Metodi Numerici dell'Informatica

Discesa del gradiente

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SAPIENZA
UNIVERSITÀ DI ROMA

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Is there a general recipe to solve problems of this form, with f differentiable?

$$\min_{\mathbf{x}} f(\mathbf{x})$$

Gradient descent: Intuition

Gradient descent is a first-order iterative minimization algorithm.

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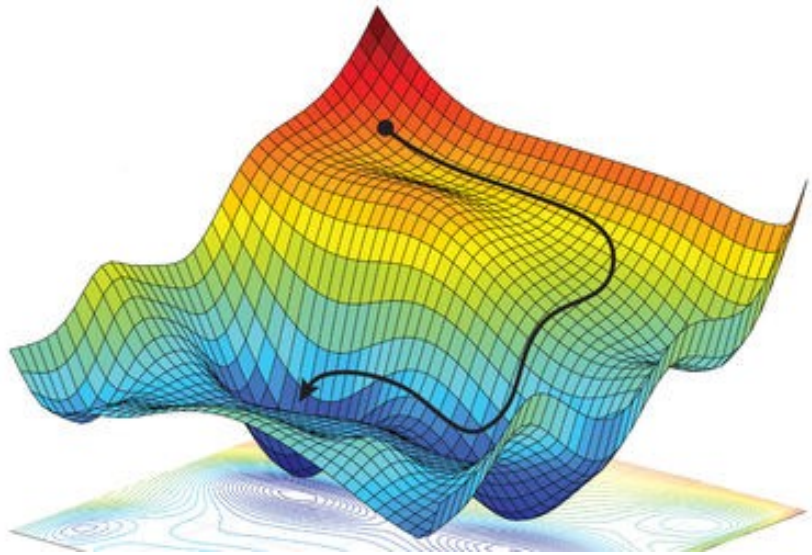
Example of an energy $f : \mathbb{R}^2 \to \mathbb{R}$:



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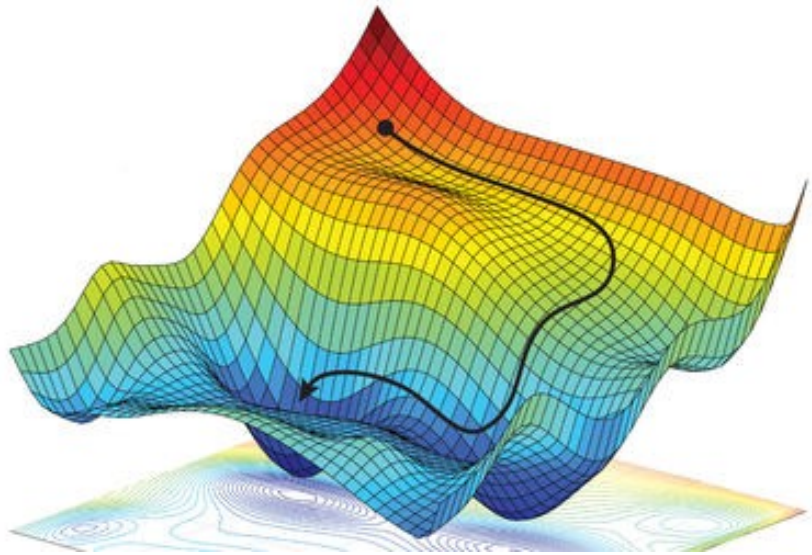

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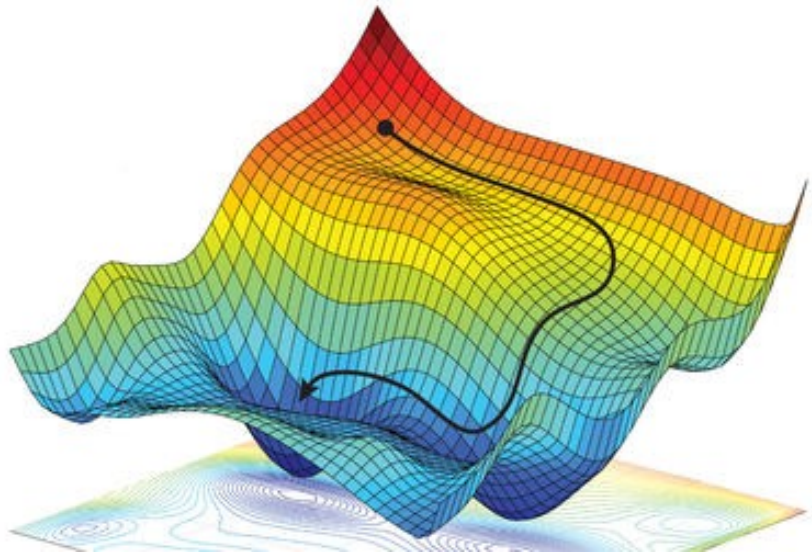

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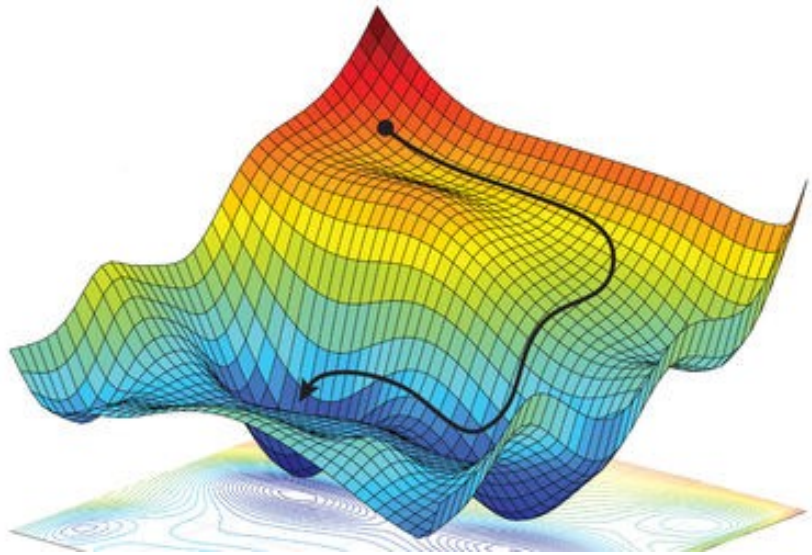

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3. Stop when a minimum is reached.

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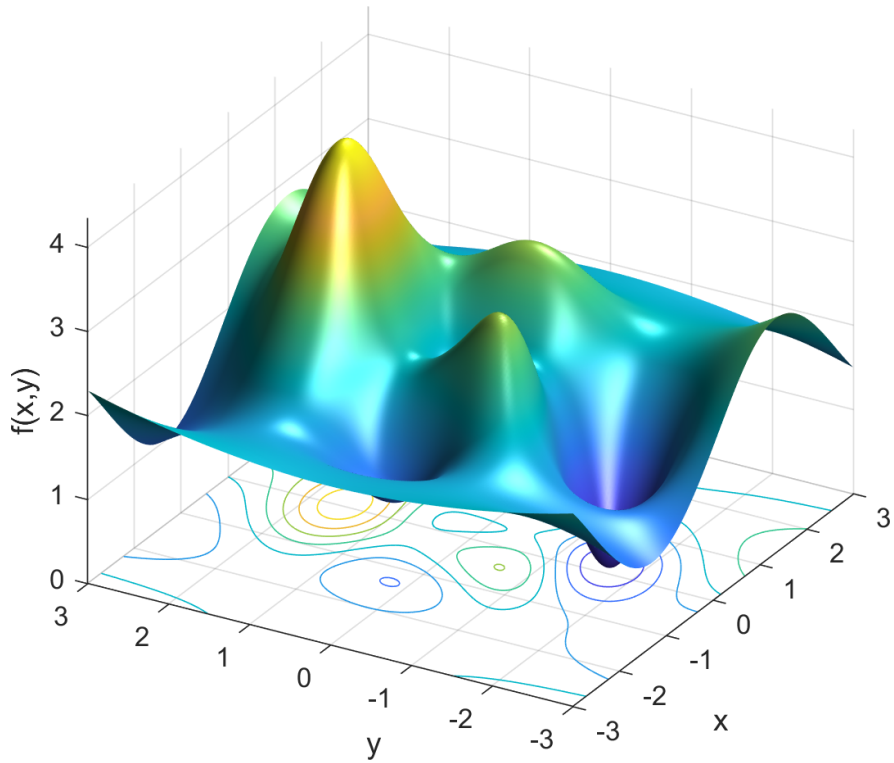

