Neural networks

STAT 4710

November 16, 2023

Where we are

✓ **Unit 1:** R for data mining

✓ **Unit 2:** Prediction fundamentals

✓ **Unit 3:** Regression-based methods

✓ **Unit 4:** Tree-based methods

Unit 5: Deep learning

Lecture 1: Deep learning preliminaries

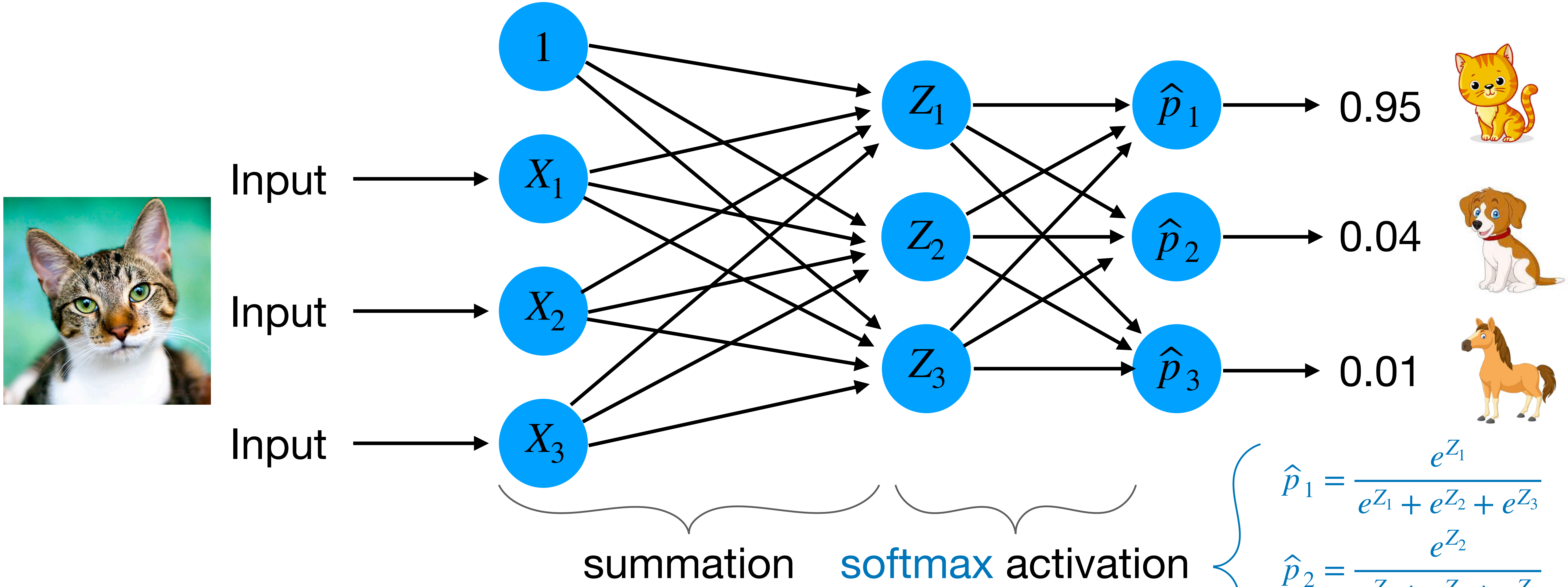
Lecture 2: Neural networks

Lecture 3: Deep learning for images

Lecture 4: Deep learning for text

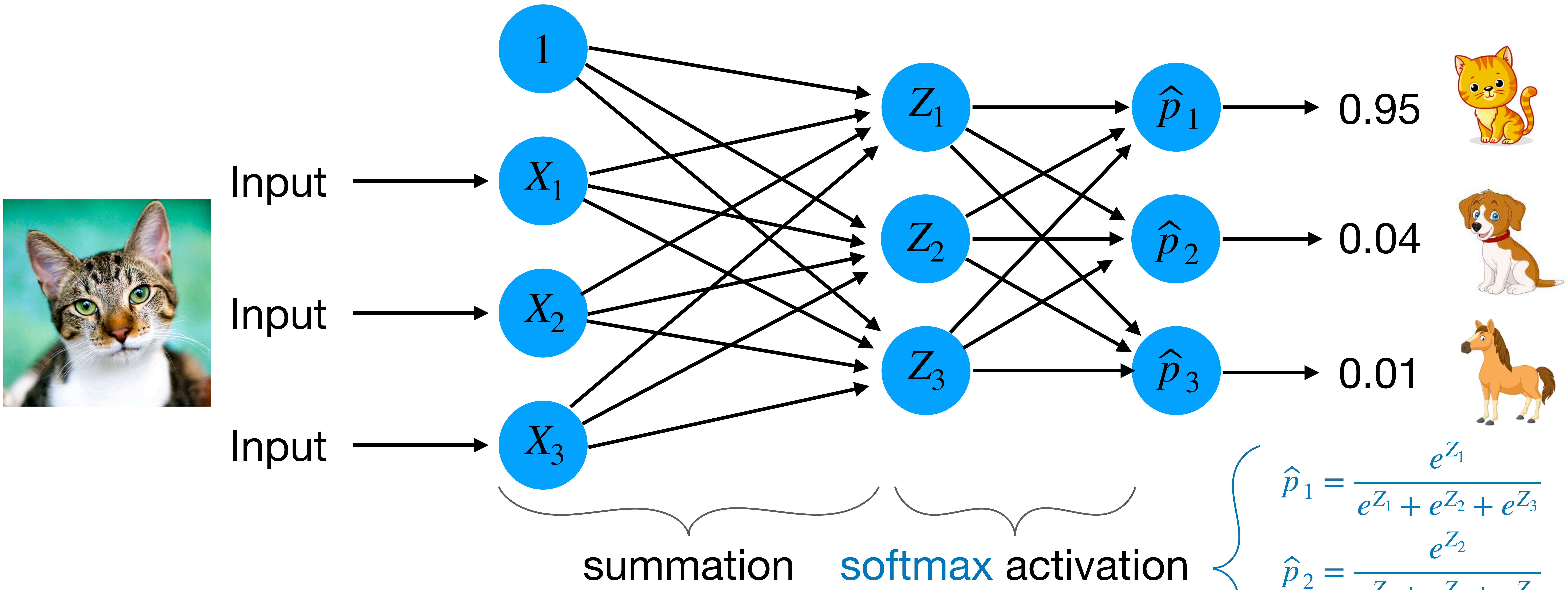
Lecture 5: Unit review and quiz in class

Recall: Multi-class logistic model



$$\begin{cases} \hat{p}_1 = \dfrac{e^{Z_1}}{e^{Z_1} + e^{Z_2} + e^{Z_3}} \\ \hat{p}_2 = \dfrac{e^{Z_2}}{e^{Z_1} + e^{Z_2} + e^{Z_3}} \\ \hat{p}_3 = \dfrac{e^{Z_3}}{e^{Z_1} + e^{Z_2} + e^{Z_3}} \end{cases}$$

Recall: Multi-class logistic model



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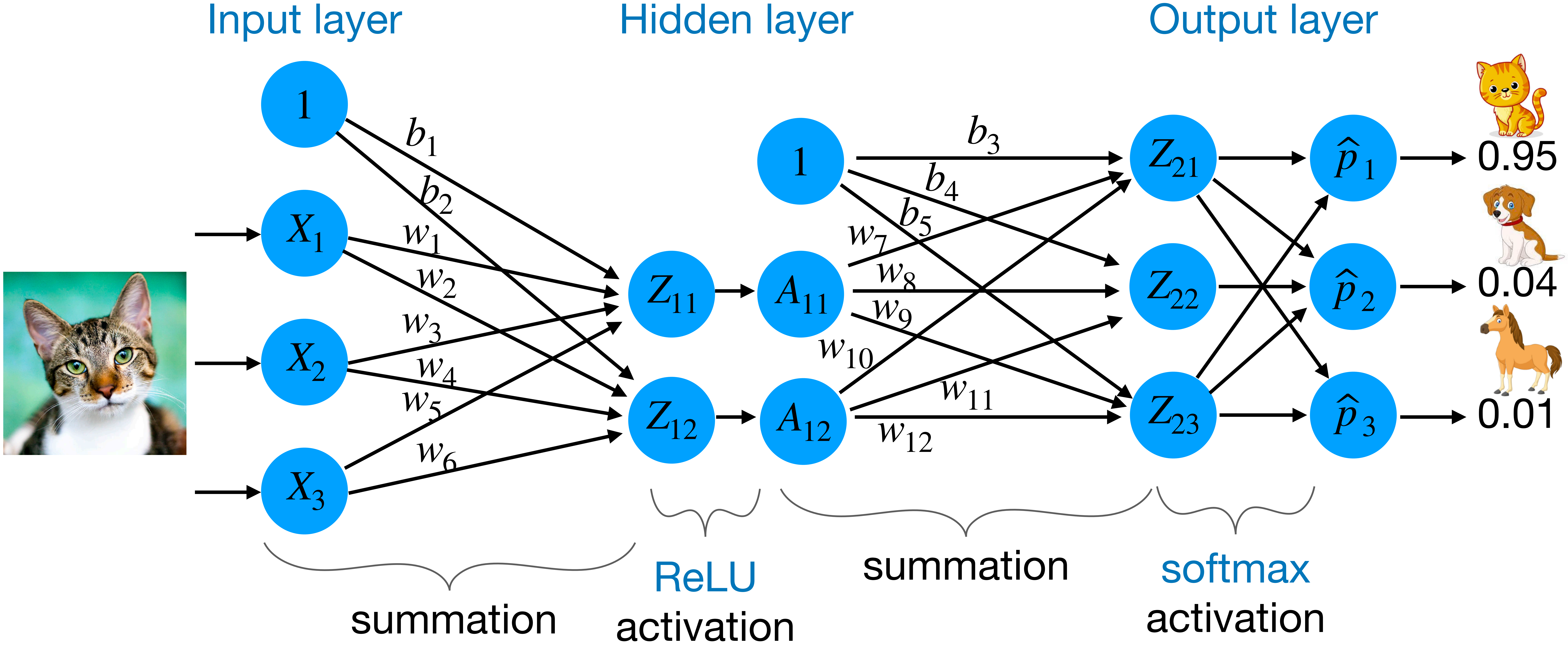
This simple architecture directly uses raw pixel features.
Intuitively, a good classifier would pick up on cat’s eyes, ears, etc.

One-hidden-layer neural network

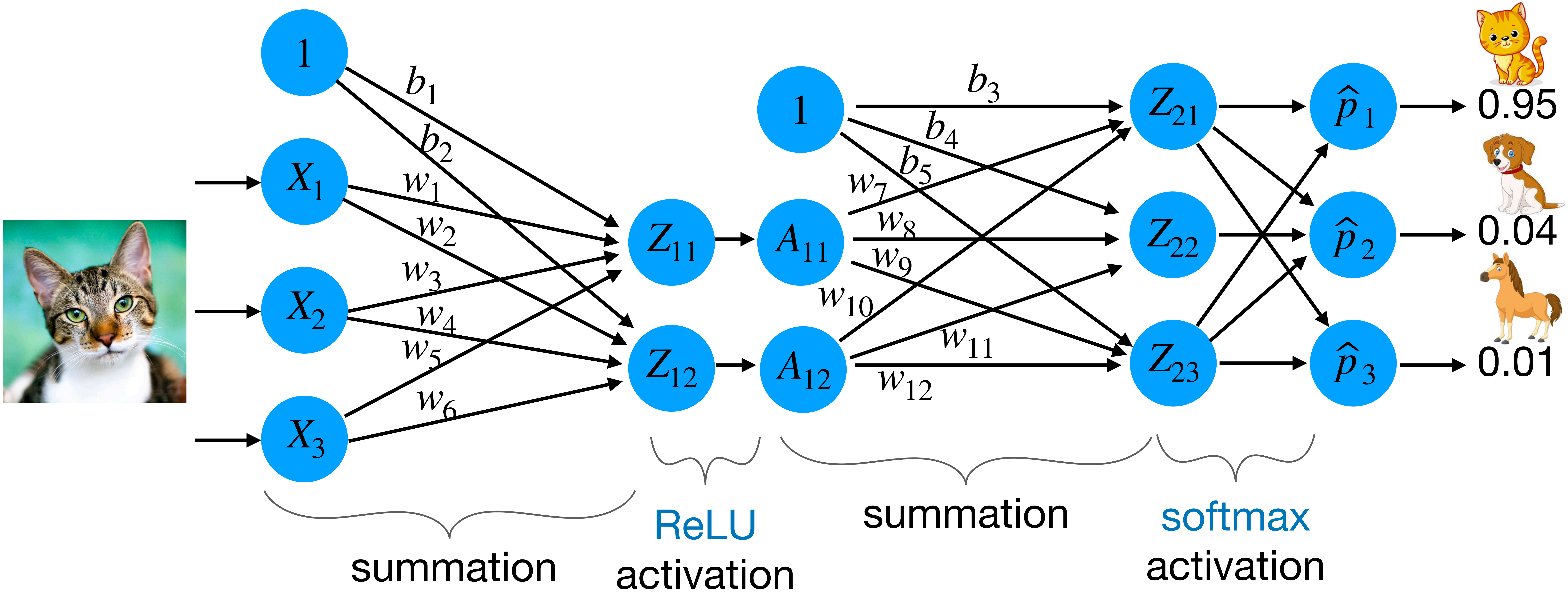


One-hidden-layer neural network

Input layer

Hidden layer

Output layer



summation

ReLU activation

summation

softmax activation

E.g., $Z_{12} = b_2 + w_2X_1 + w_4X_2 + w_6X_3$

One-hidden-layer neural network

Input layer

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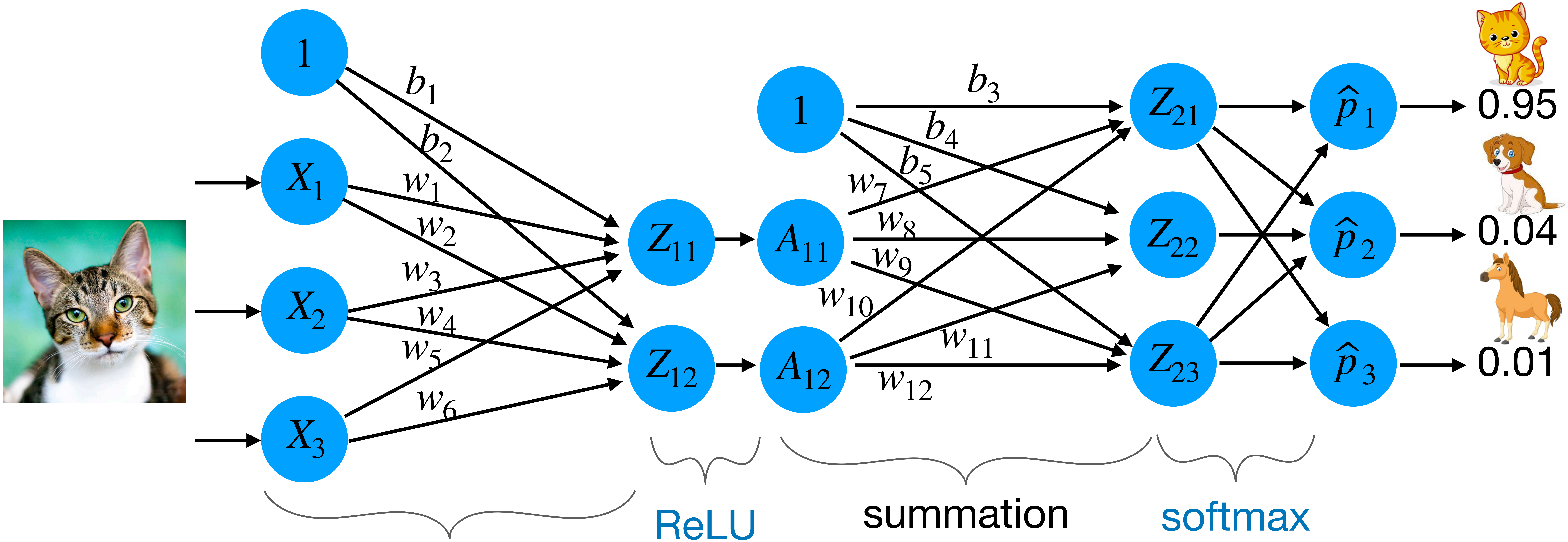
Output layer

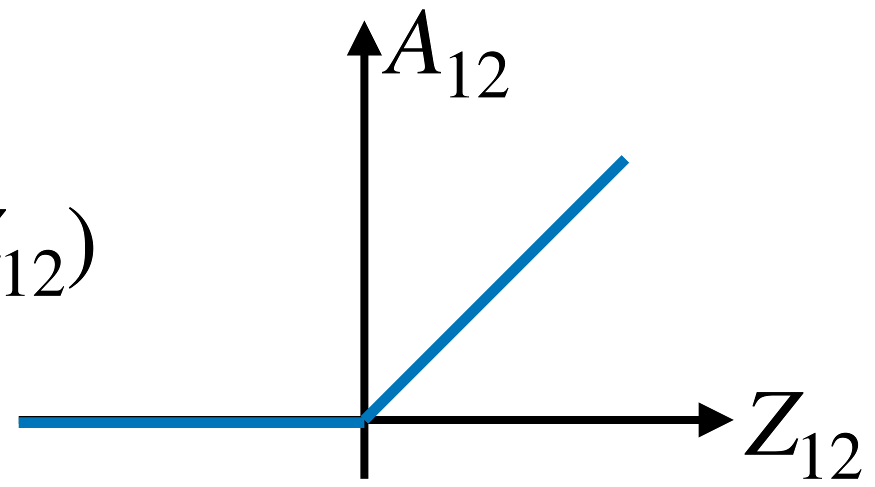


summation

E.g., $Z_{12} = b_2 + w_2X_1 + w_4X_2 + w_6X_3$

ReLU activation

E.g., $A_{12} = \max(0, Z_{12})$



summation

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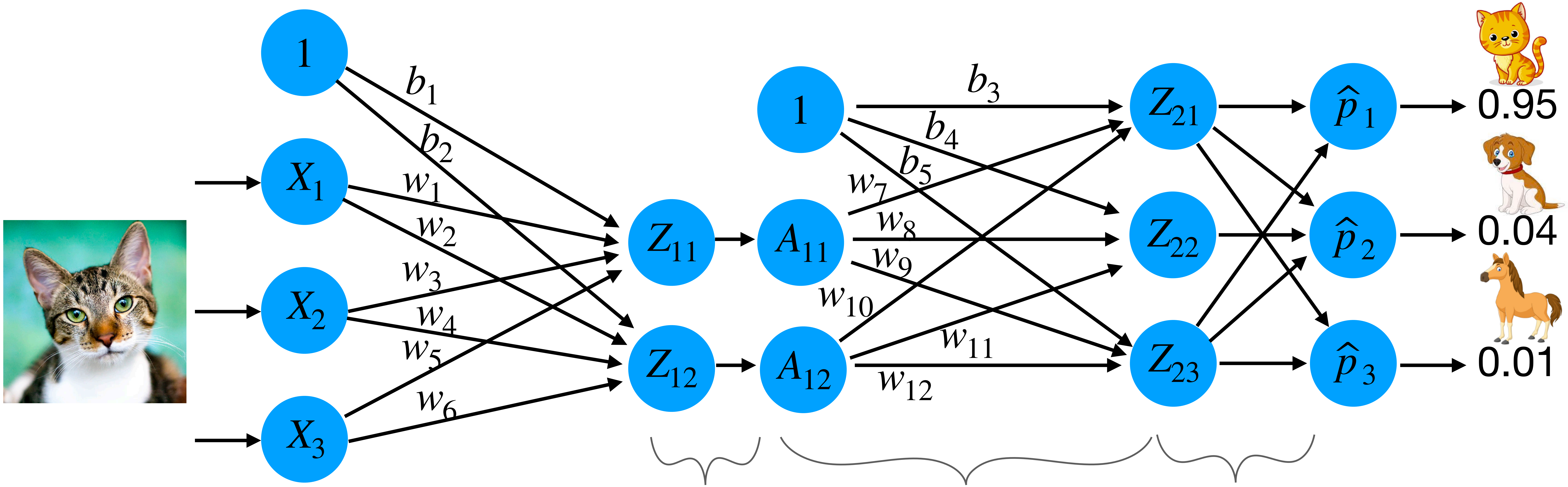

