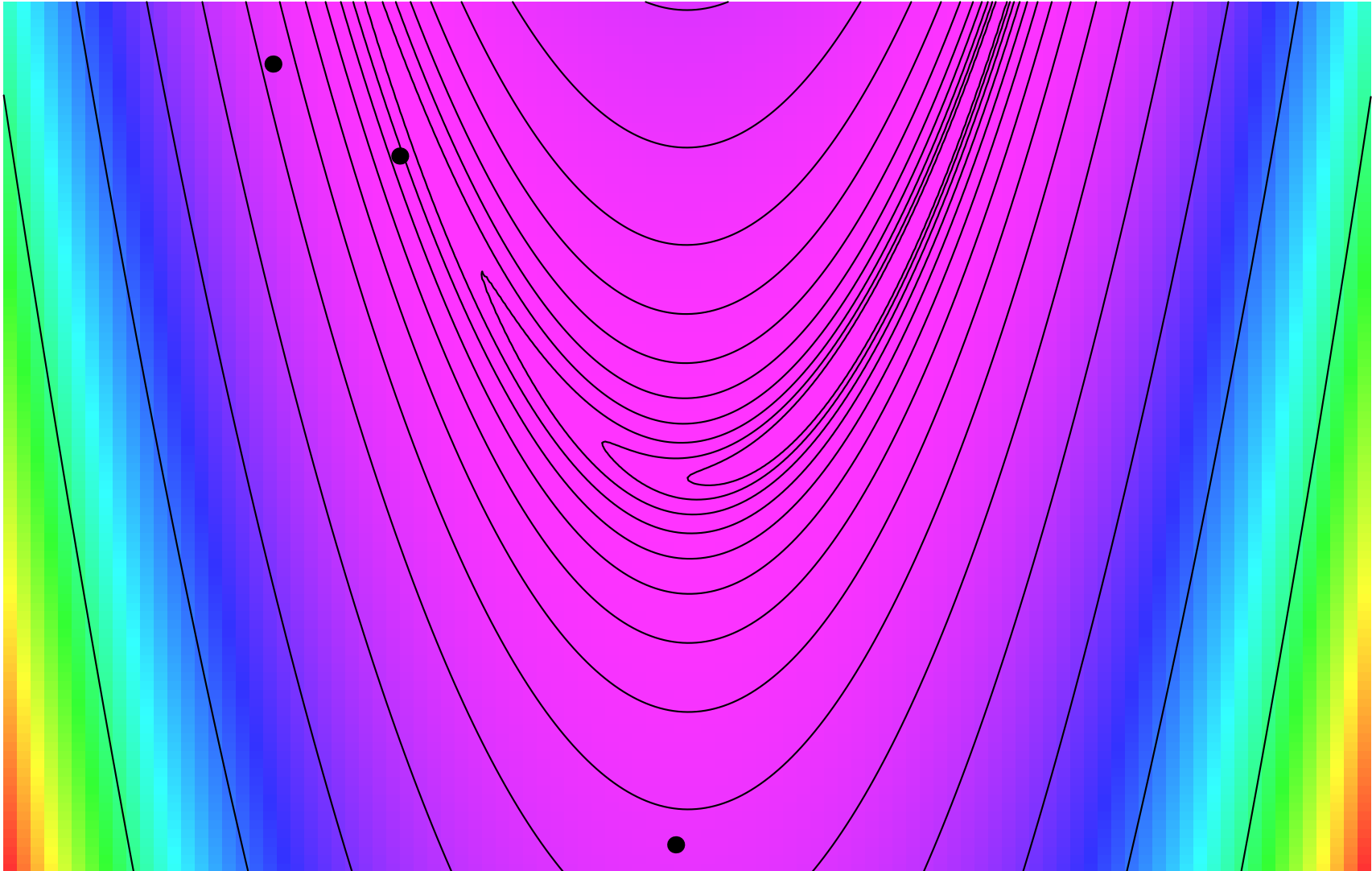
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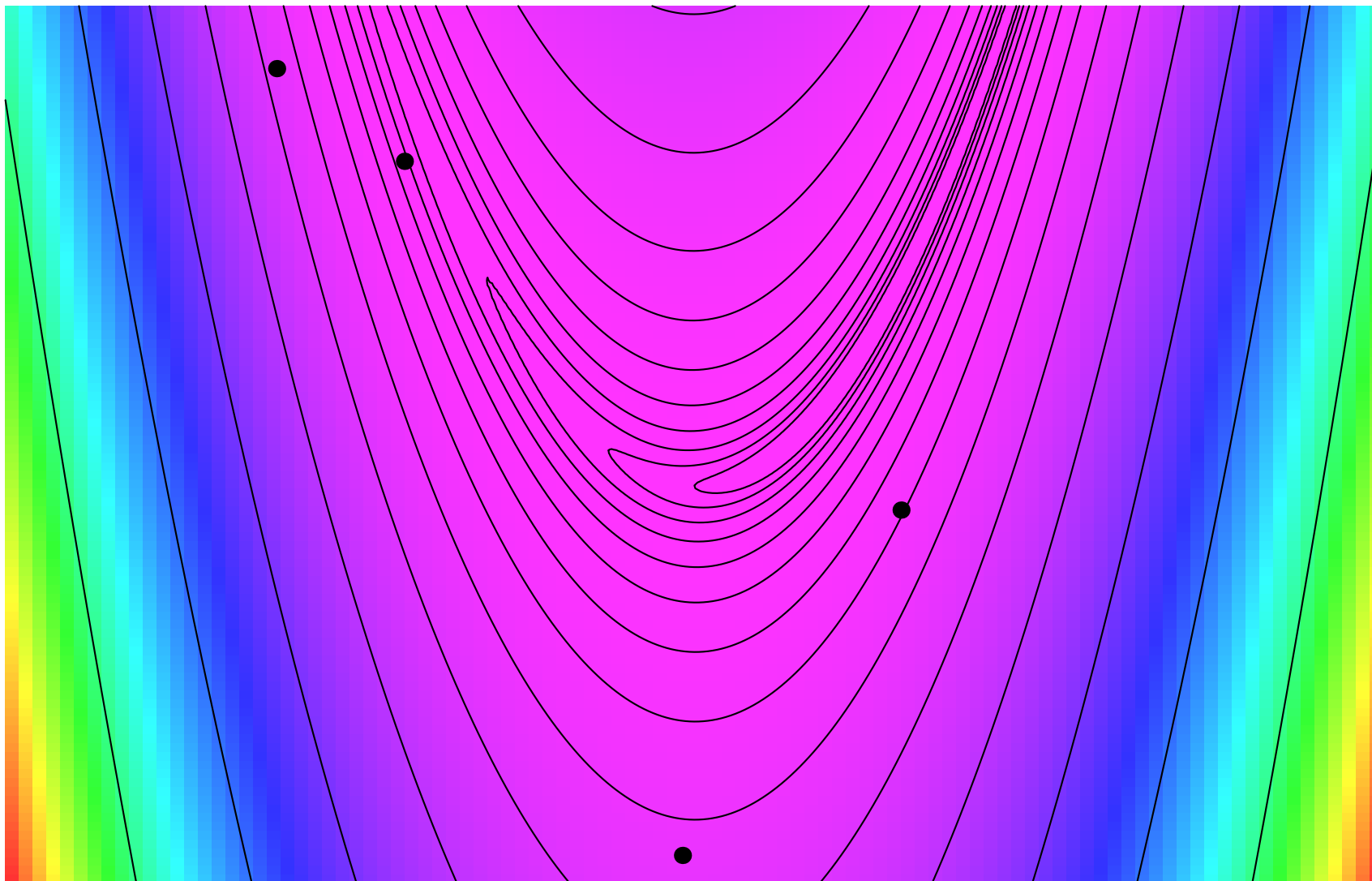
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