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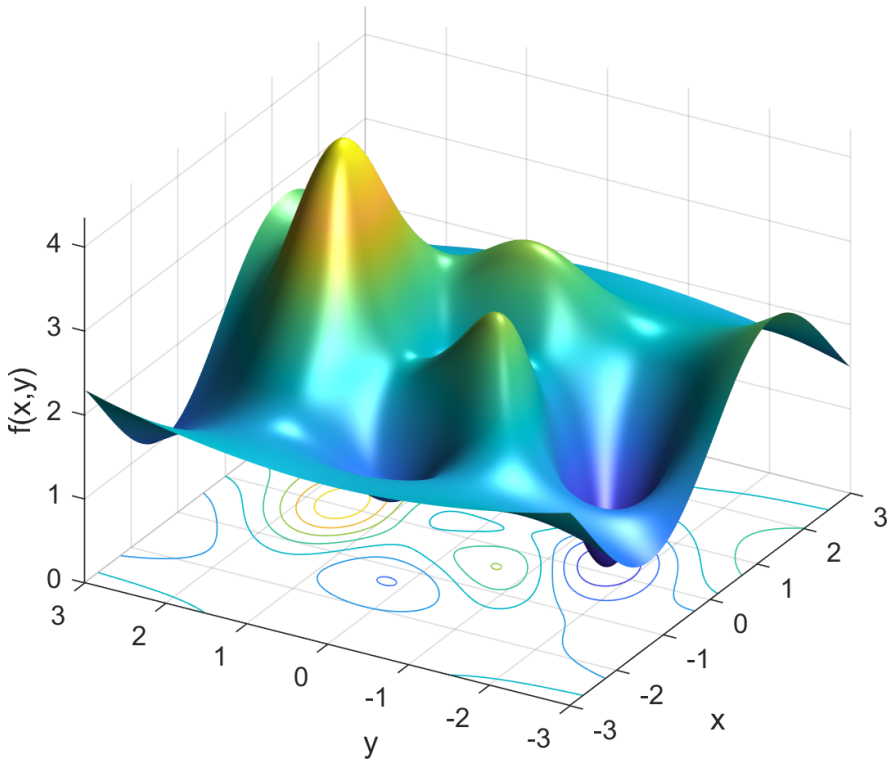

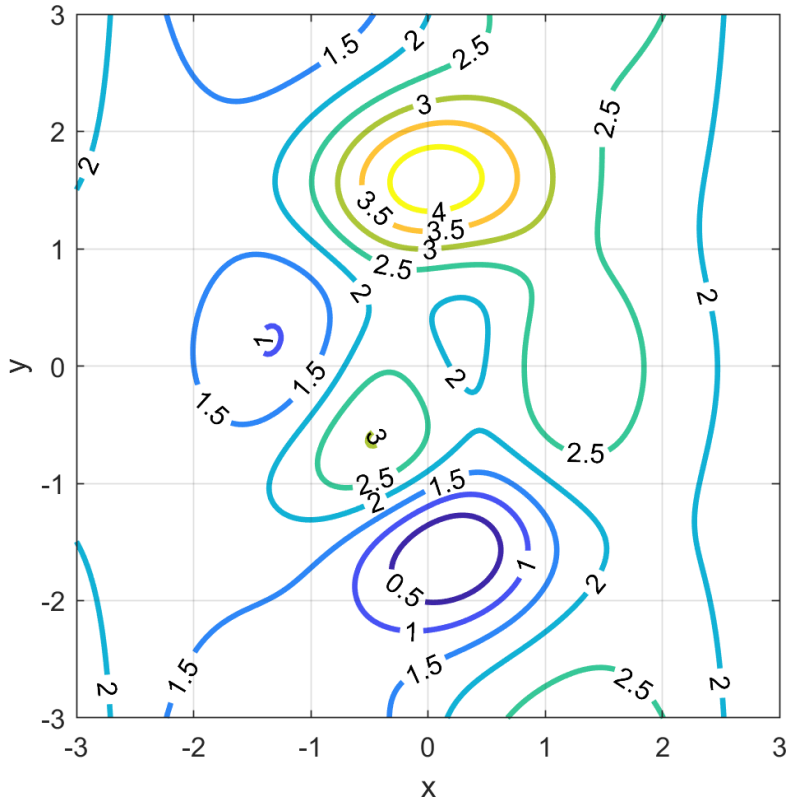

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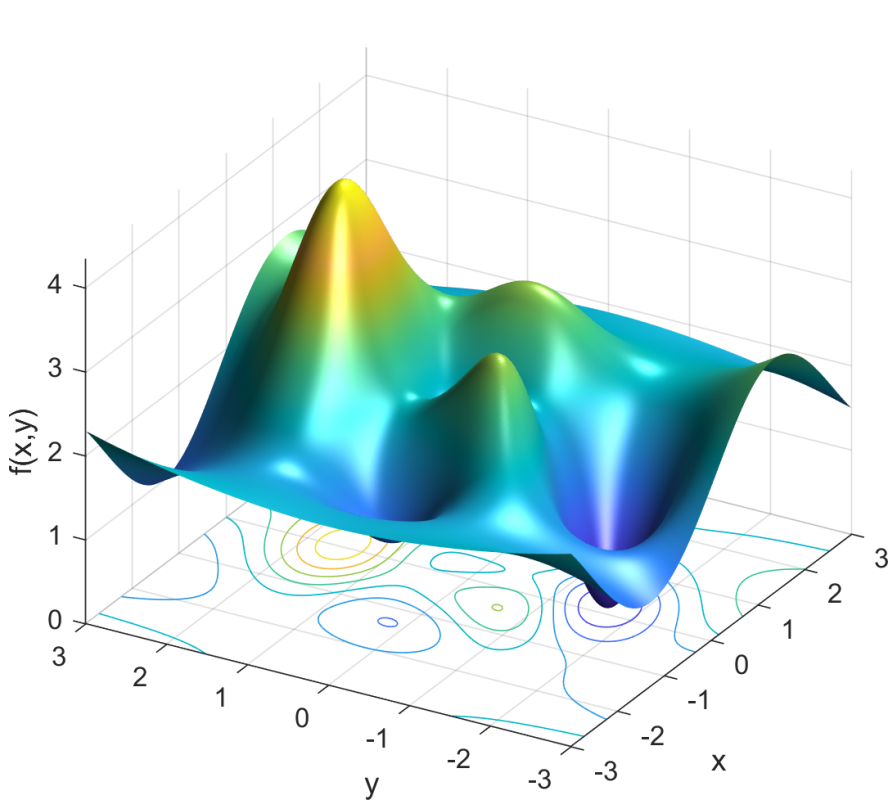

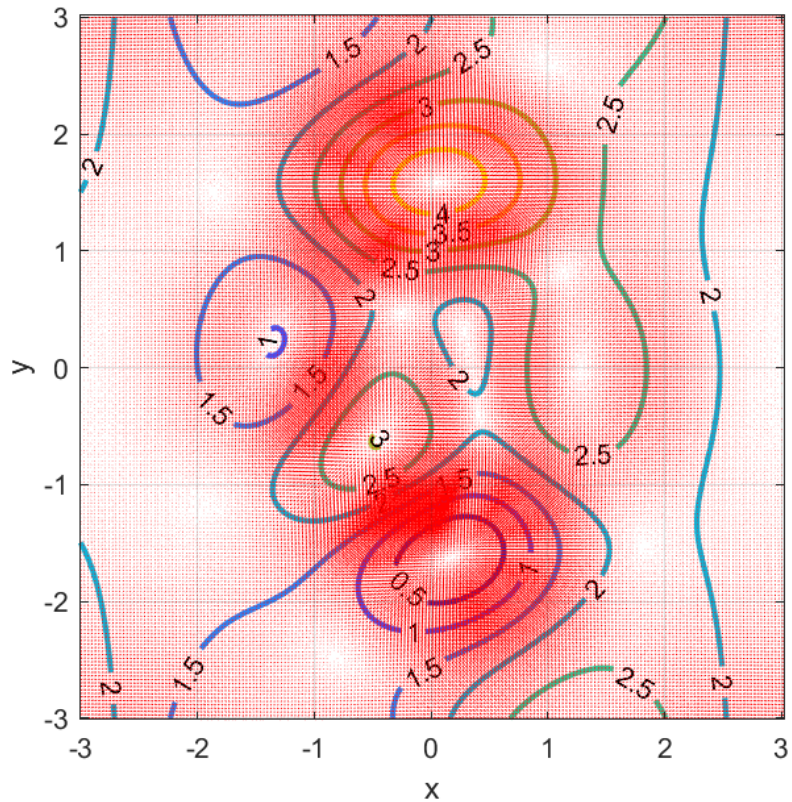

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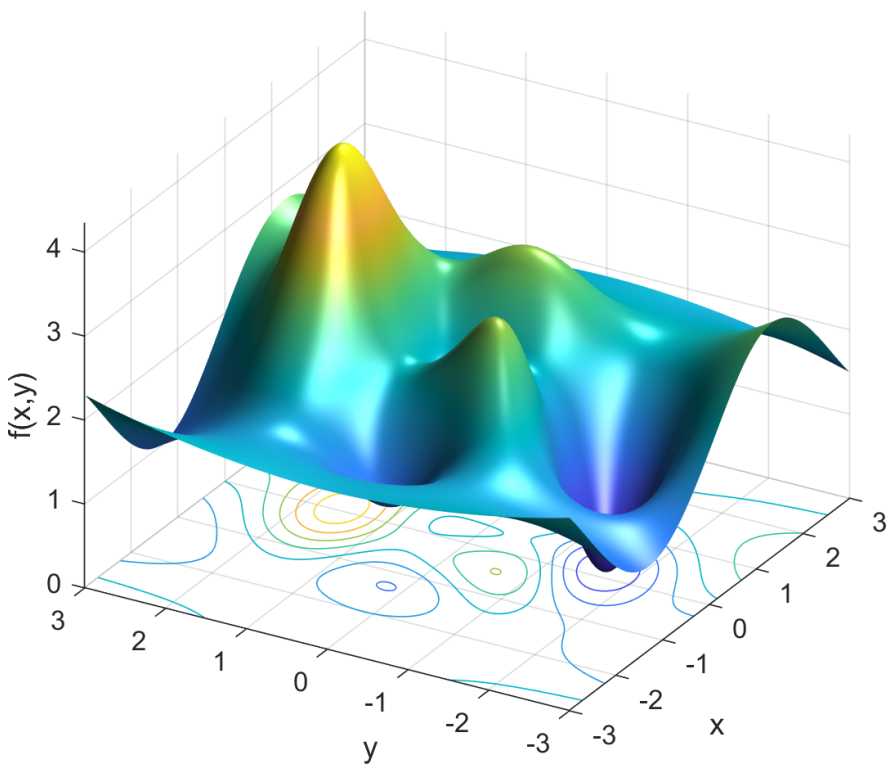