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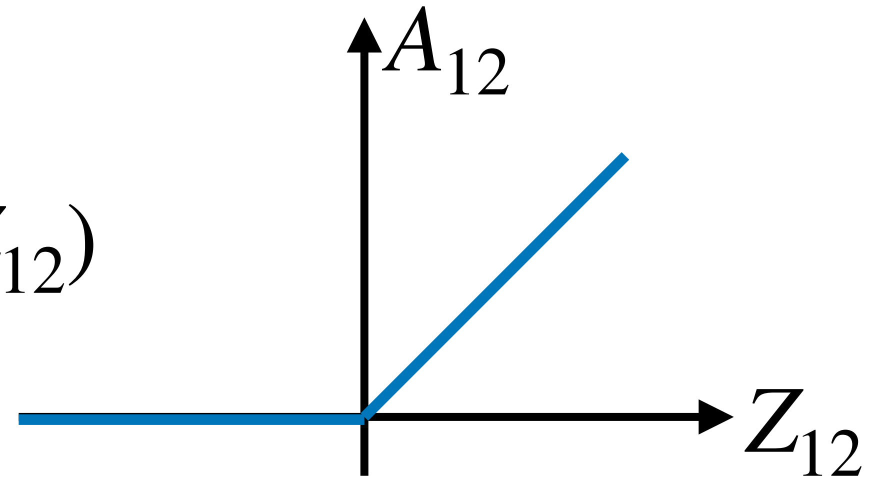


summation

softmax

activation

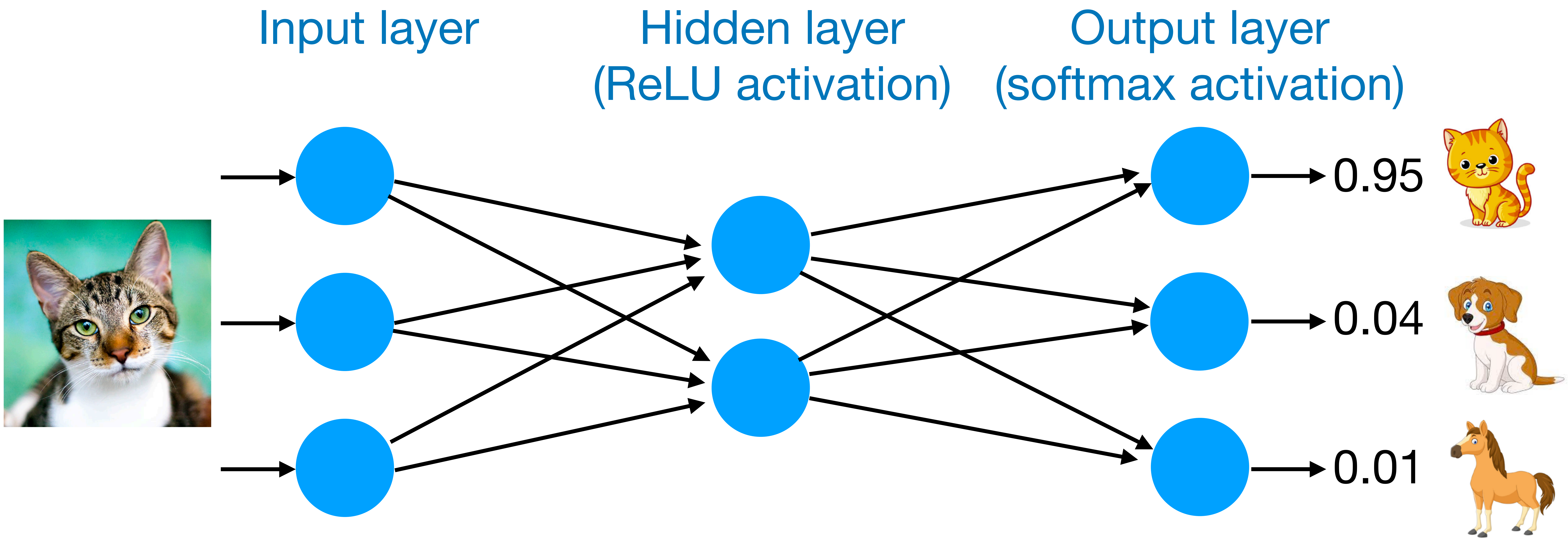
Terminology:

b_j: biases

w_j: weights

One-hidden-layer neural network

Concise representation



Input layer

Hidden layer
(ReLU activation)

Output layer
(softmax activation)

One-hidden-layer neural network

Concise representation

Input layer

Hidden layer
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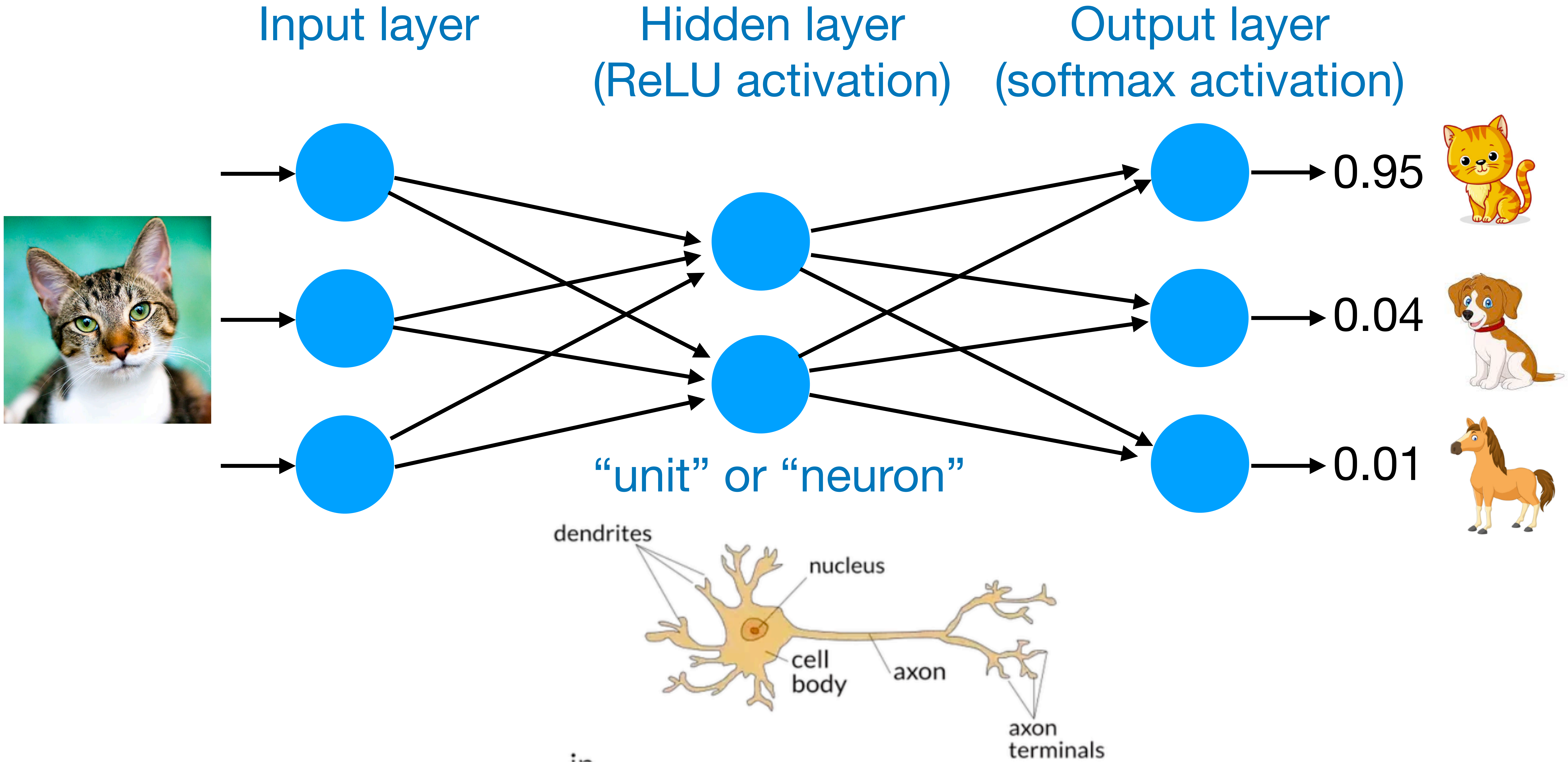

"unit" or "neuron"

One-hidden-layer neural network

Concise representation

Input layer

Hidden layer
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Output layer
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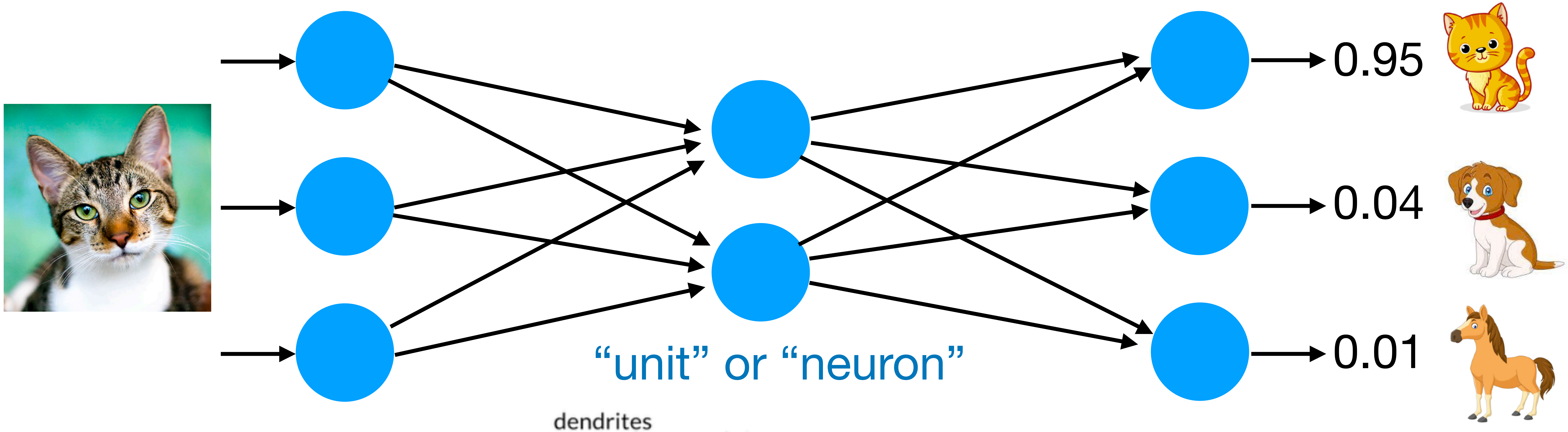

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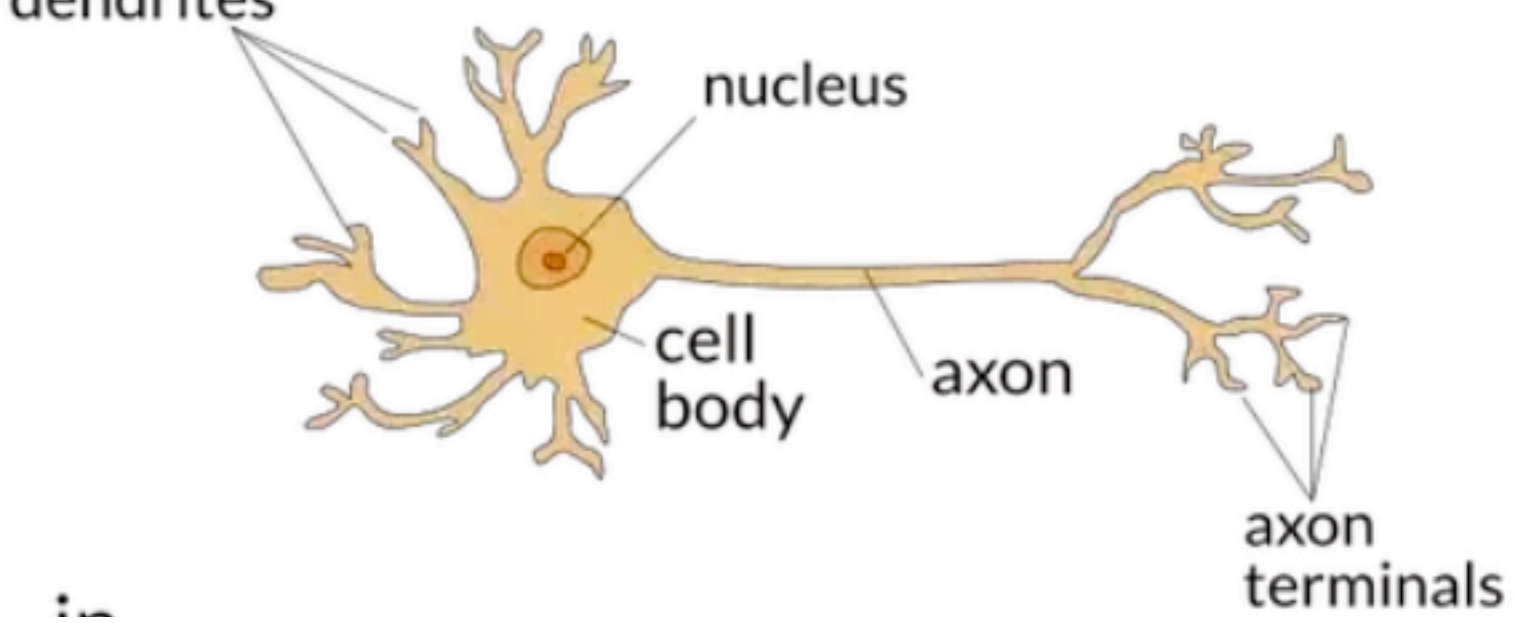
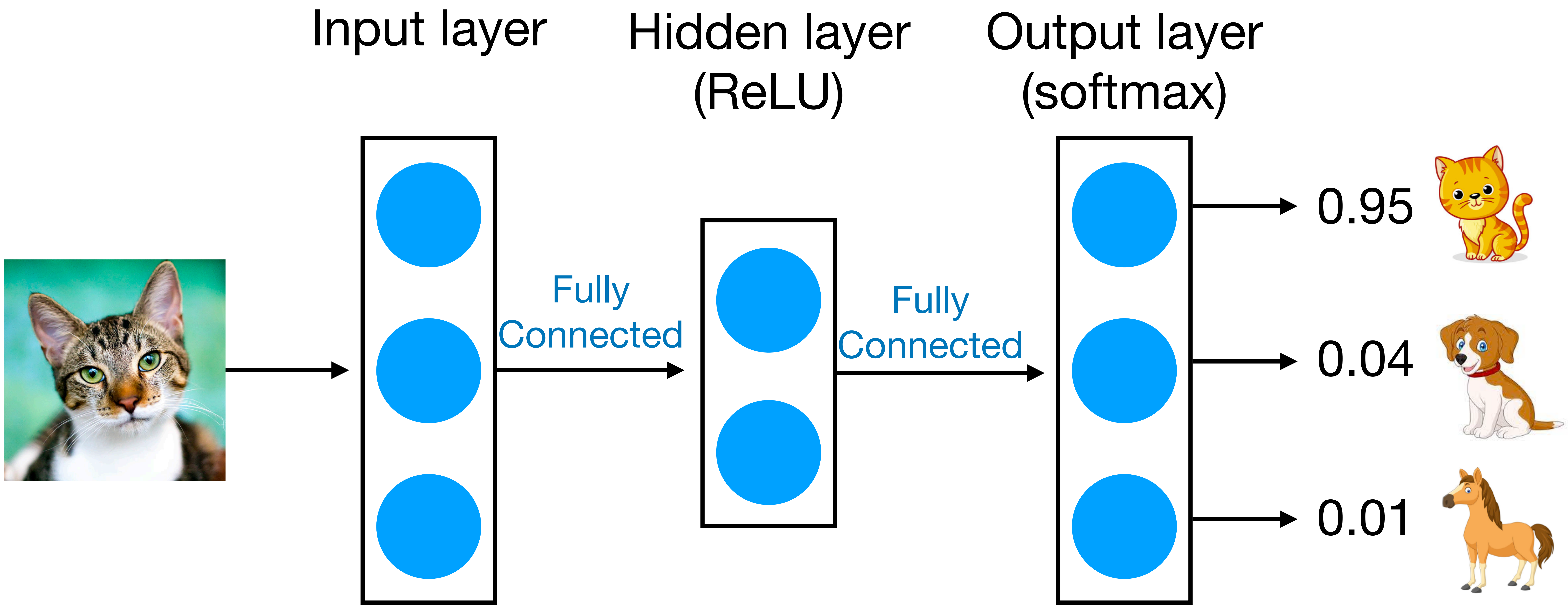


Notes:

- Bias terms left implicit.
- Fully connected architecture.
- Hidden layer: learned features.