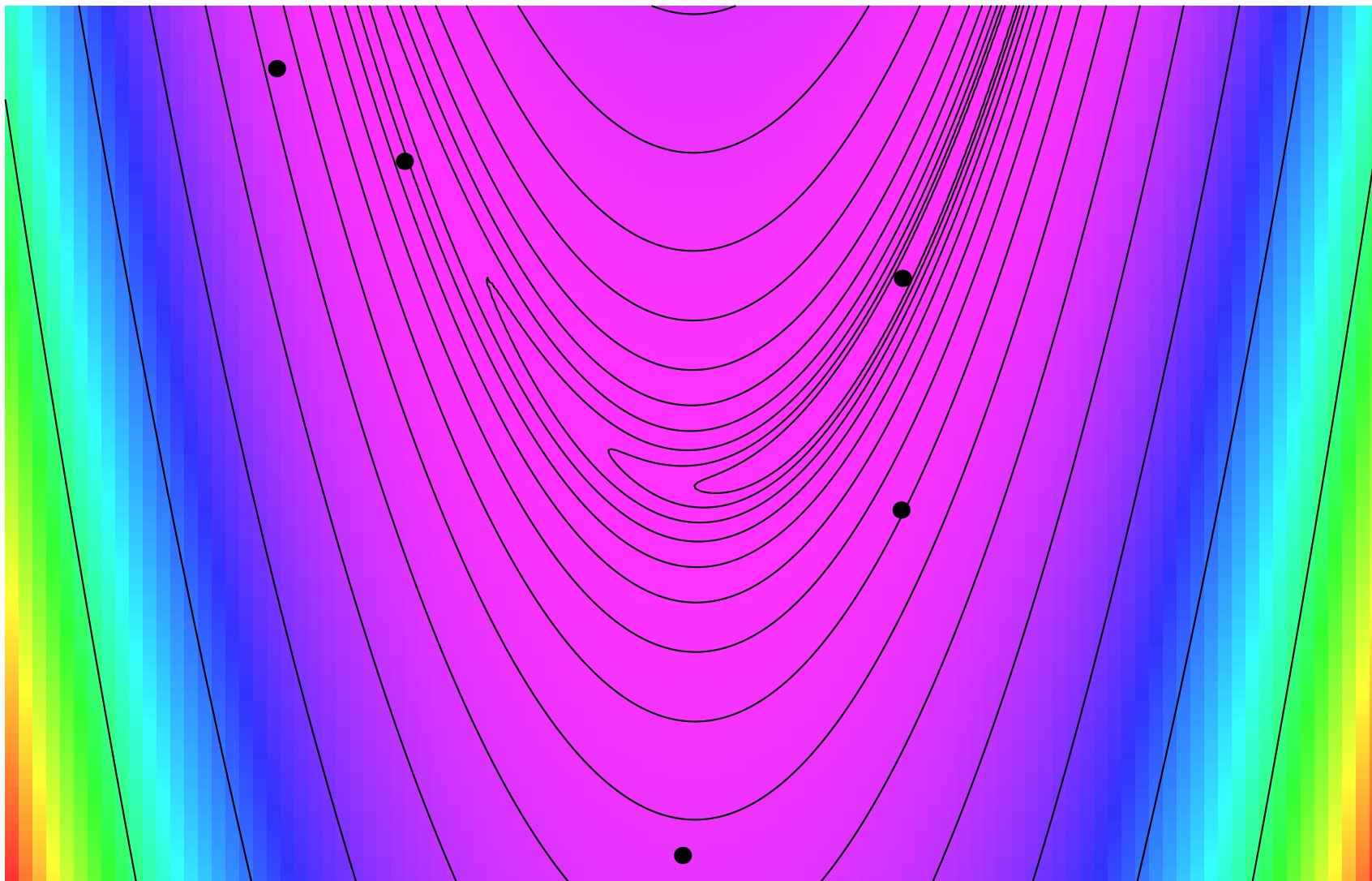
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Summary

- 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
- There exist a number of **pseudo-Newton methods** (conjugate gradient, Levenberg-Marquardt, etc.) that approximates Newton's method often without explicitly computing the Hessian

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