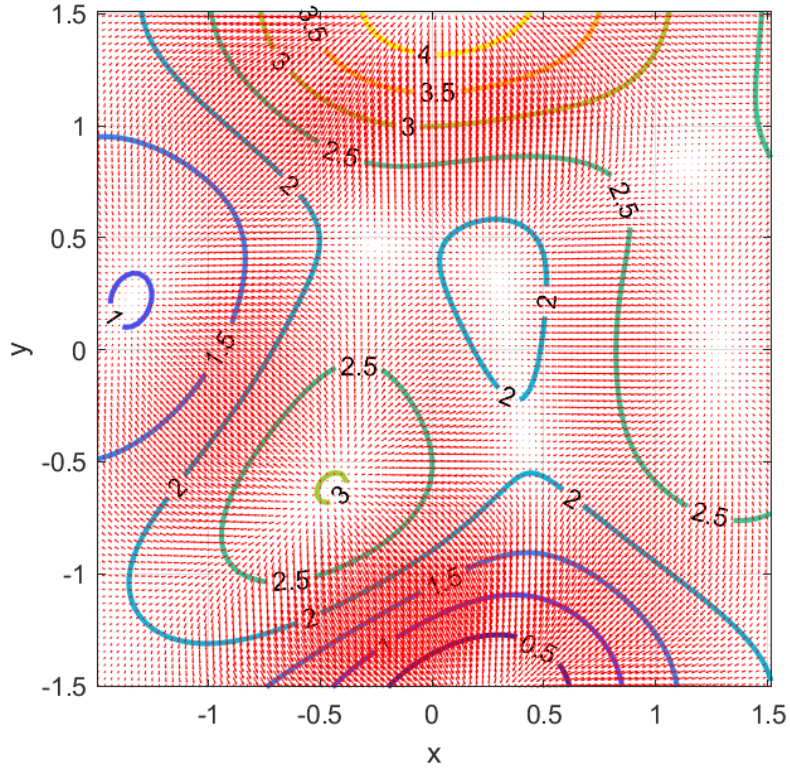

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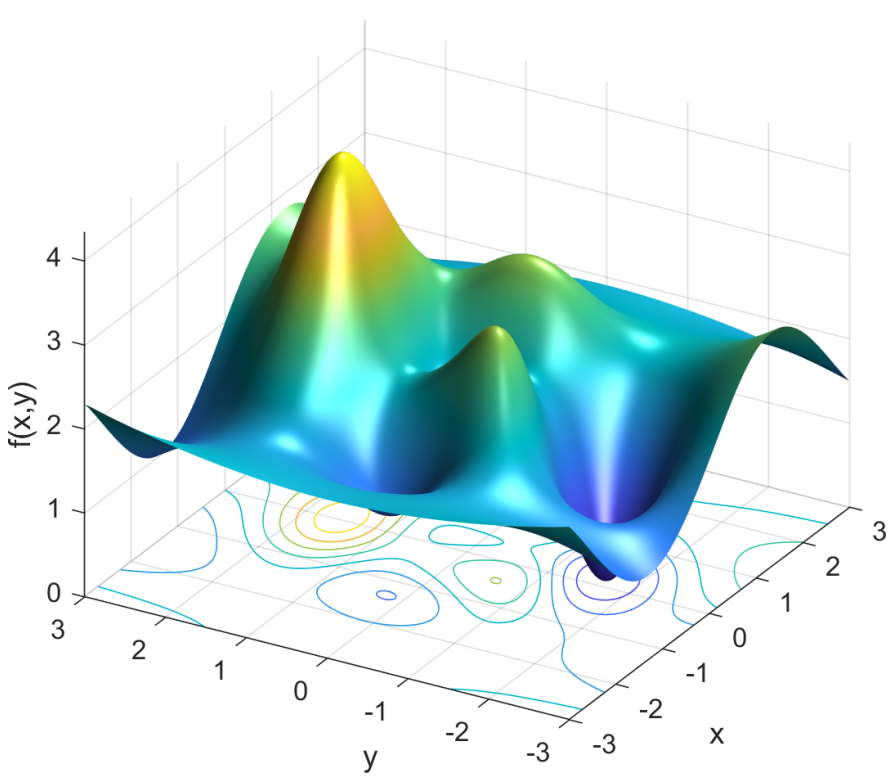

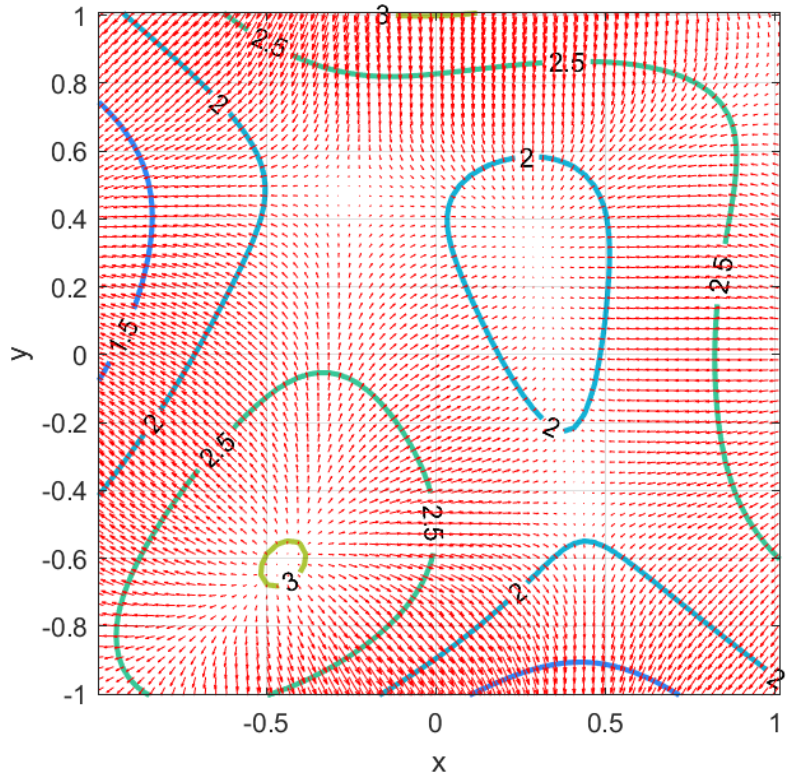

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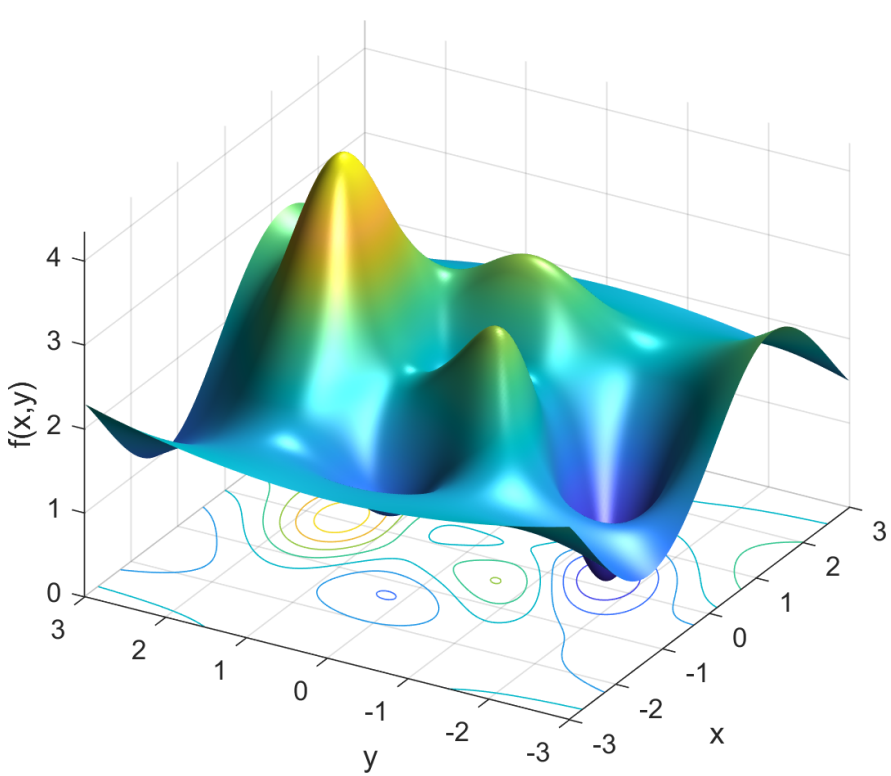