One-hidden-layer neural network

Even more concise representation



Input layer

Hidden layer (ReLU)

Output layer (softmax)

Fully Connected

Fully Connected

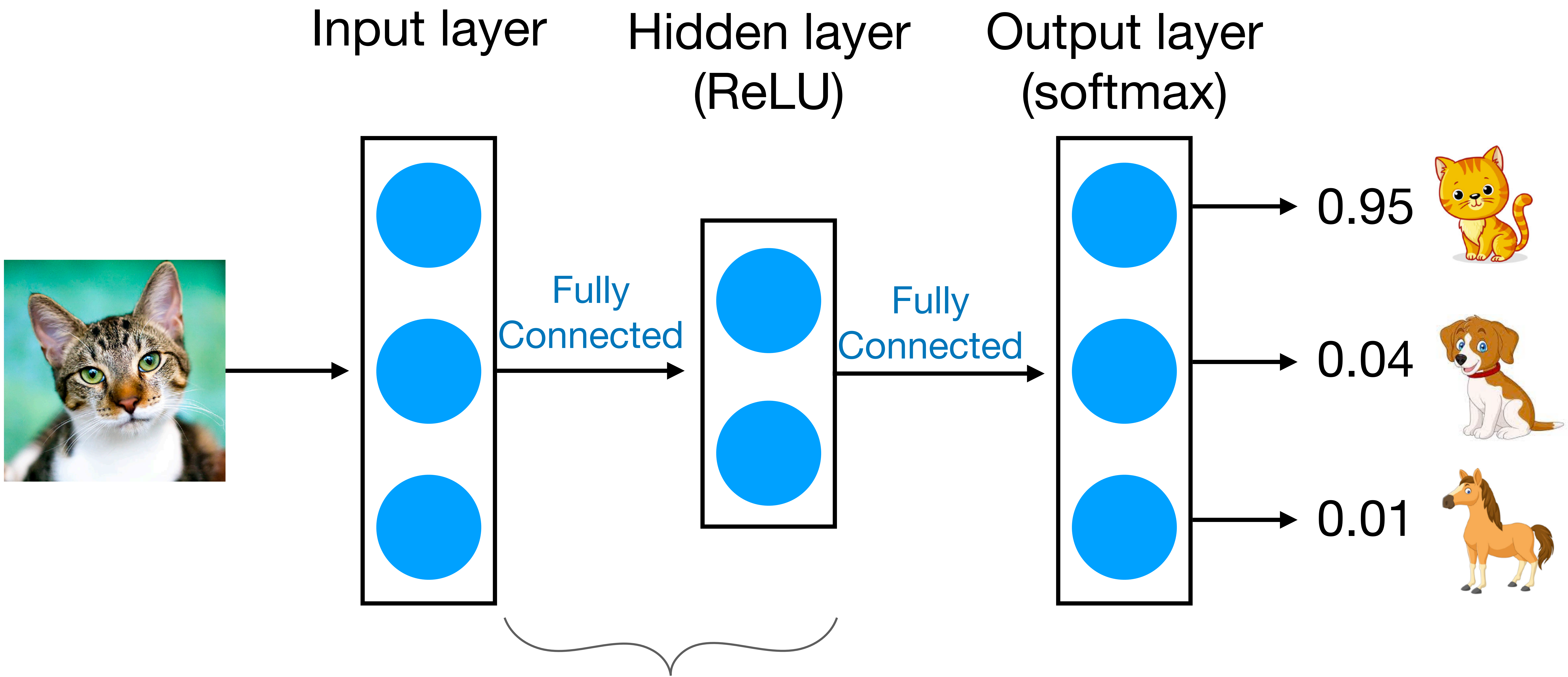
0.95

0.04

0.01

One-hidden-layer neural network

Even more concise representation



Input layer

Hidden layer (ReLU)

Output layer (softmax)

Fully Connected

Fully Connected

0.95

0.04

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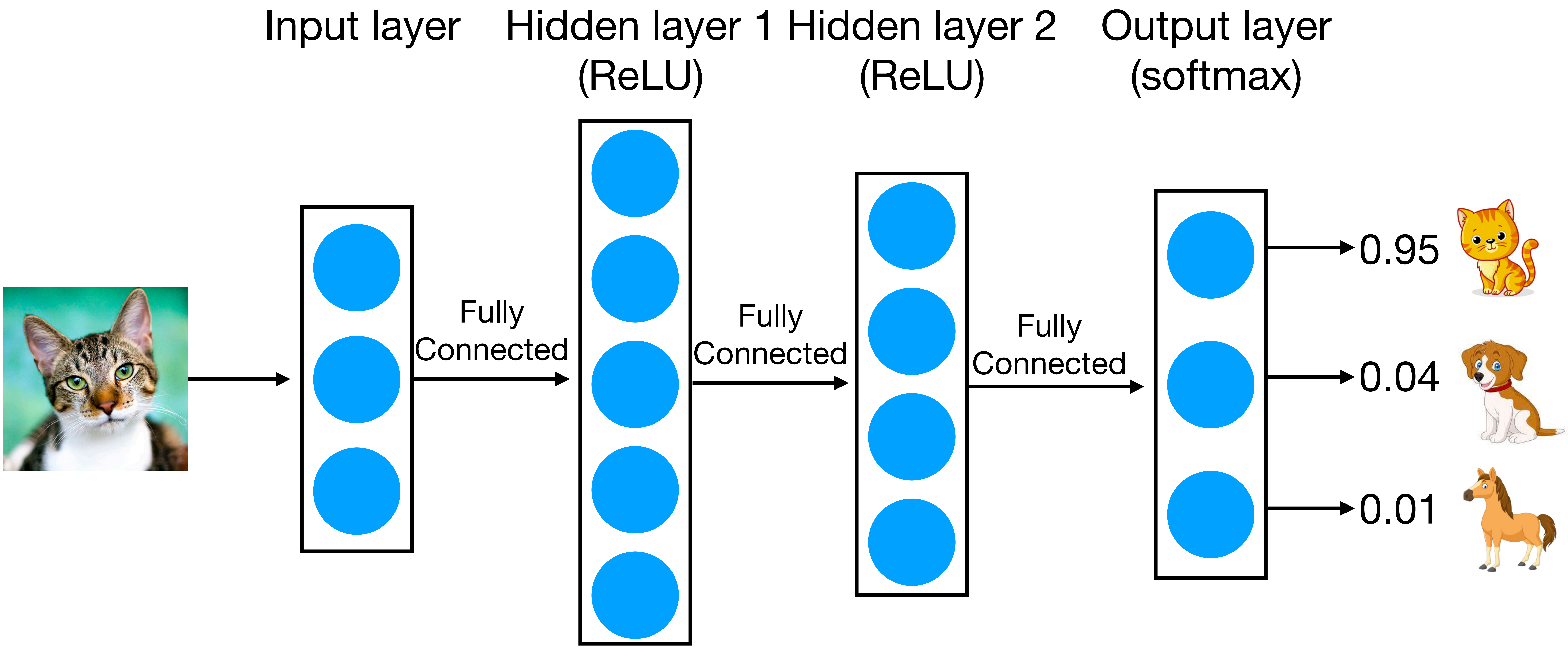
Number of parameters in FC layer =

(# units in previous layer + 1) × (# units in this layer)

Multi-layer fully connected neural networks



Input layer

Hidden layer 1 (ReLU)

Hidden layer 2 (ReLU)

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Fully Connected

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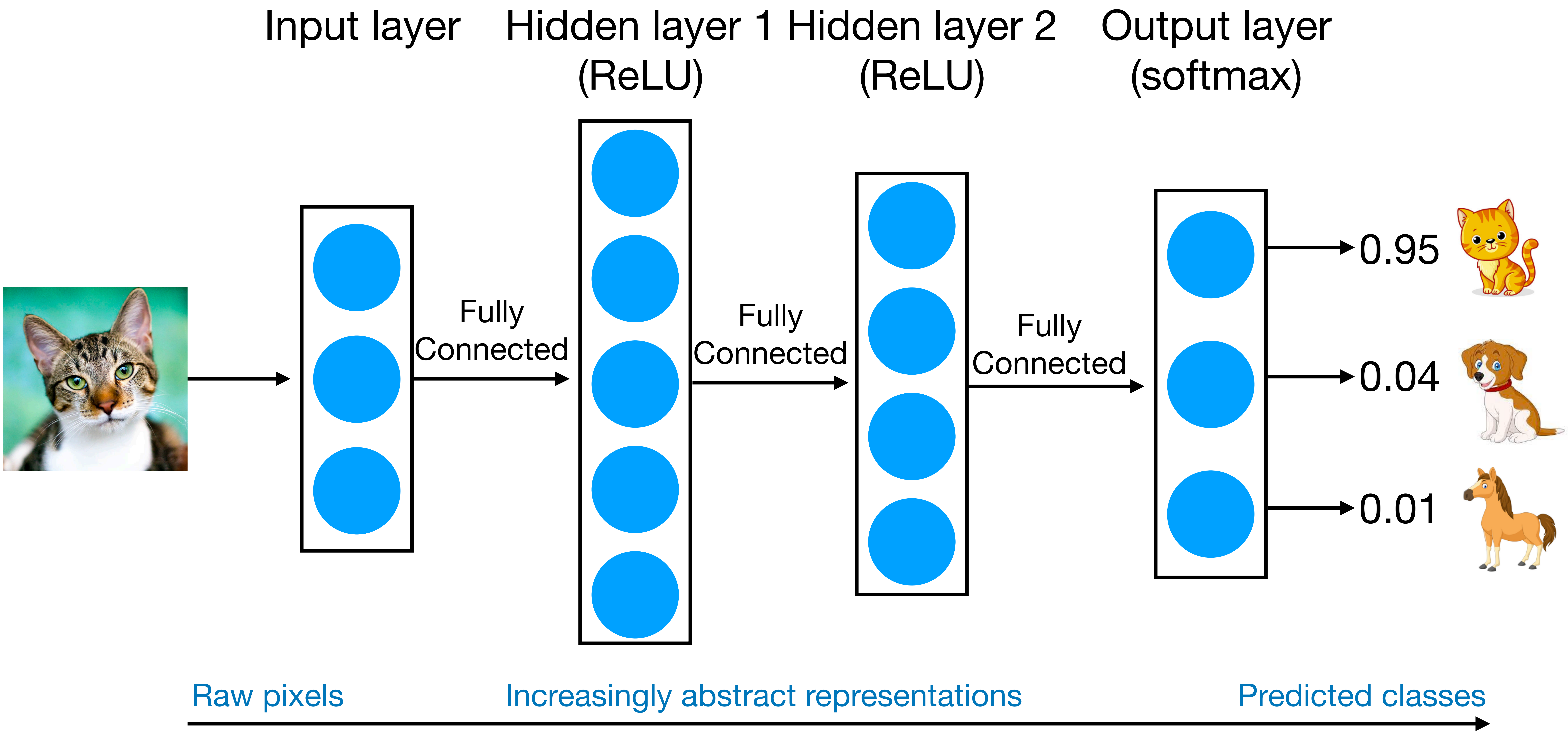

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Fully Connected

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Raw pixels

Increasingly abstract representations

Predicted classes

Training deep learning models

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Training a neural network amounts to solving our usual optimization problem:

$$\widehat{\beta} = \arg\min_{\beta} \frac{1}{n}\sum_{i=1}^{n} L(Y_i, f_\beta(X_i)) + \lambda \cdot \text{penalty}(\beta) = \arg\min_{\beta} F(\beta)\,.$$

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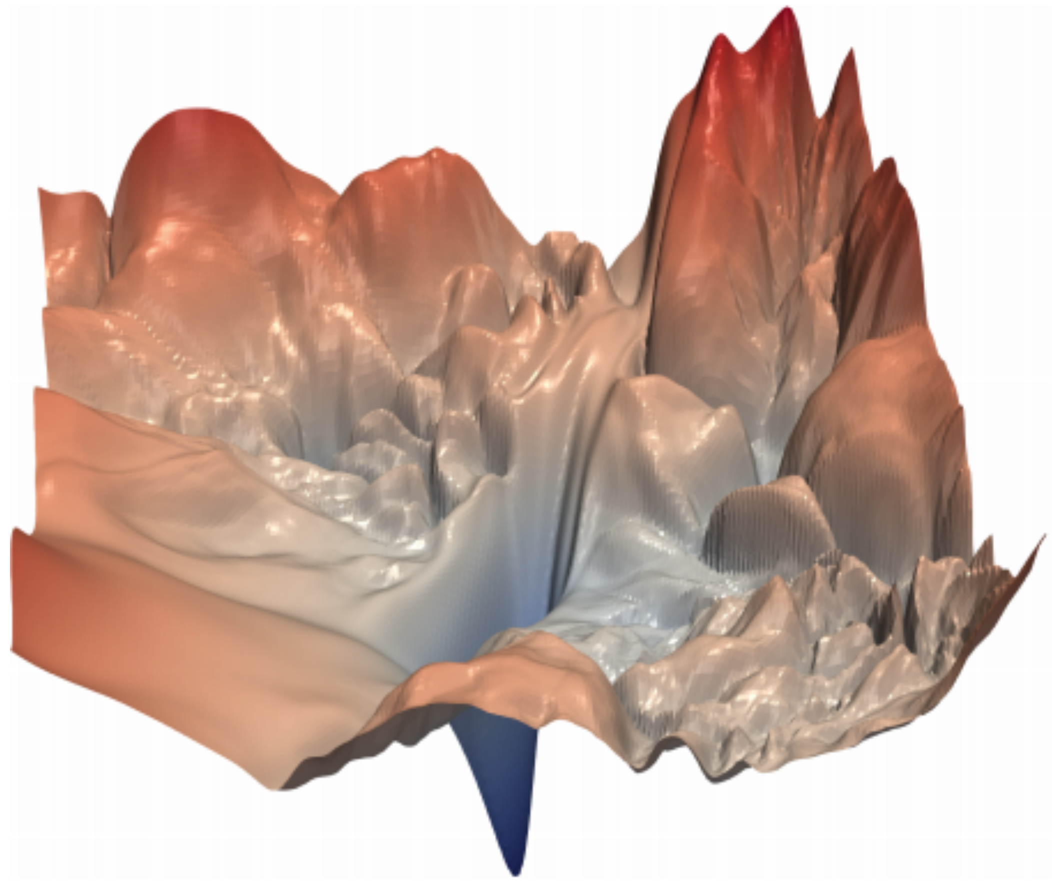

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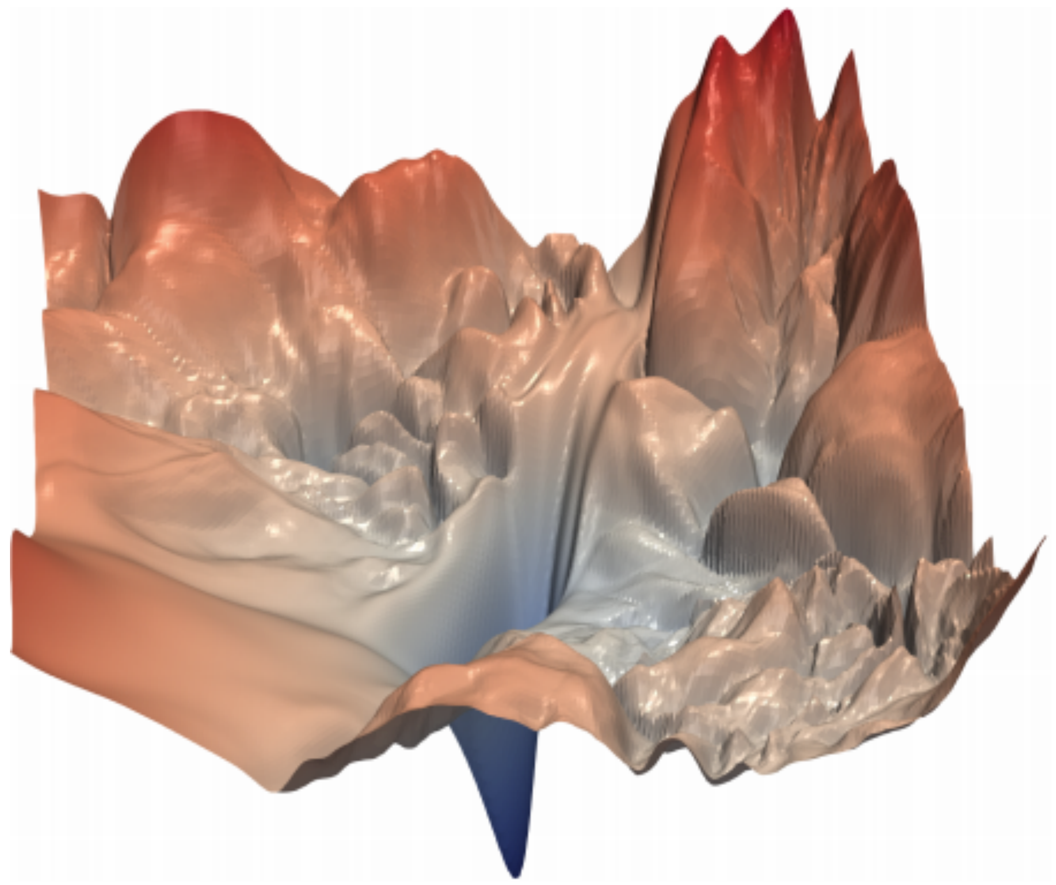

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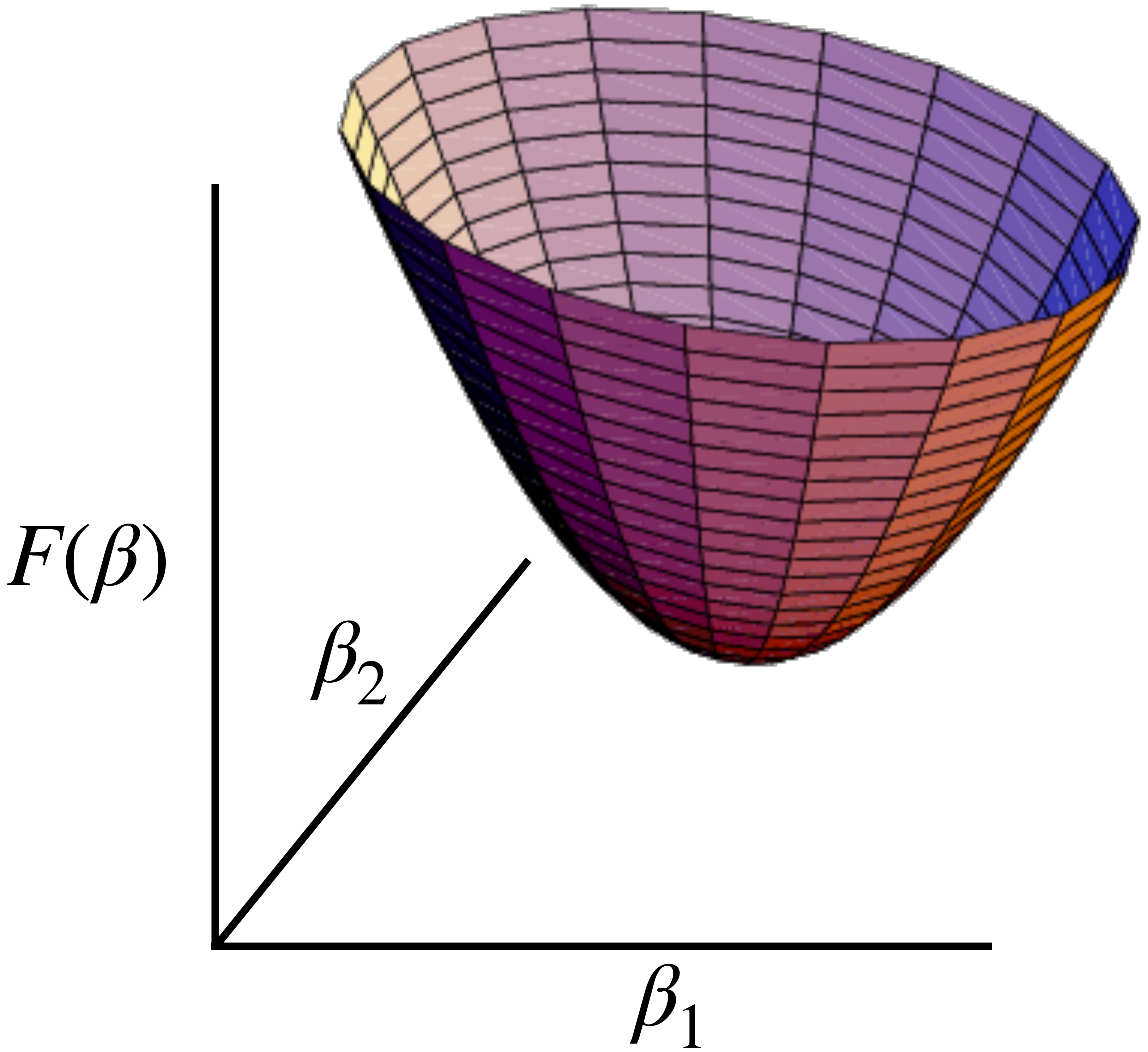

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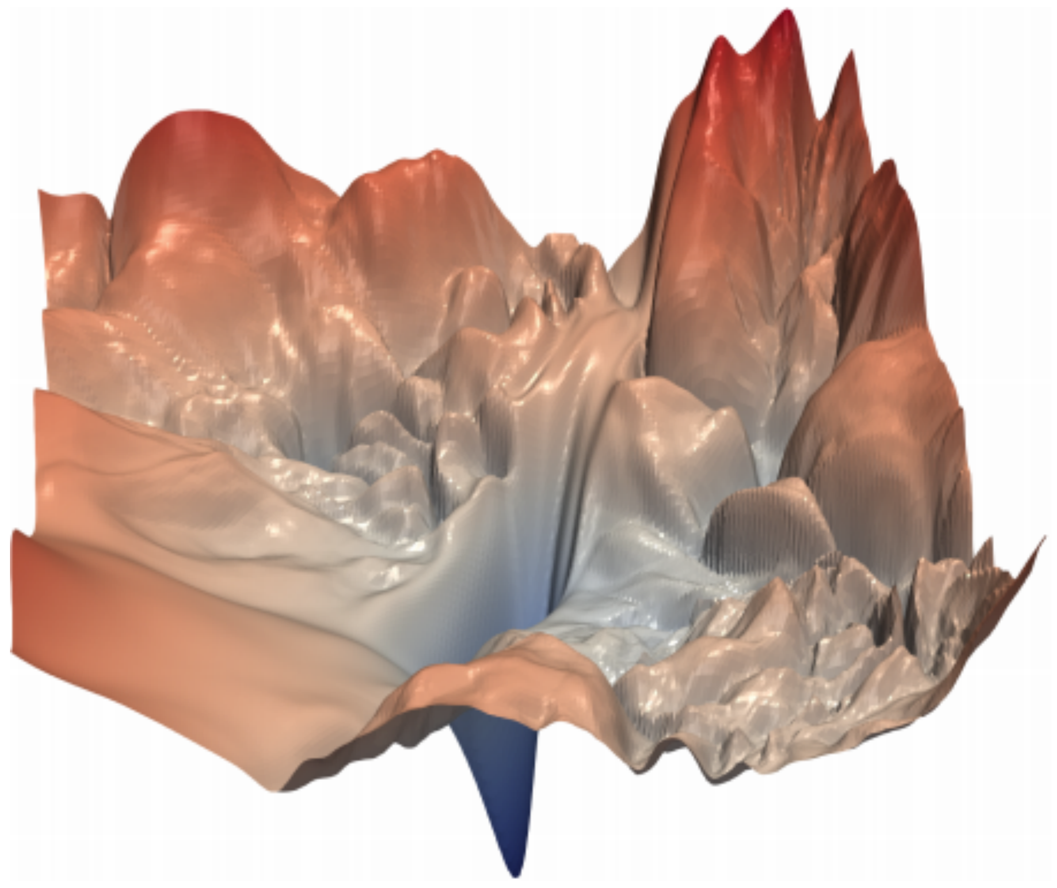

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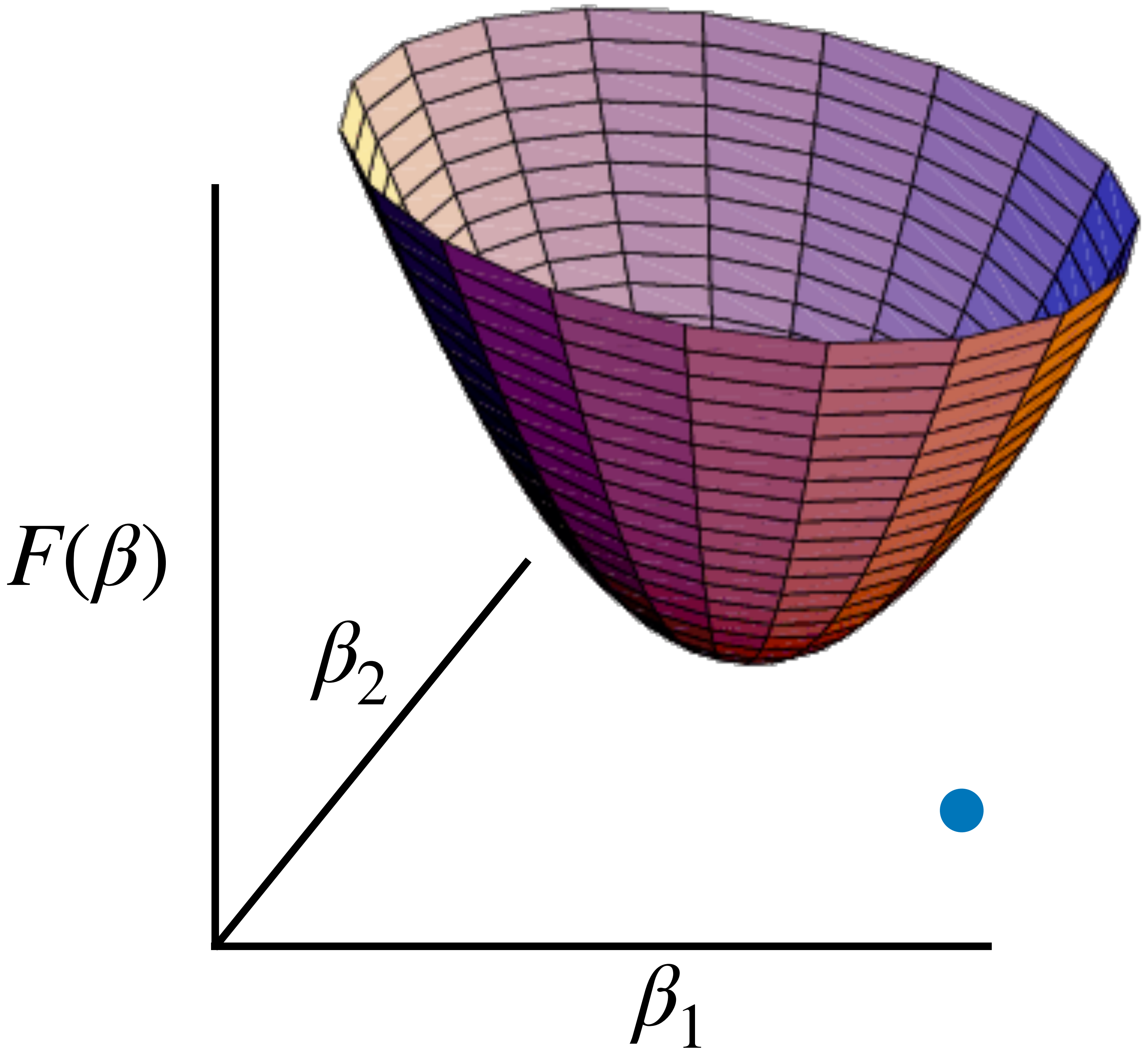

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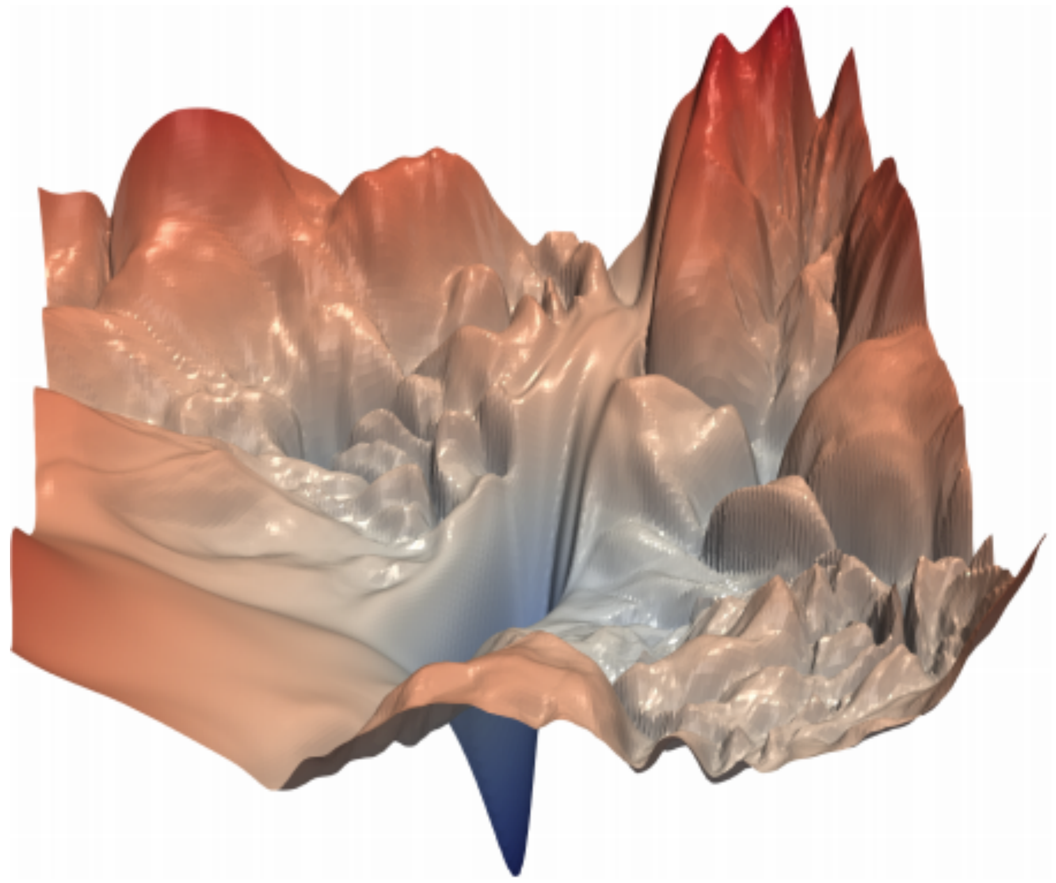

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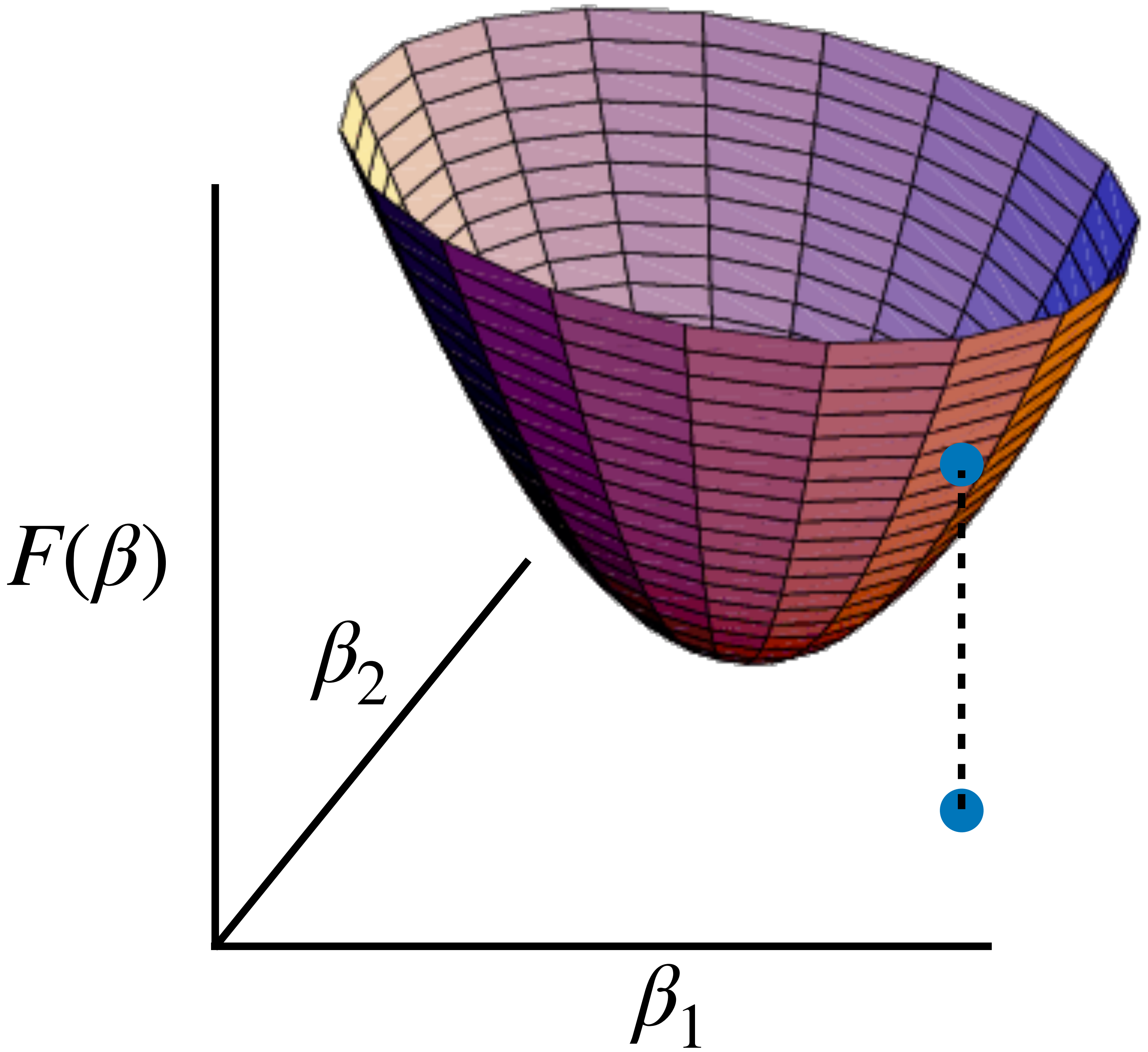

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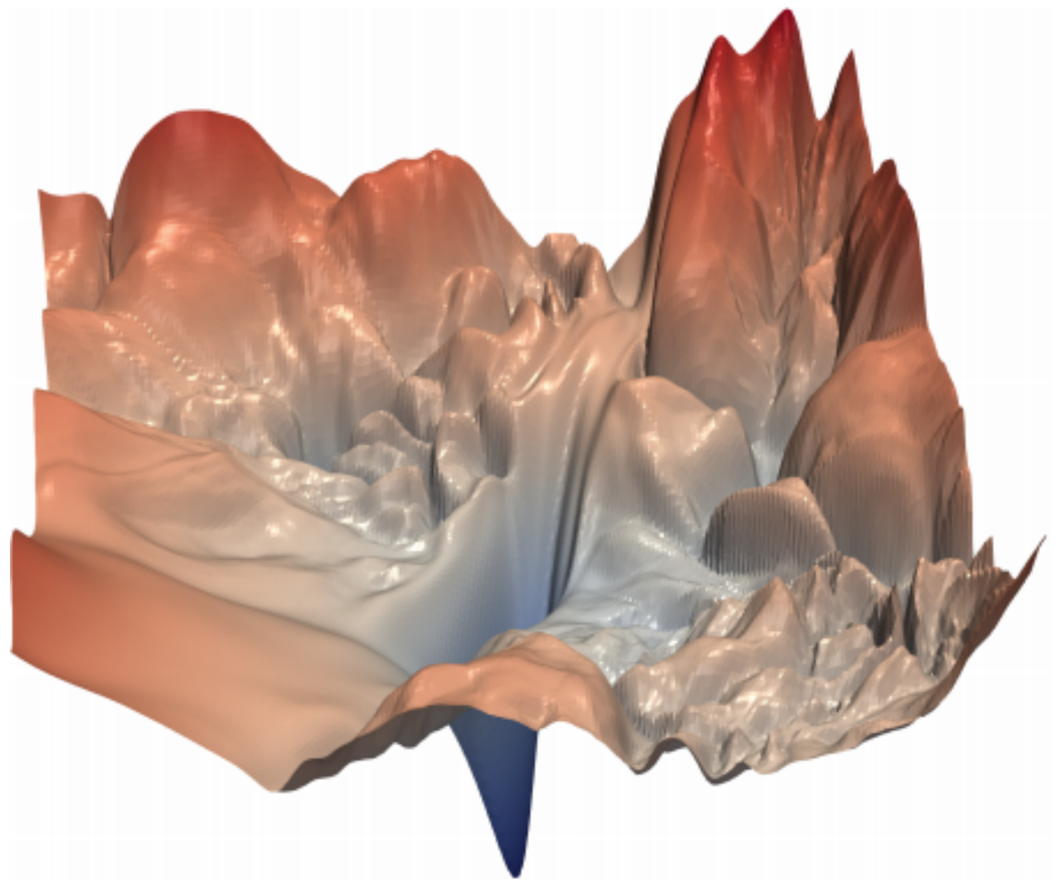