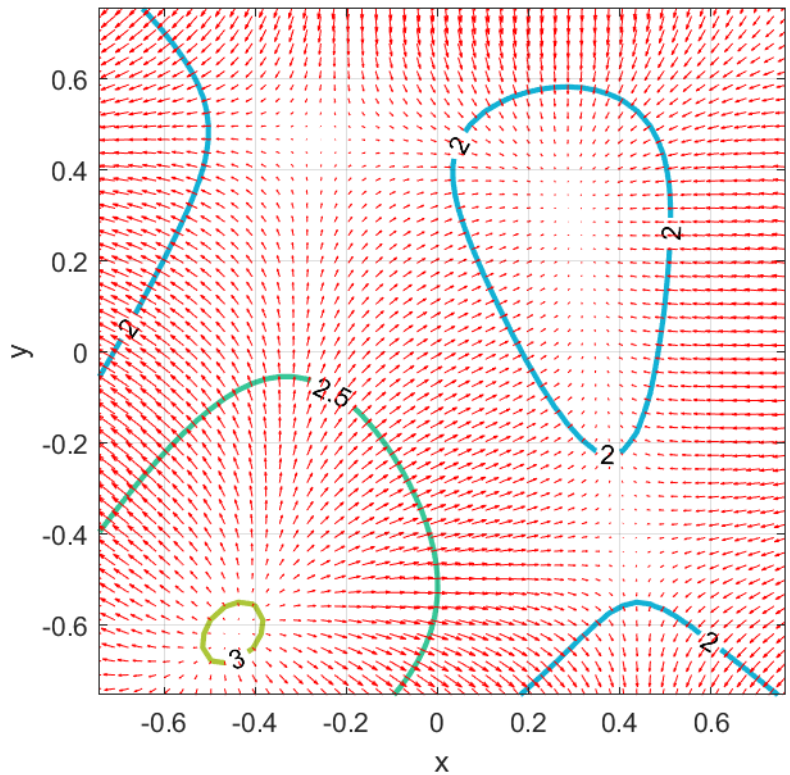

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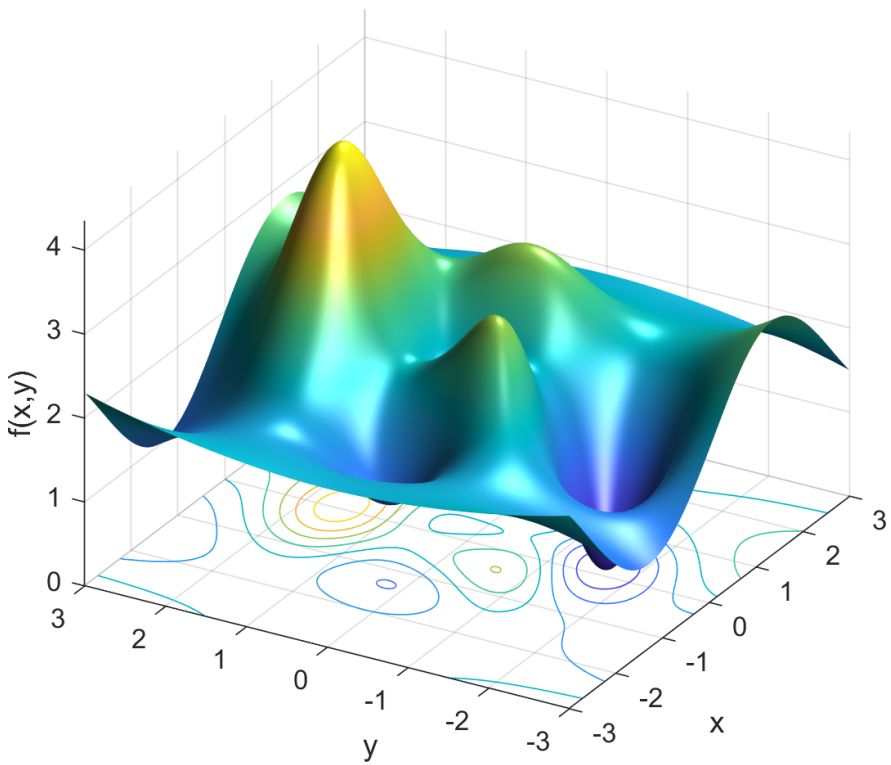

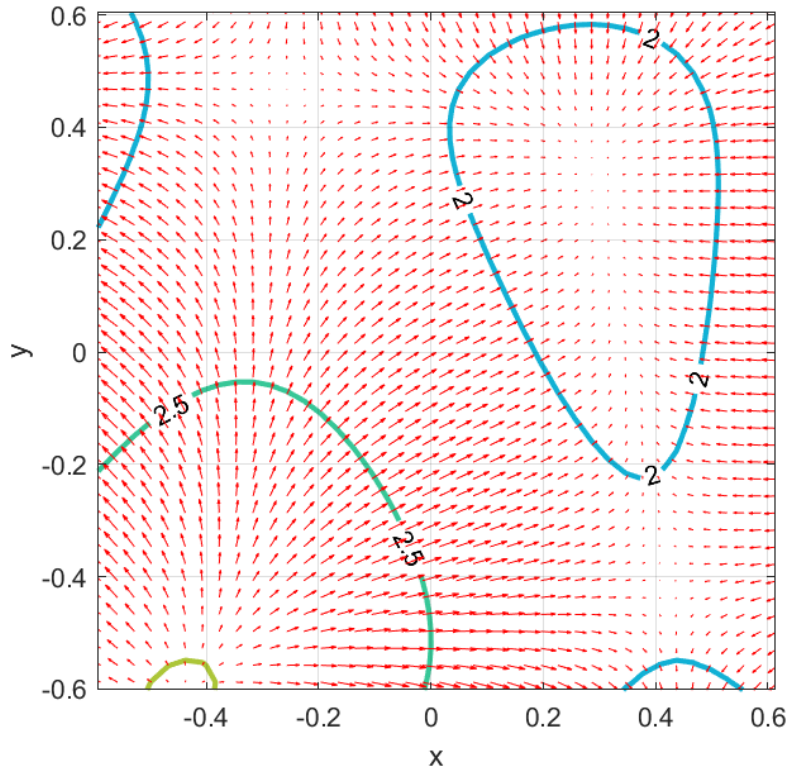

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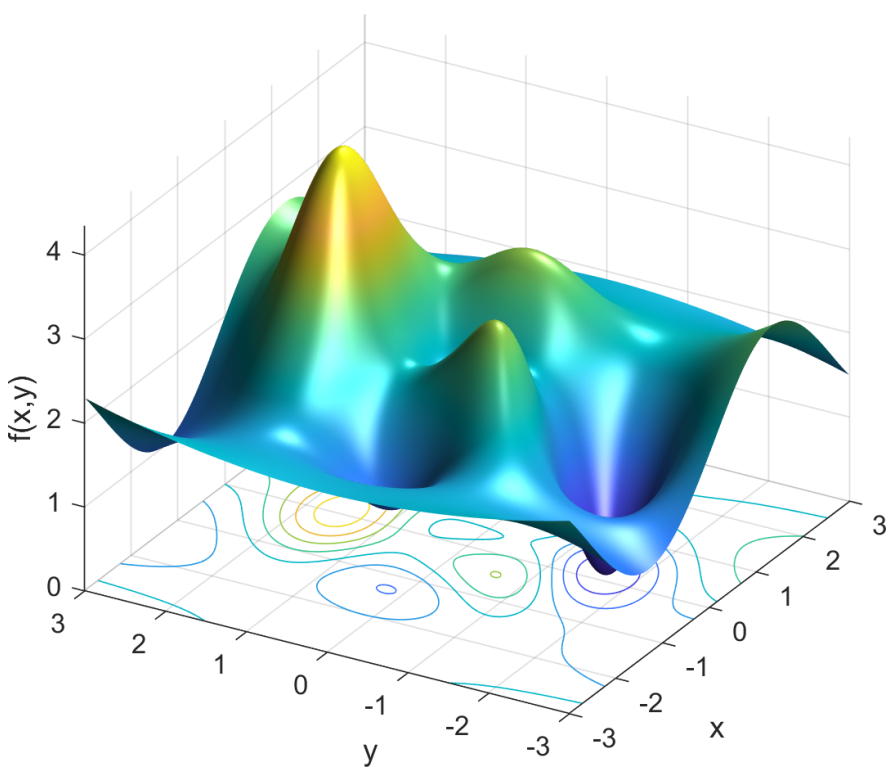
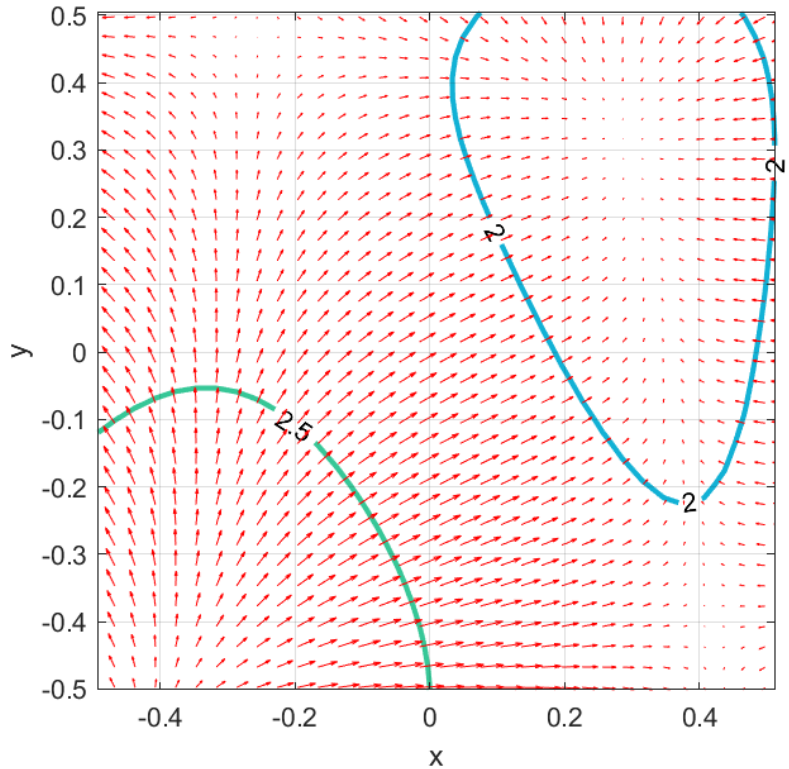
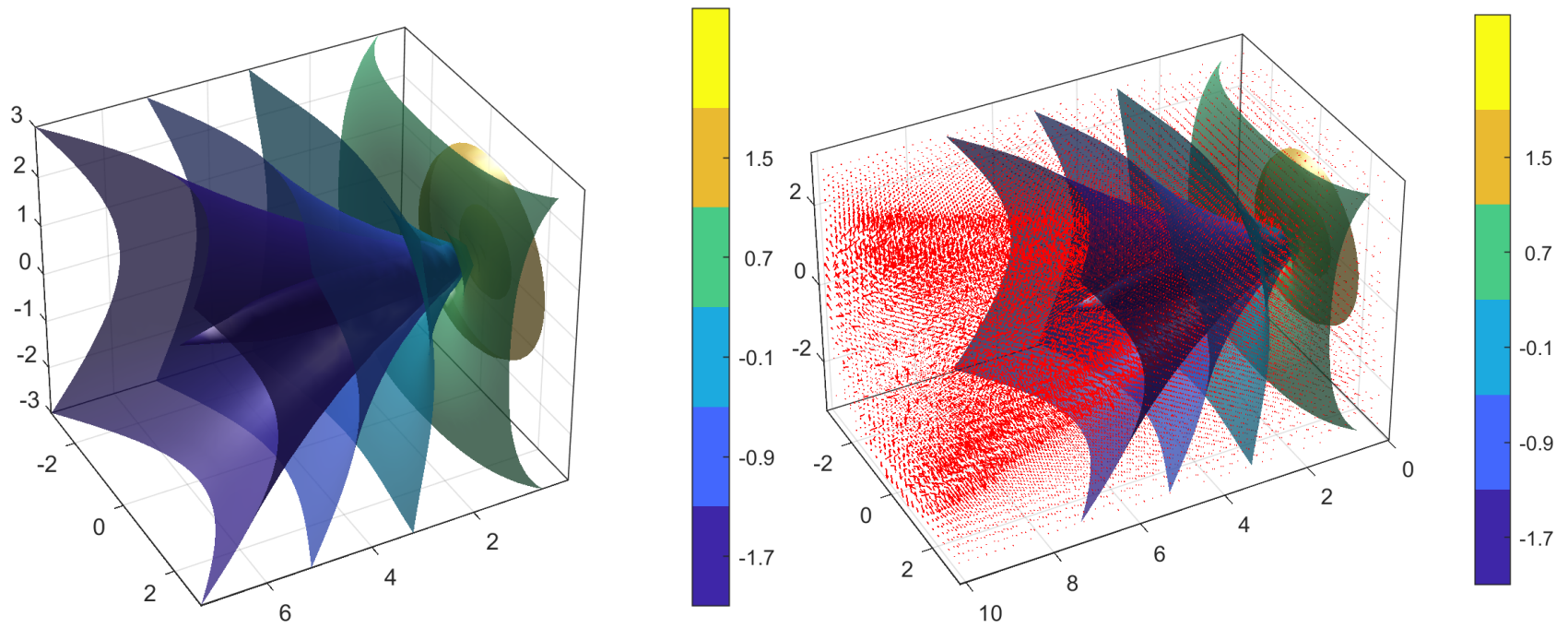




Gradient descent: High dimensions

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$



All we say is also valid in $\gg 2$ dimensions.

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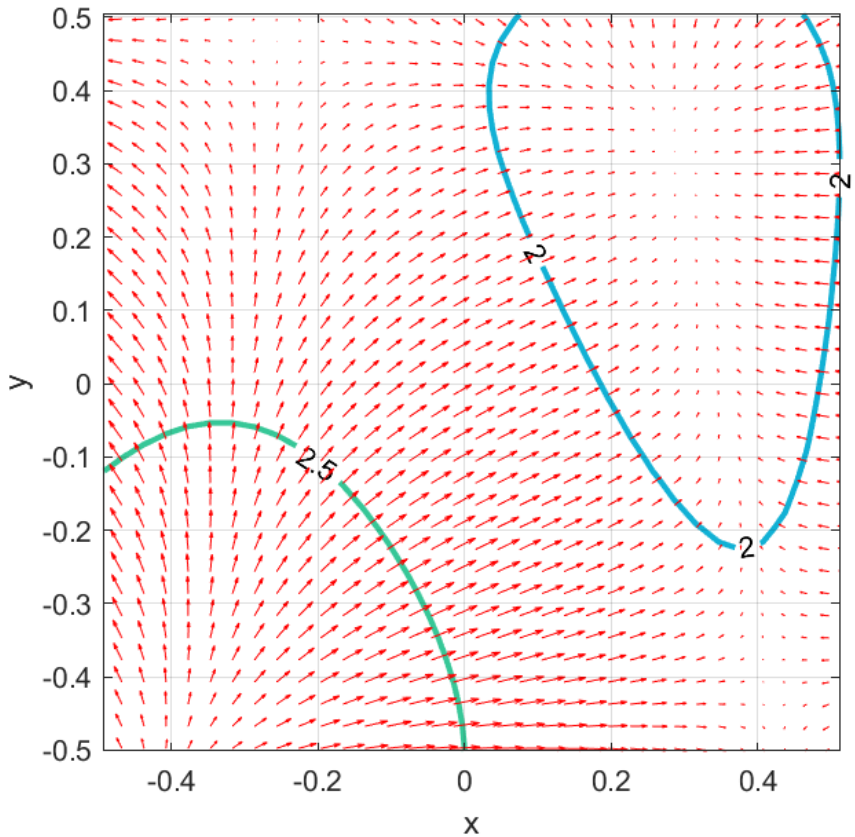
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

The gradient is orthogonal to level curves / level surfaces.



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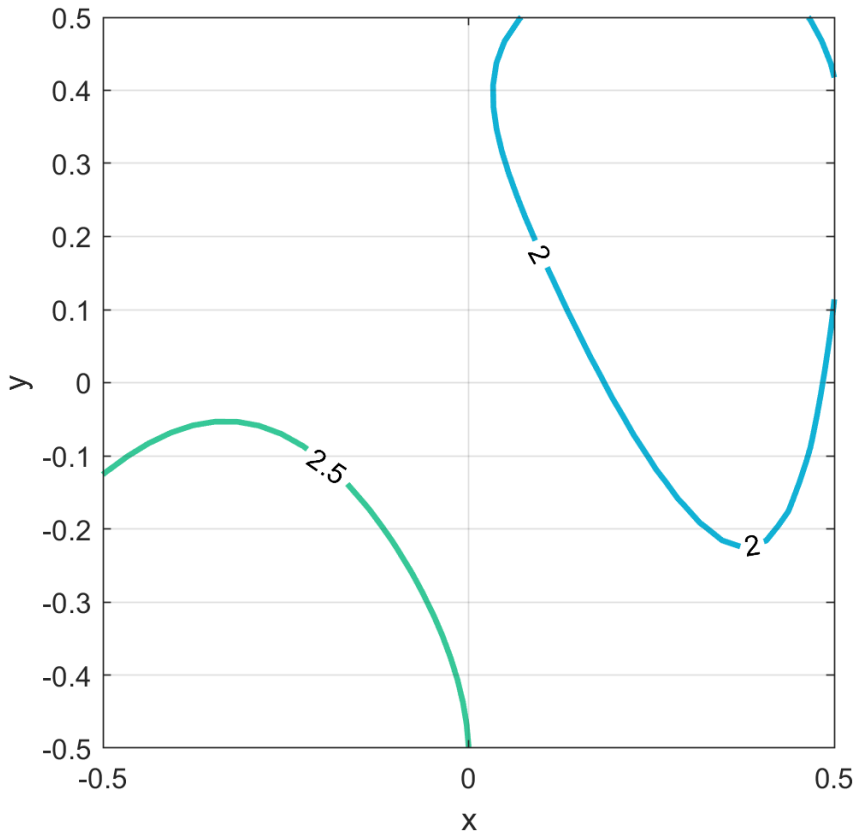

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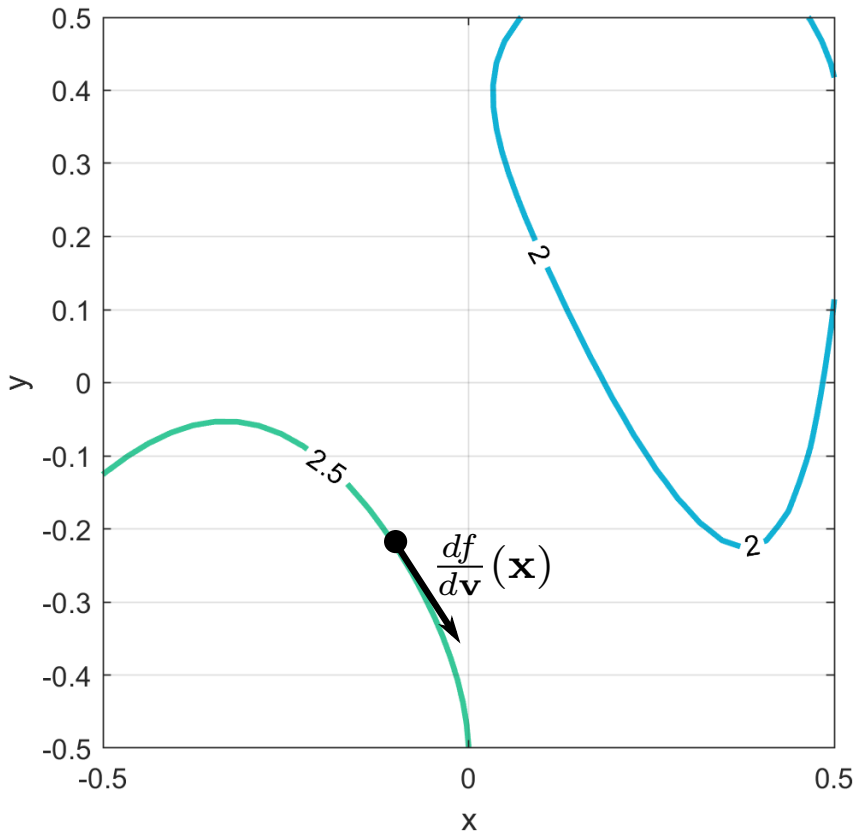