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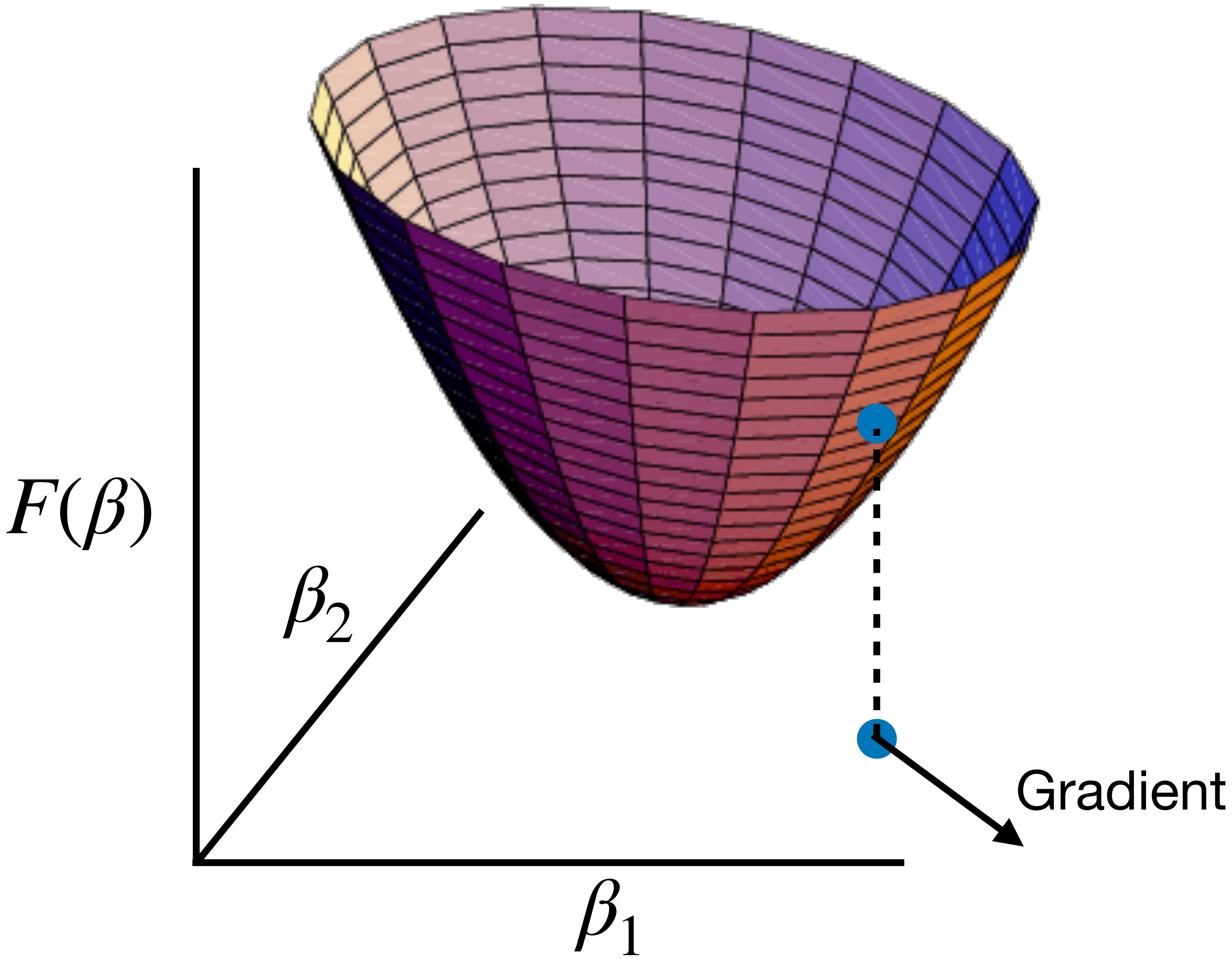

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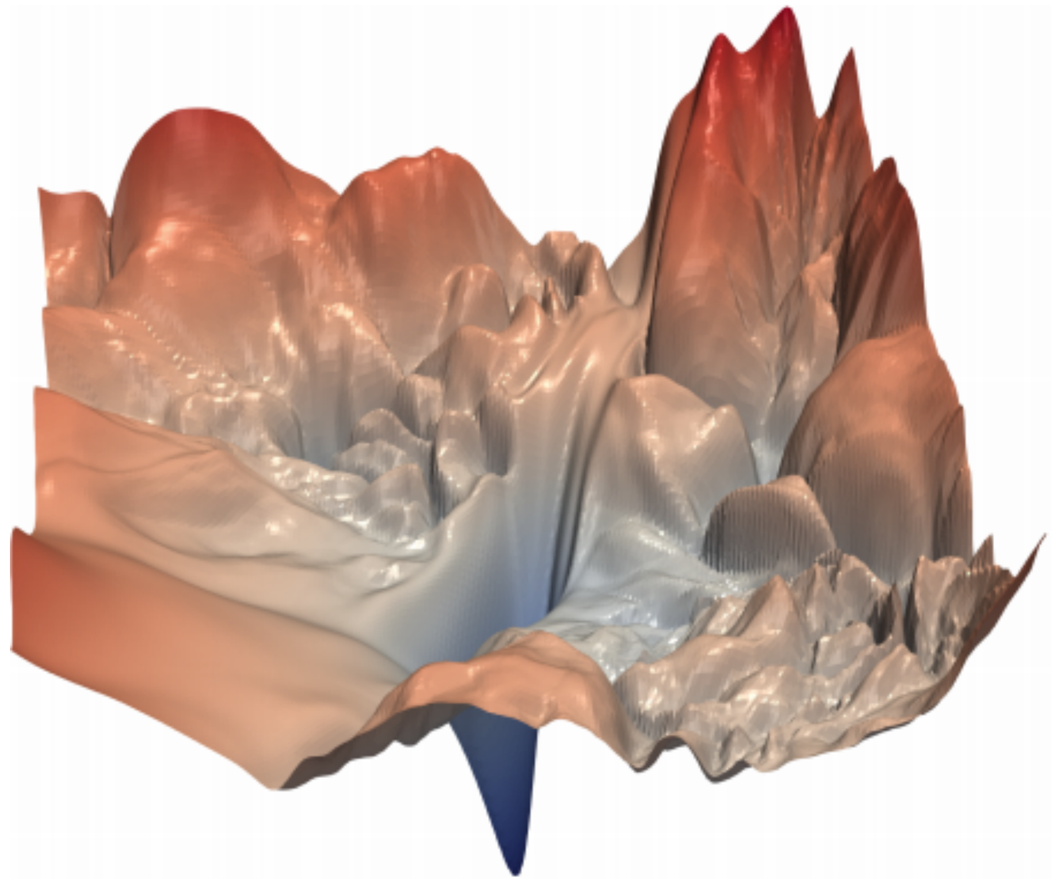

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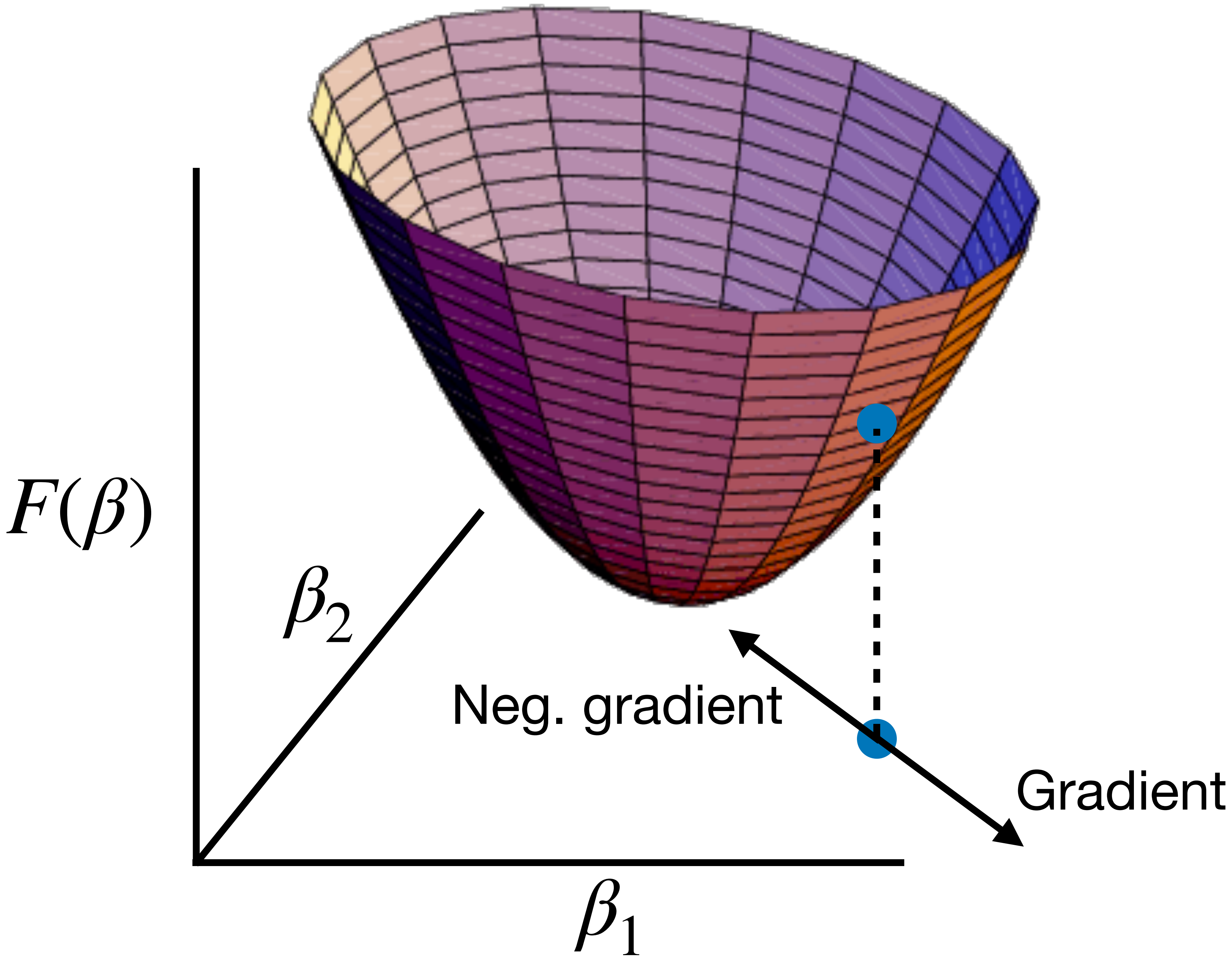

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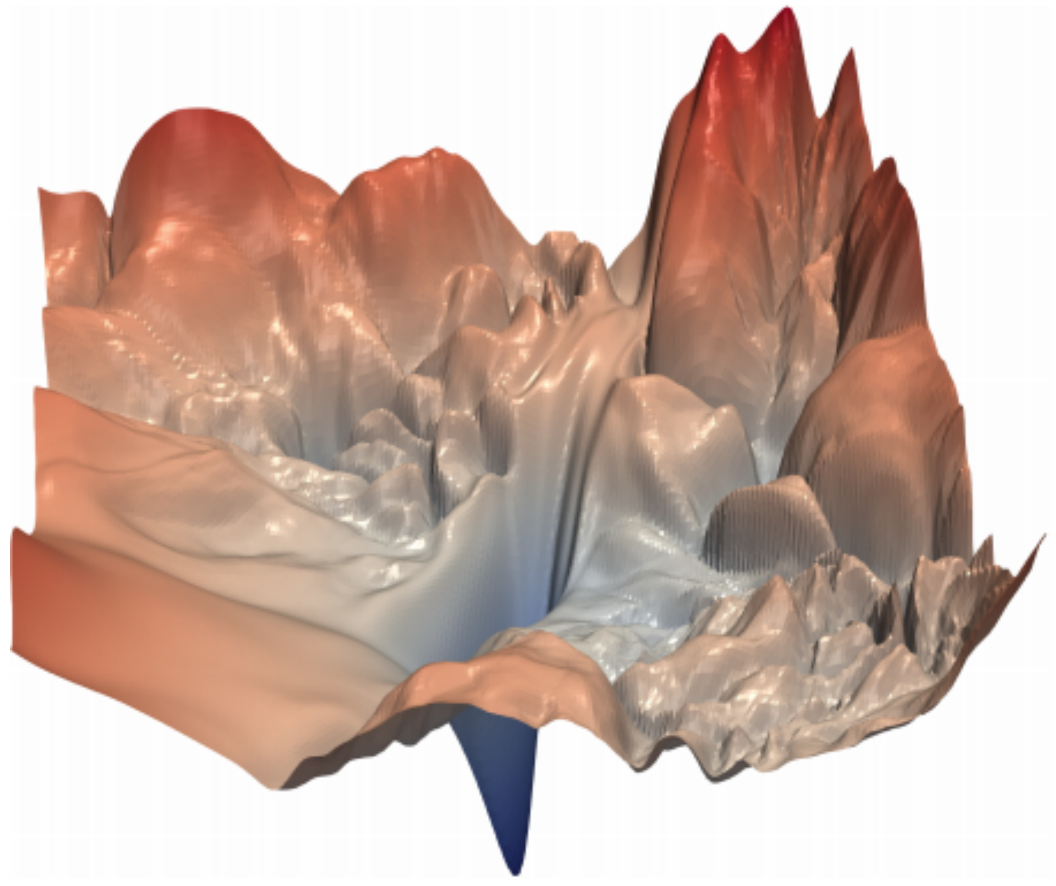

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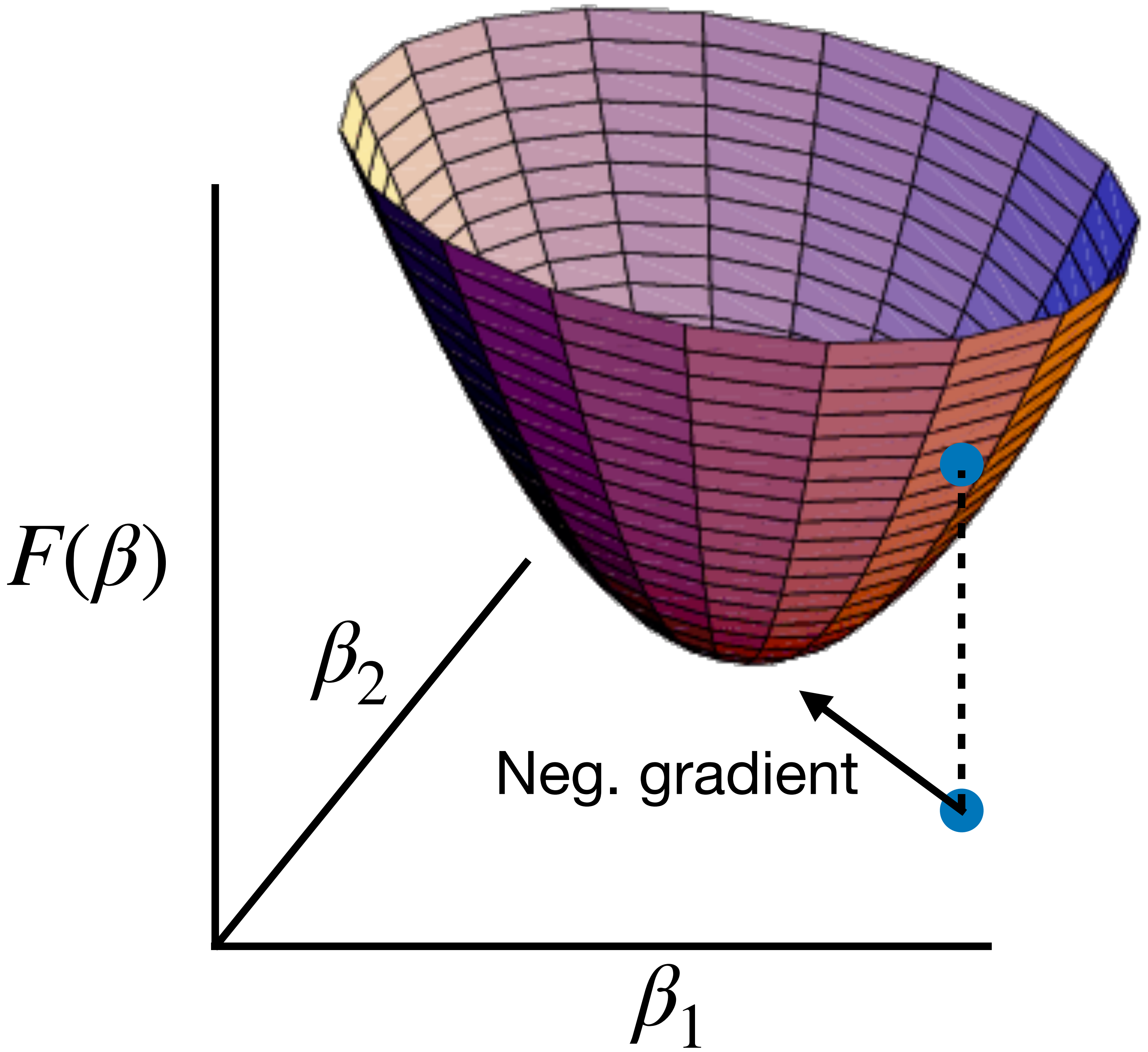