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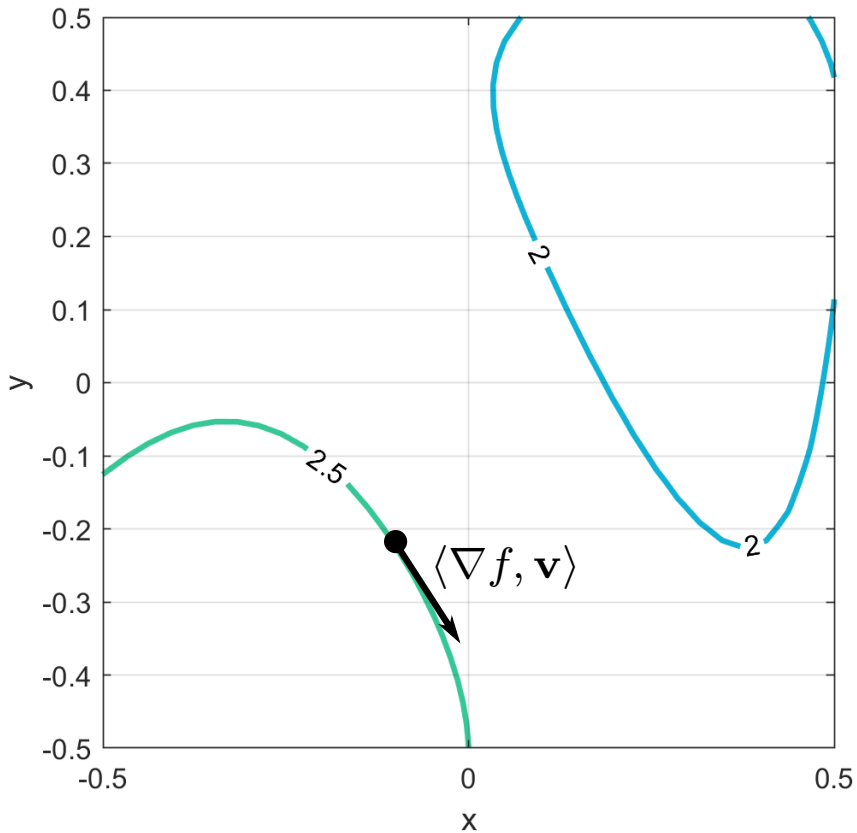

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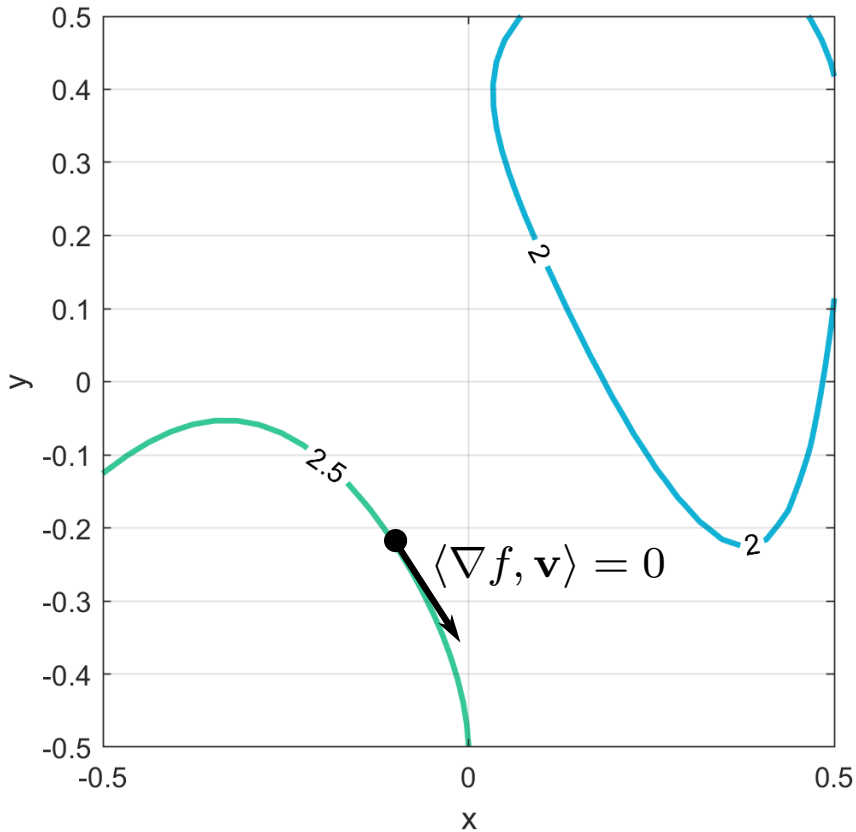

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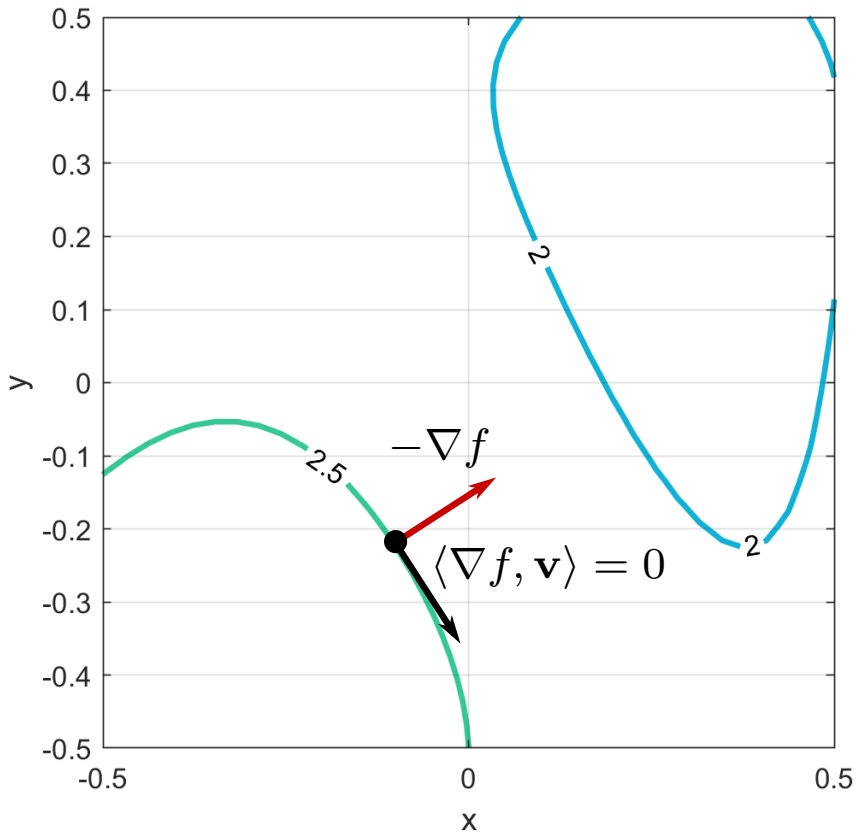

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See examples at: `https://mathinsight.org/differentiability_multivariable_subtleties`

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A stationary point is such that:

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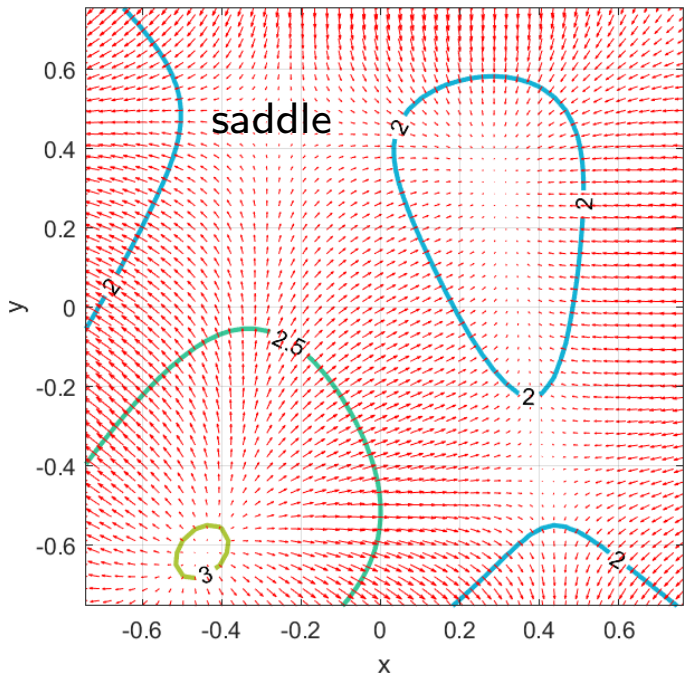

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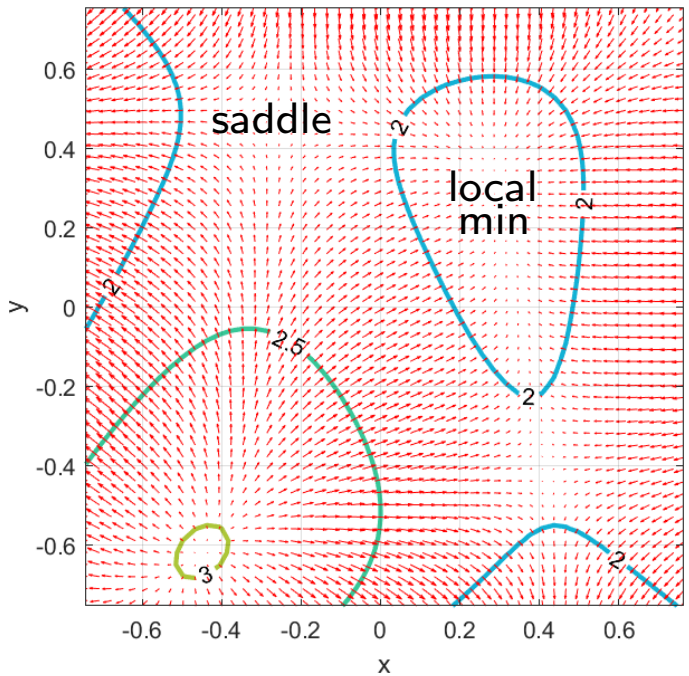

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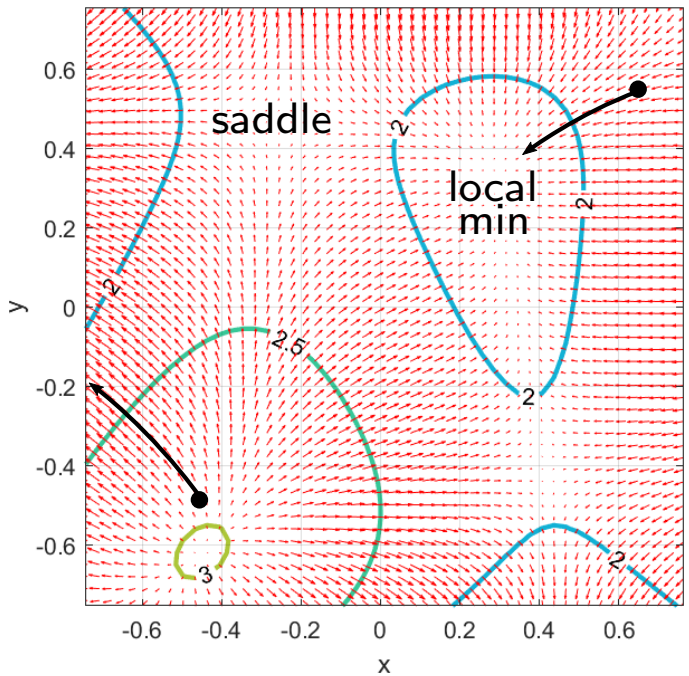
- Which stationary point depends on the initialization.



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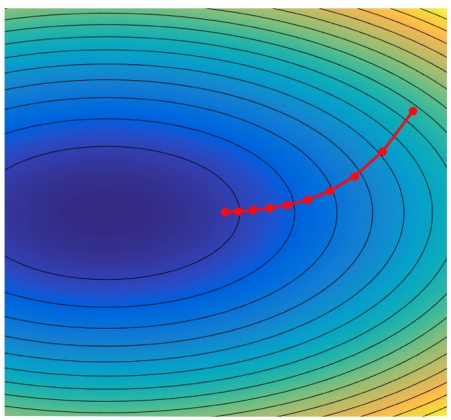

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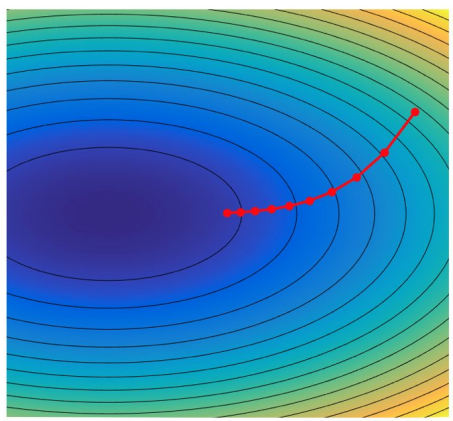

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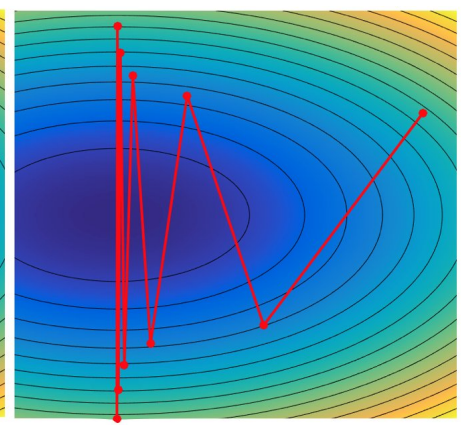

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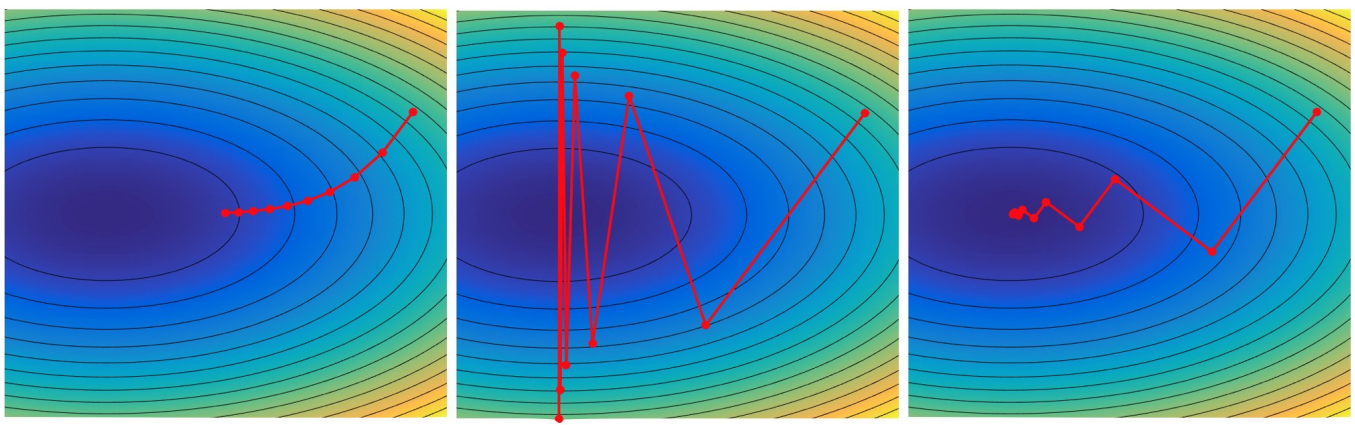
- Too small: slow convergence speed
- Too big: risk of overshooting
- Optimal values can be found via line search algorithms



small α | large α | optimal α

$\arg\min_\alpha f(\mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)}))$

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  Examples:

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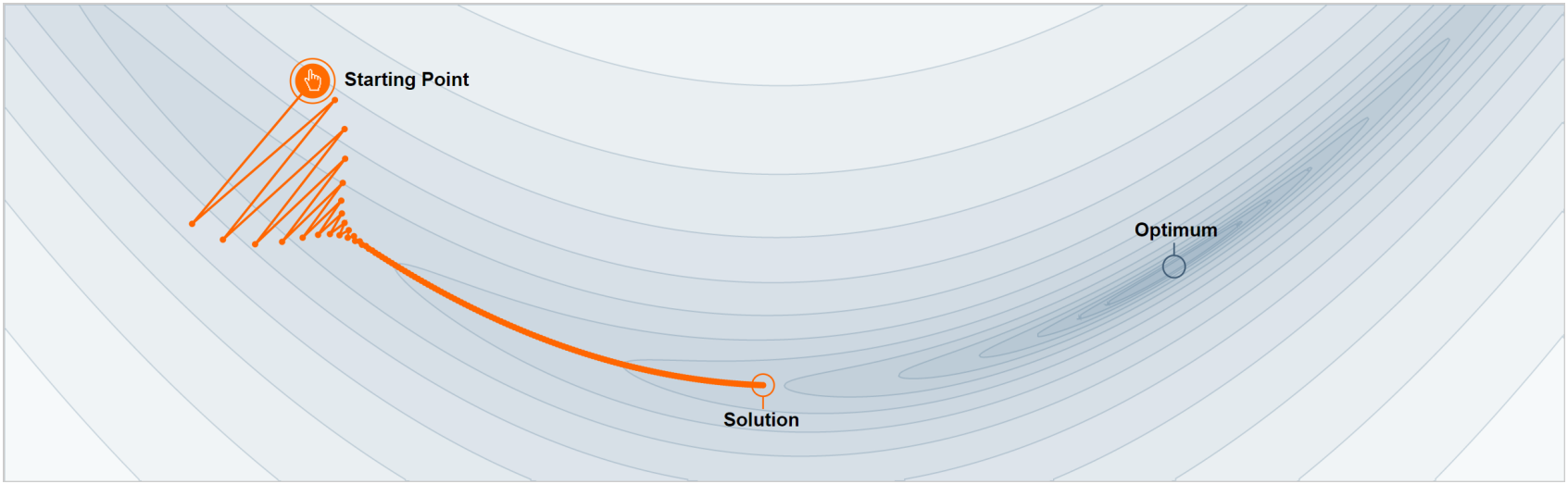
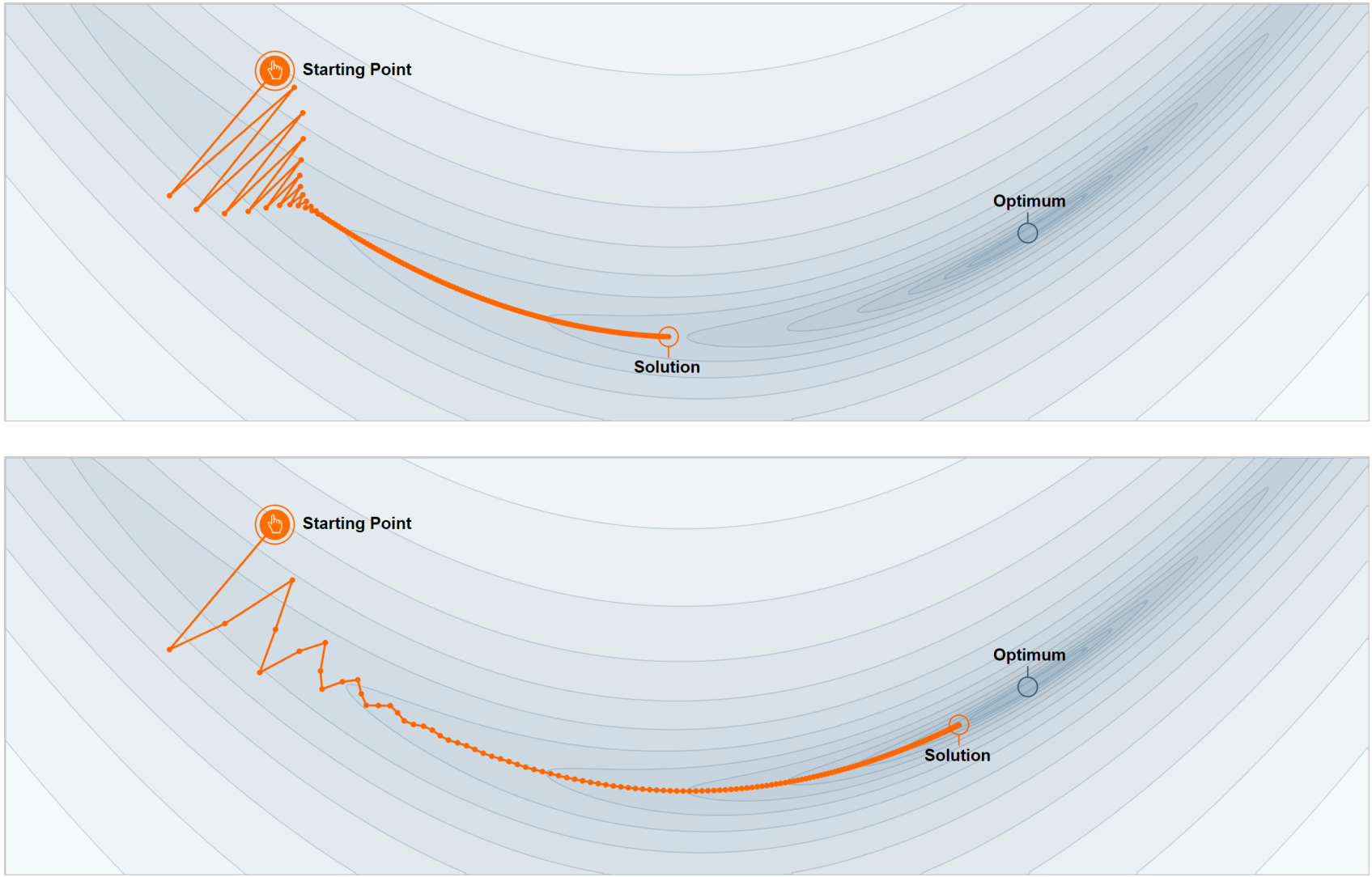
  Acceleration effect for big λ + escape from local minima.

Momentum



Goh, "Why momentum really works", Distill 2017

Momentum



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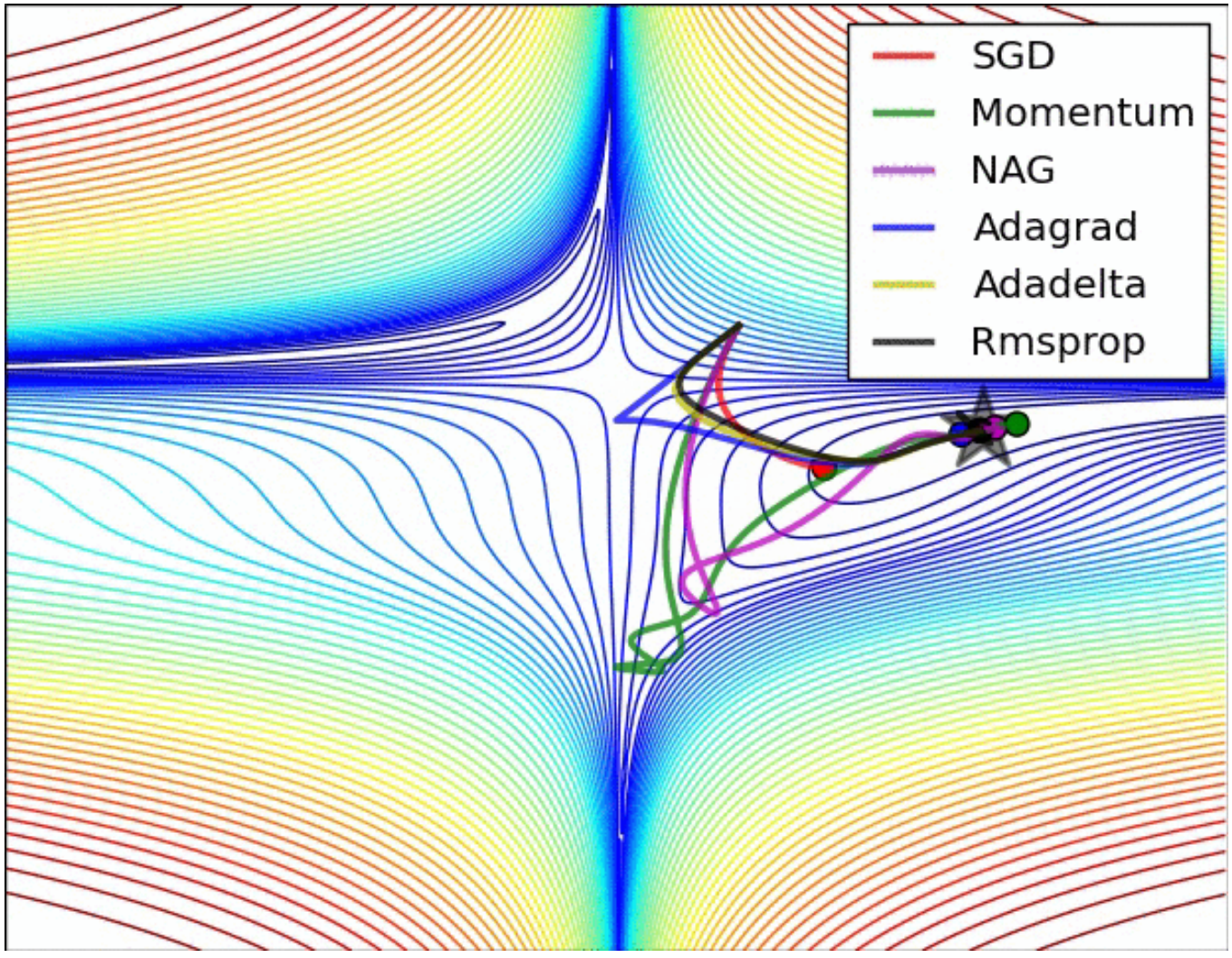
SGD
Momentum
NAG
Adagrad
Adadelta
Rmsprop

First-order acceleration methods

Let us try to unroll gradient descent:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \alpha \nabla f(\mathbf{x}^{(t)})$$

First-order acceleration methods

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First-order acceleration methods

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$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} - \alpha \nabla f(\mathbf{x}^{(1)})$$

First-order acceleration methods

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$$\begin{aligned}\mathbf{x}^{(1)} &= \mathbf{x}^{(0)} - \alpha\nabla f(\mathbf{x}^{(0)}) \\ \mathbf{x}^{(2)} &= \mathbf{x}^{(1)} - \alpha\nabla f(\mathbf{x}^{(1)}) \\ &= \mathbf{x}^{(0)} - \alpha\nabla f(\mathbf{x}^{(0)}) - \alpha\nabla f(\mathbf{x}^{(1)})\end{aligned}$$

First-order acceleration methods

Let us try to unroll gradient descent:

$$
\begin{aligned}
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&= \mathbf{x}^{(0)} - \alpha \nabla f(\mathbf{x}^{(0)}) - \alpha \nabla f(\mathbf{x}^{(1)}) \\
&\vdots \\
\mathbf{x}^{(t+1)} &= \mathbf{x}^{(0)} - \alpha \sum_{i=1}^{t} \nabla f(\mathbf{x}^{(i)})
\end{aligned}
$$

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With momentum:

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The more general form:

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generalizes optimization algorithms like ADAM, AdaGrad, etc.

Gradient descent as a general tool

Gradient descent can be applied to nonconvex problems, without optimality guarantees.

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