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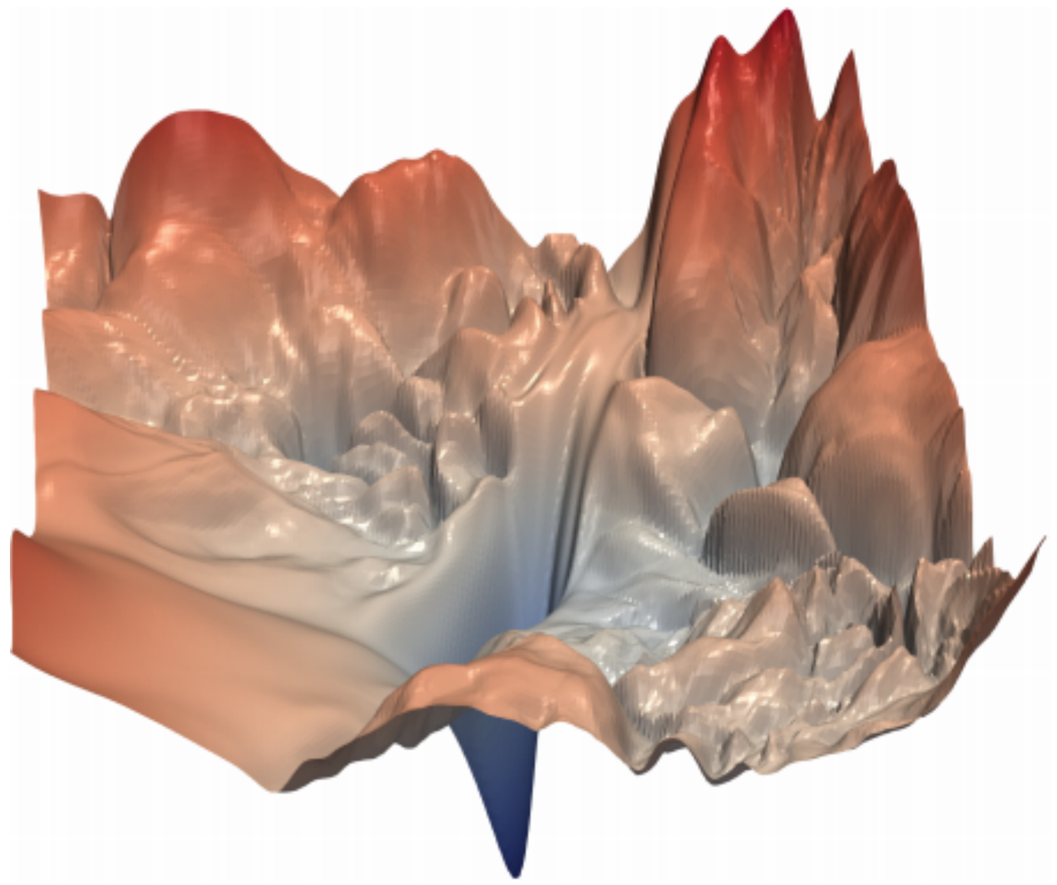

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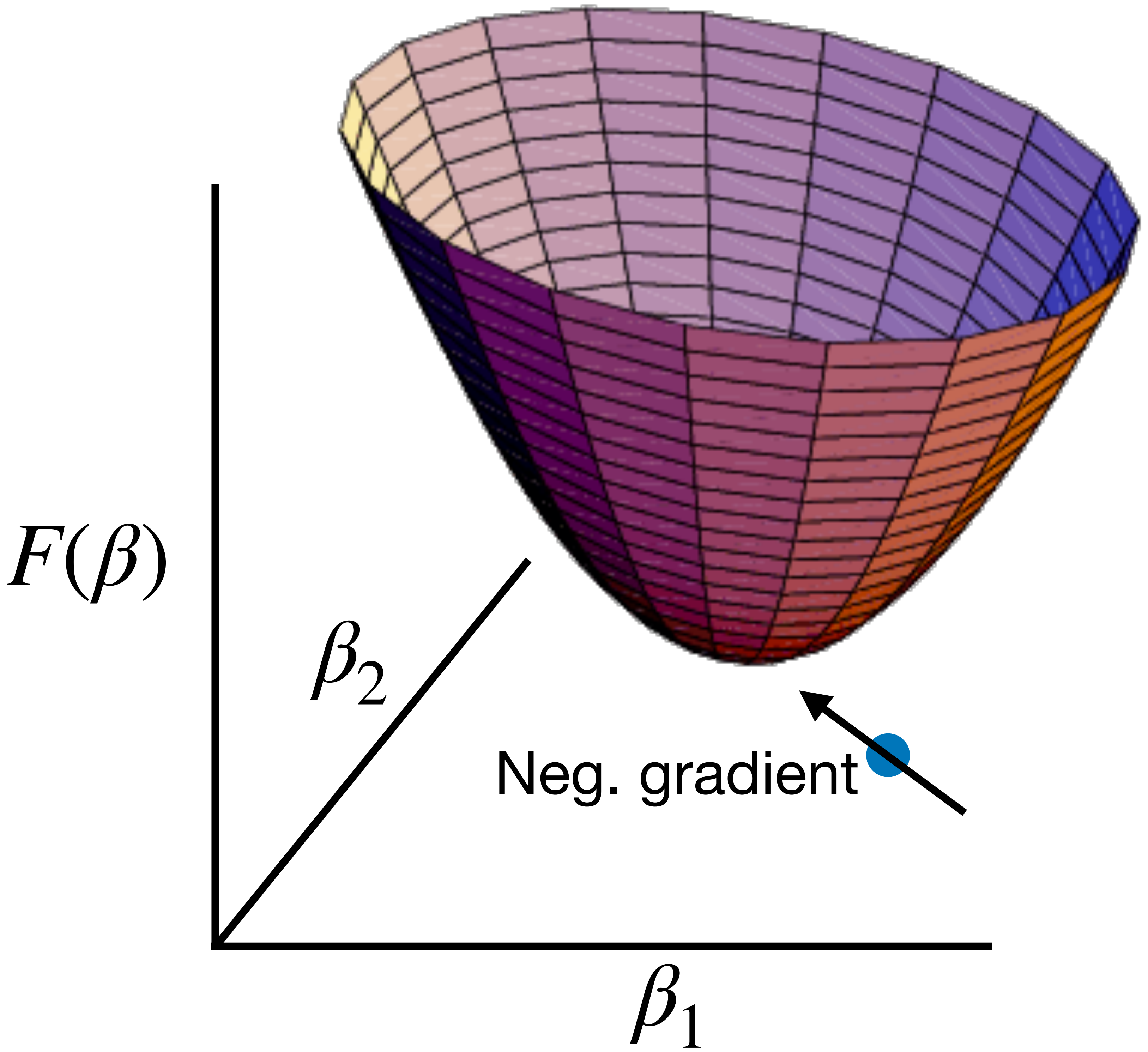

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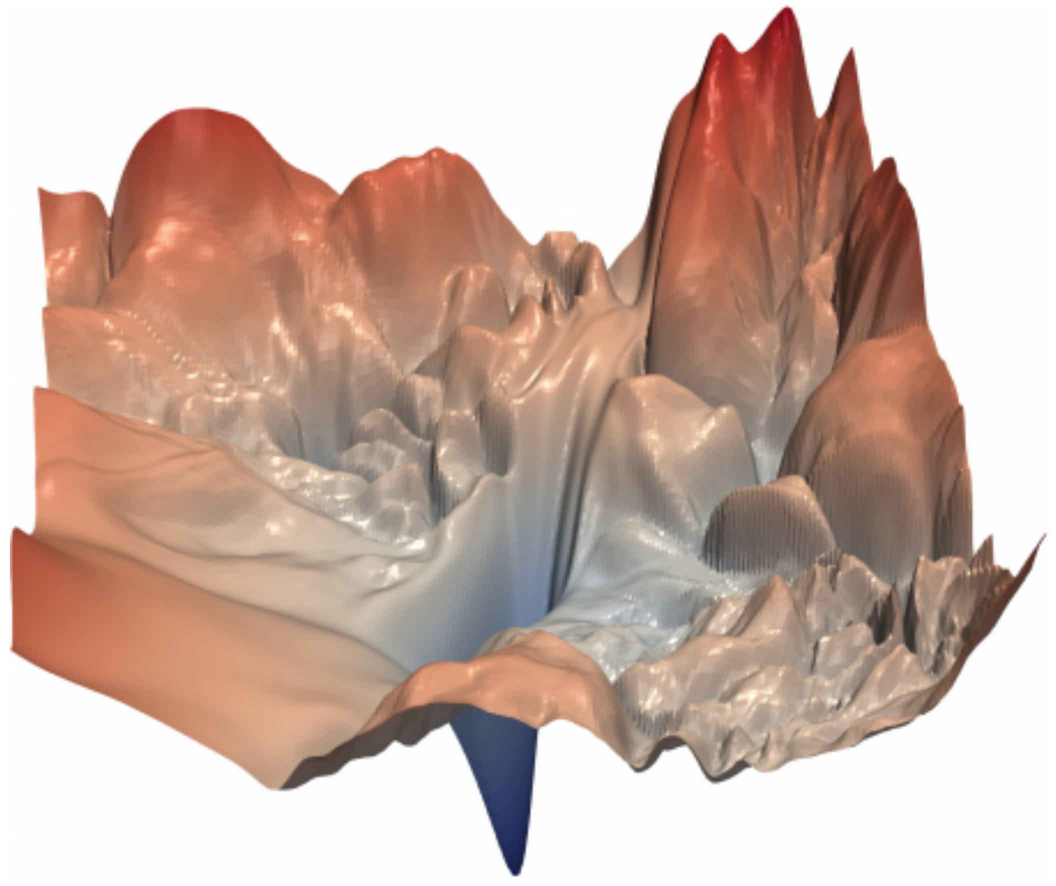

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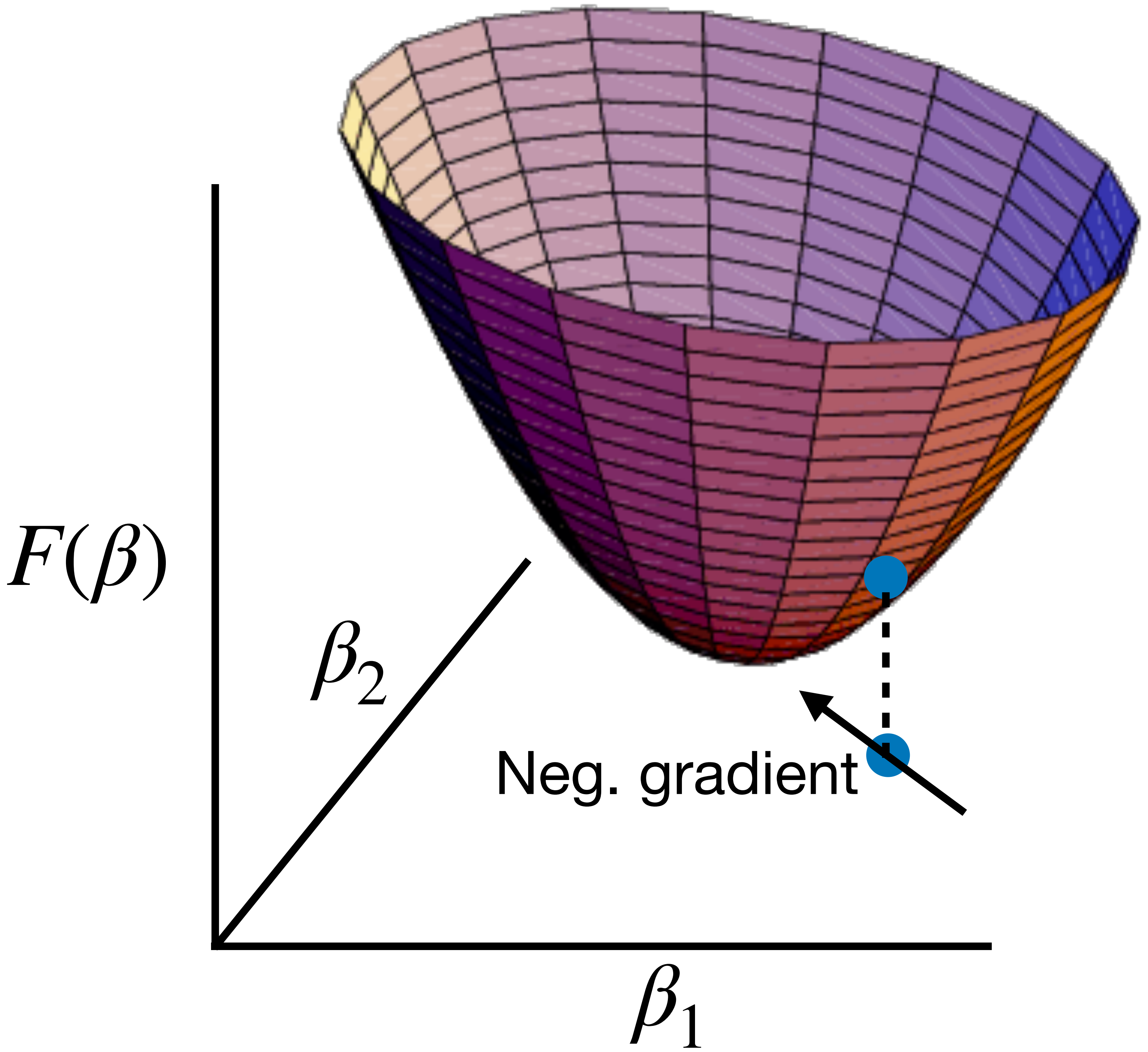

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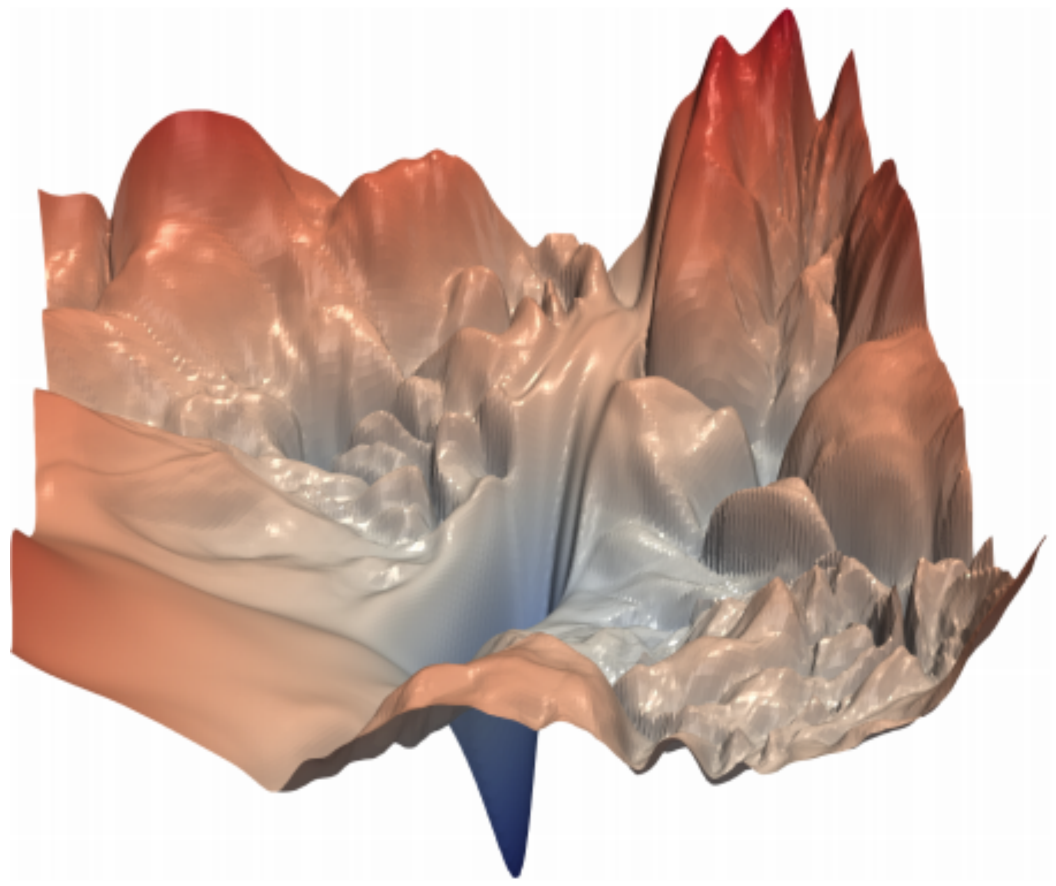

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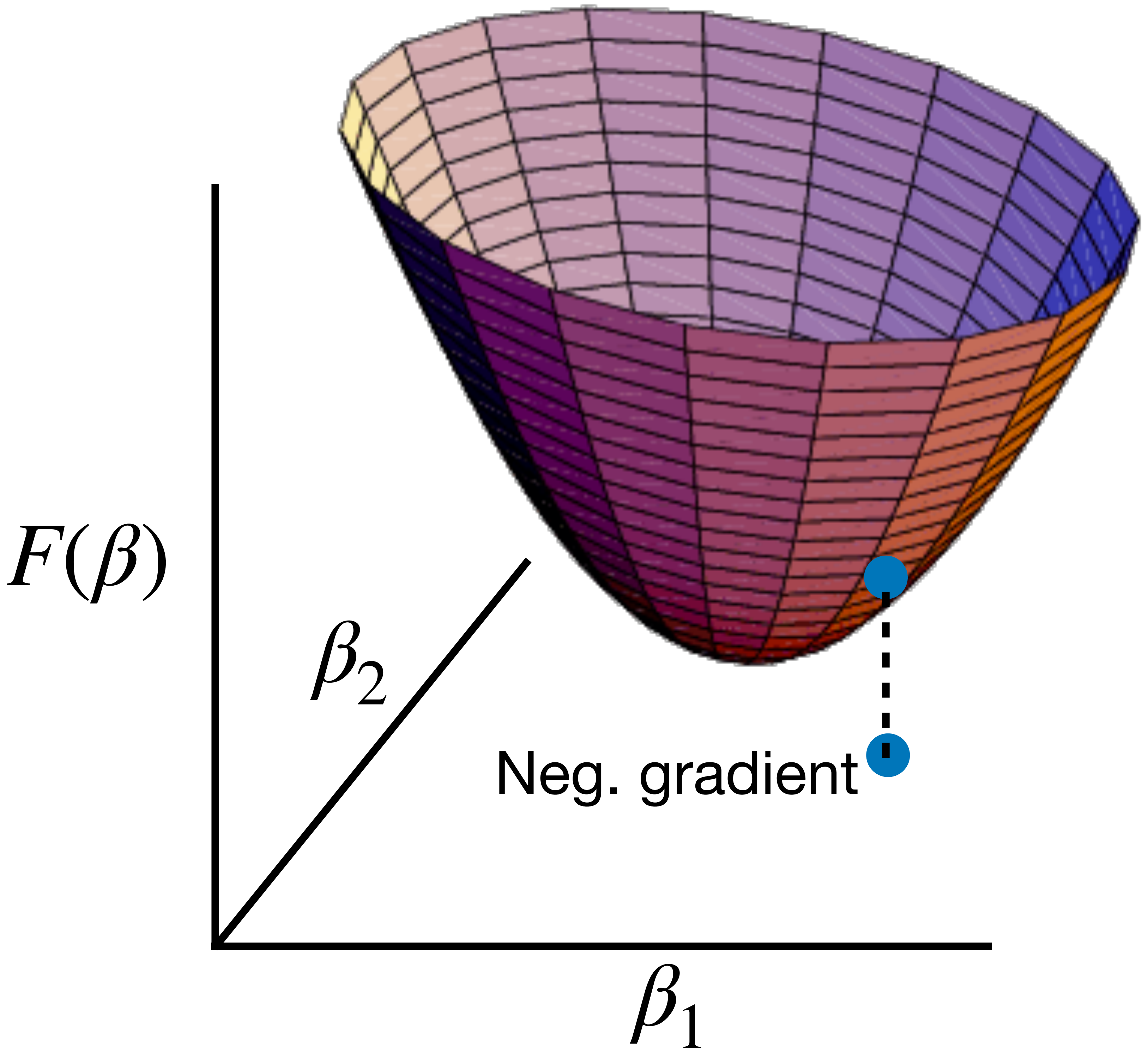

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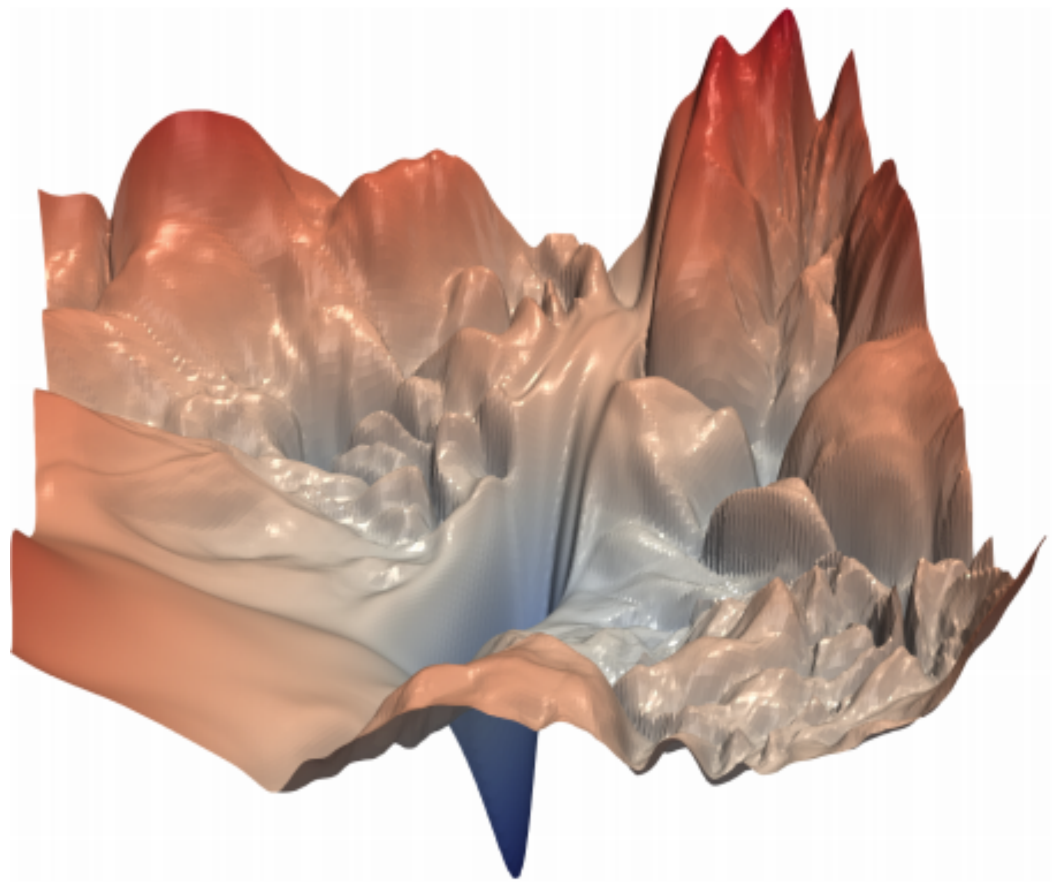

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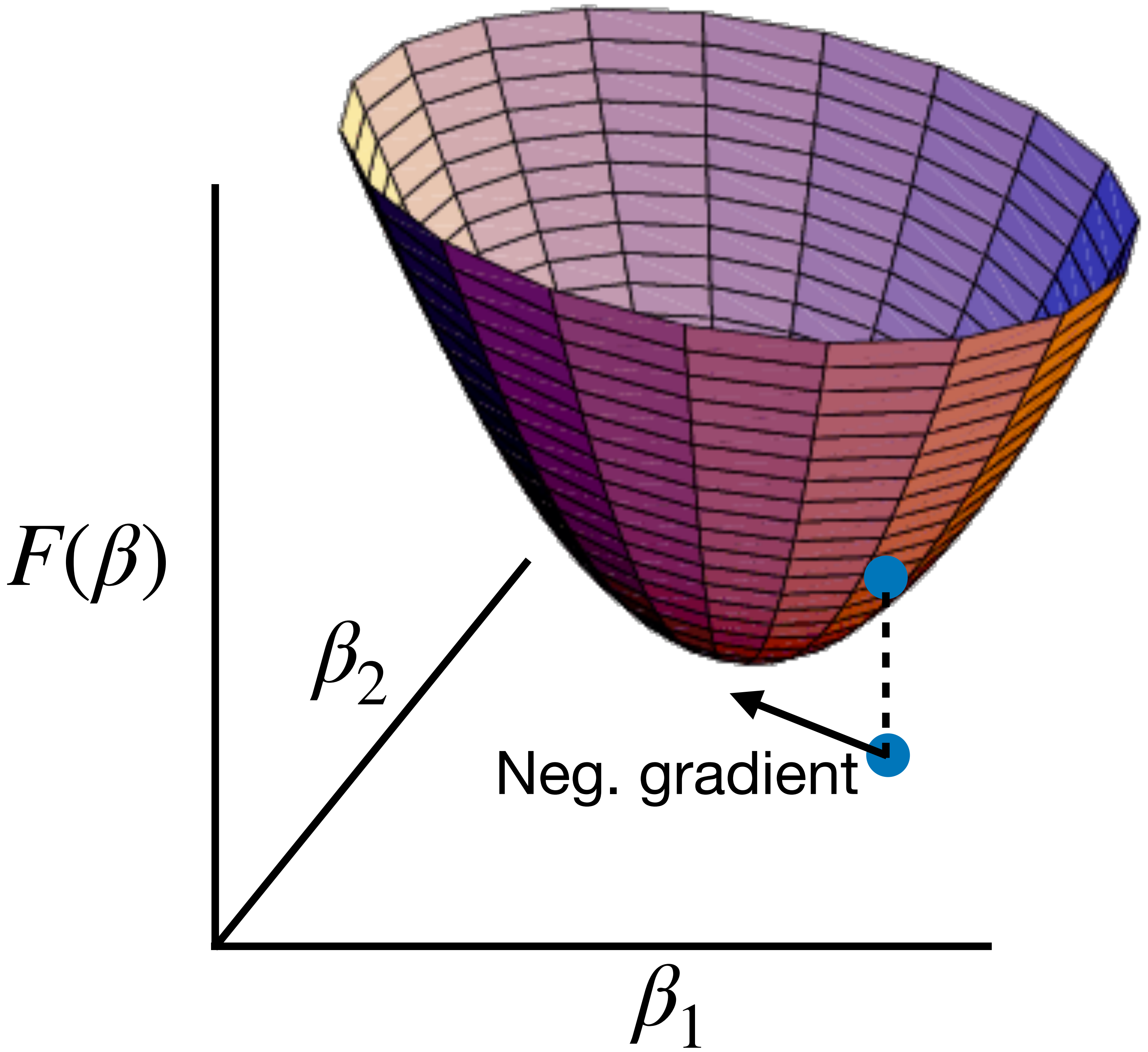

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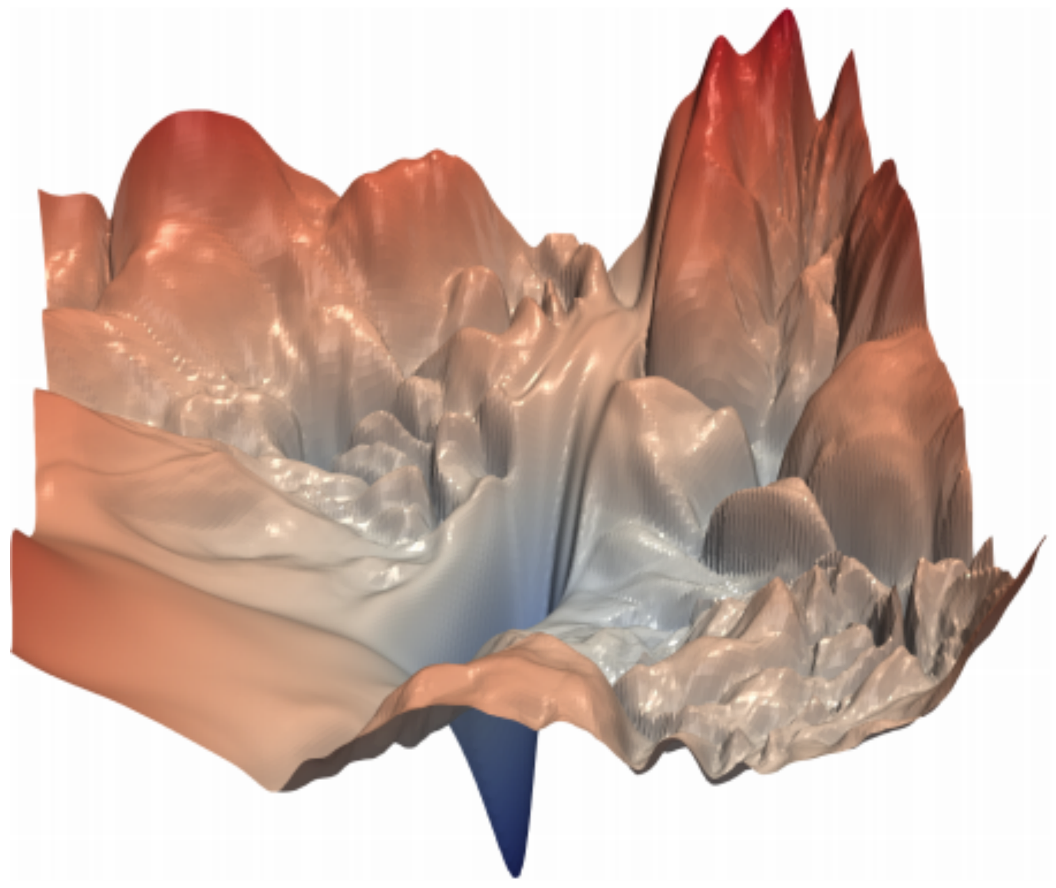

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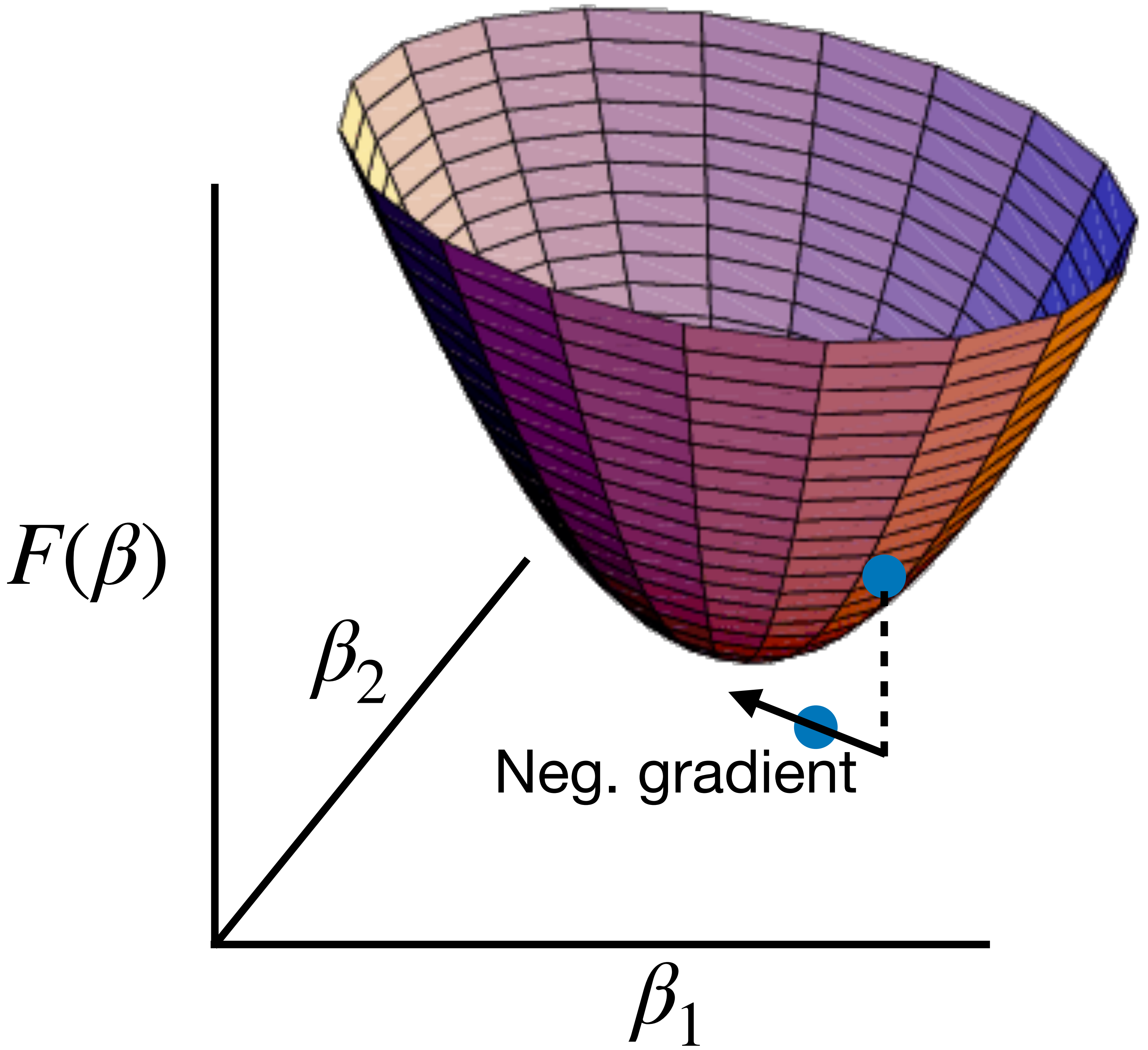

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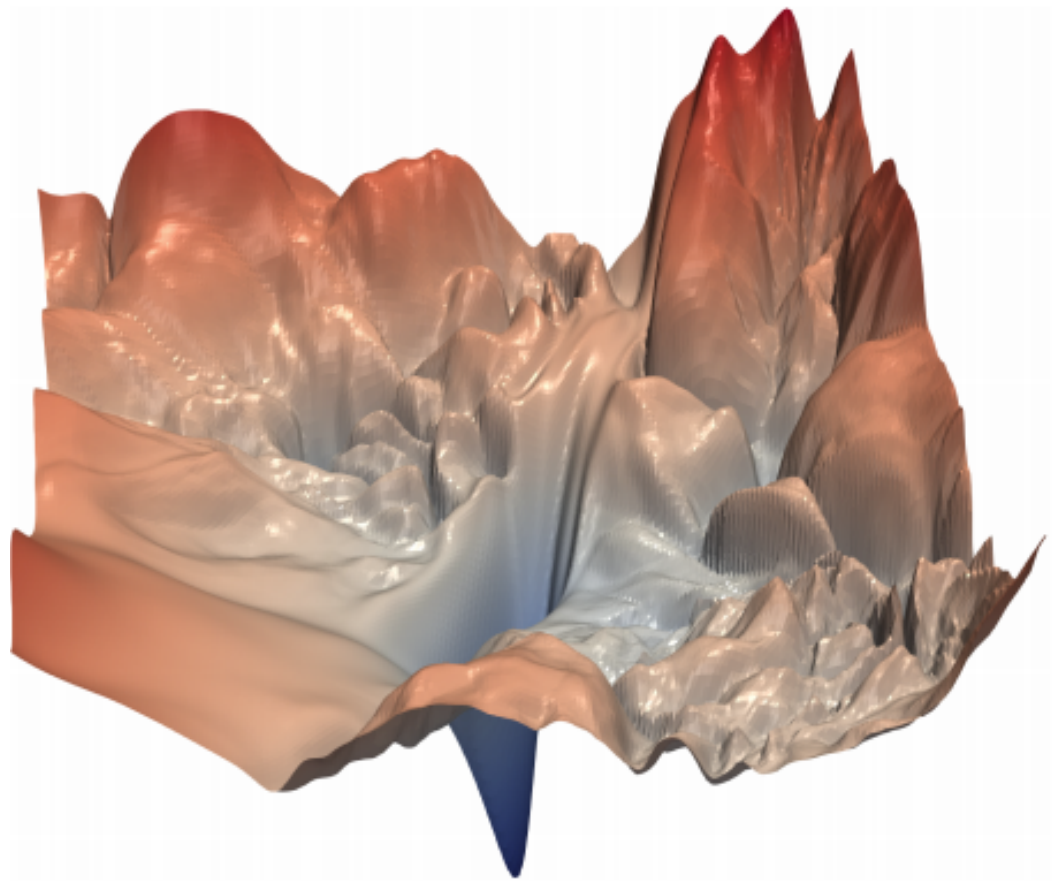

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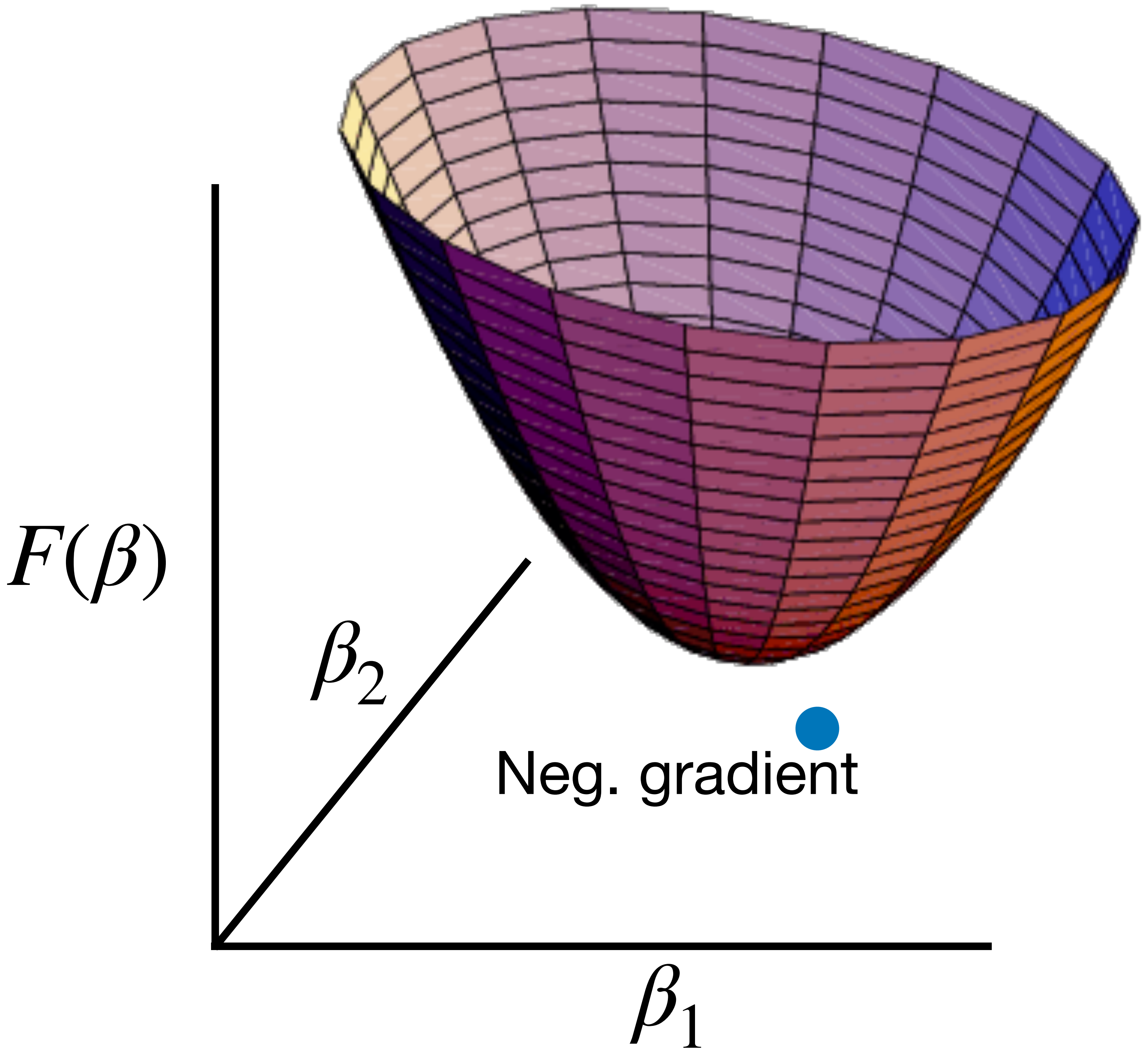

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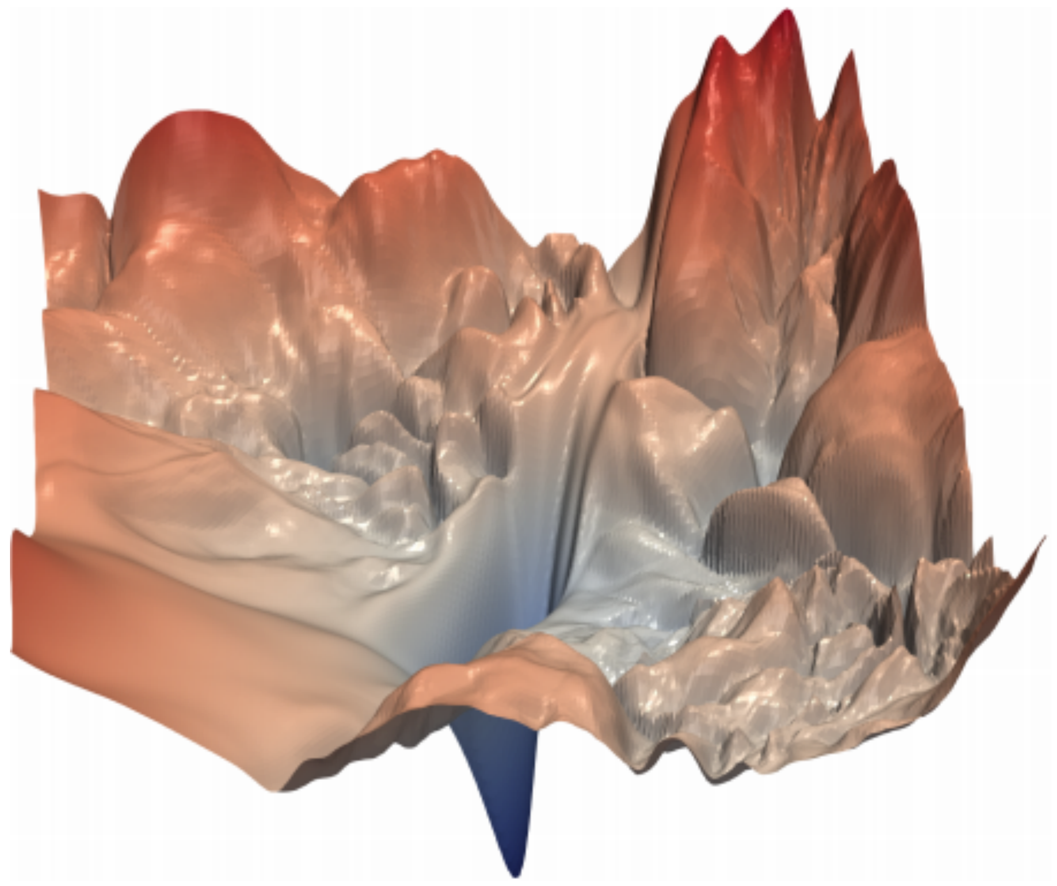

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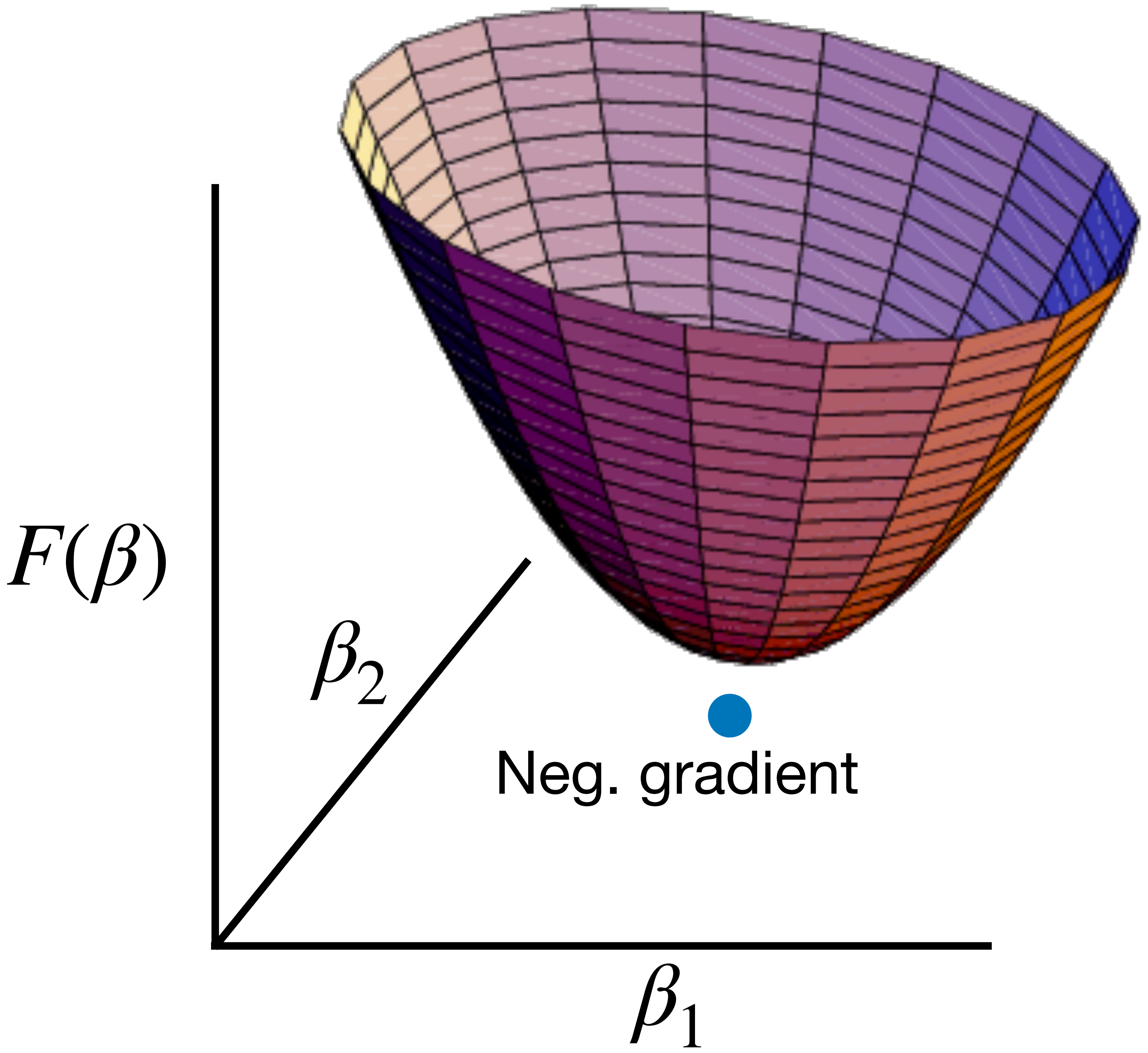

The computational cost of gradient descent

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Number of iterations has to do with the size of the learning rate (like boosting) and the shape of the objective function F.

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Cost of computing the gradient has to do with the size of the training data:

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If $F(\beta) = \frac{1}{n}\sum_{i=1}^{n} L(Y_i, f_\beta(X_i))$, then $\nabla F(\beta) = \frac{1}{n}\sum_{i=1}^{n} \nabla L(Y_i, f_\beta(X_i))$.

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This can make gradient descent prohibitively expensive.

Stochastic gradient descent

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Use subset $S \subseteq \{1, \ldots, n\}$ (mini-batch) of observations to approximate gradient:

$$\nabla F(\beta) = \frac{1}{n} \sum_{i=1}^{n} \nabla L(Y_i, f_\beta(X_i)) \approx \frac{1}{|S|} \sum_{i \in S} \nabla L(Y_i, f_\beta(X_i)).$$

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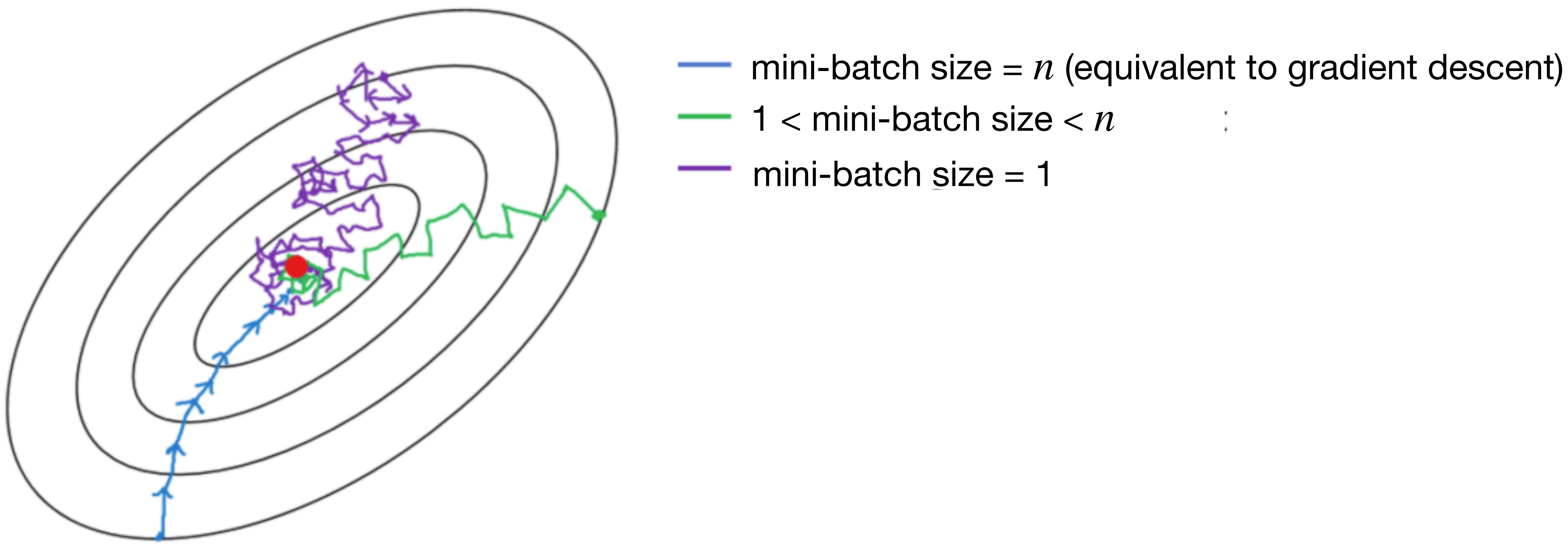
Backpropagation: An efficient algorithm to compute $\nabla L(Y_i, f_\beta(X_i))$

Behavior of stochastic gradient descent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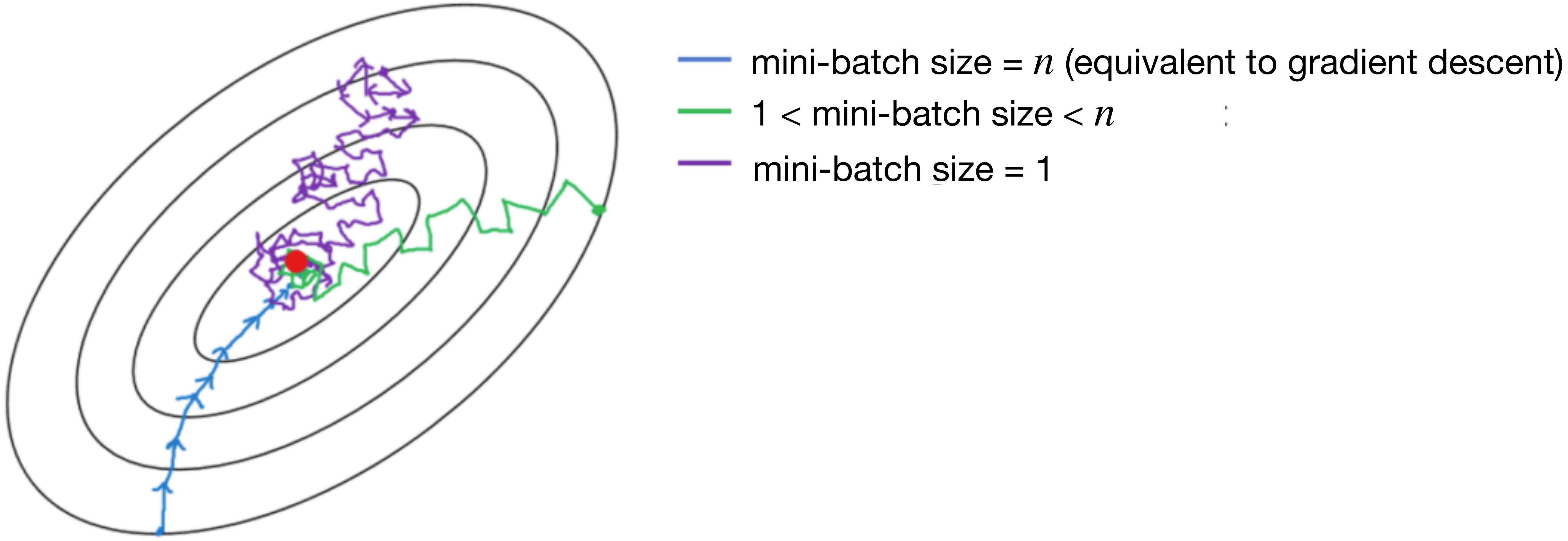
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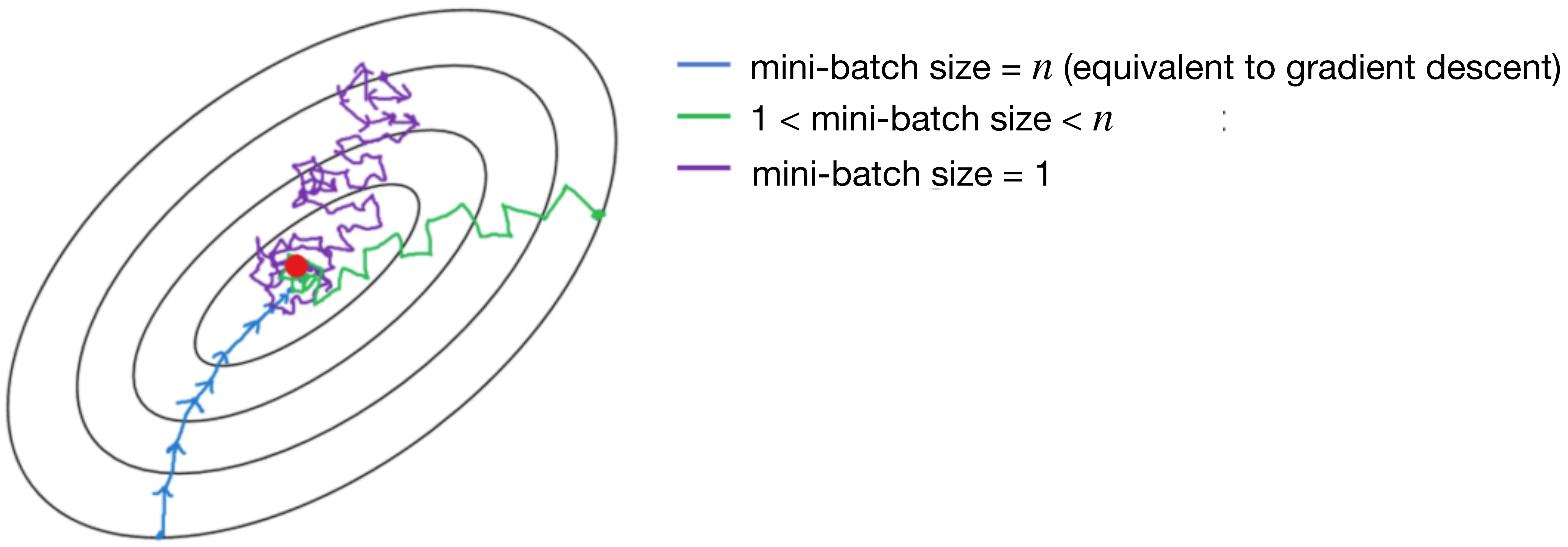
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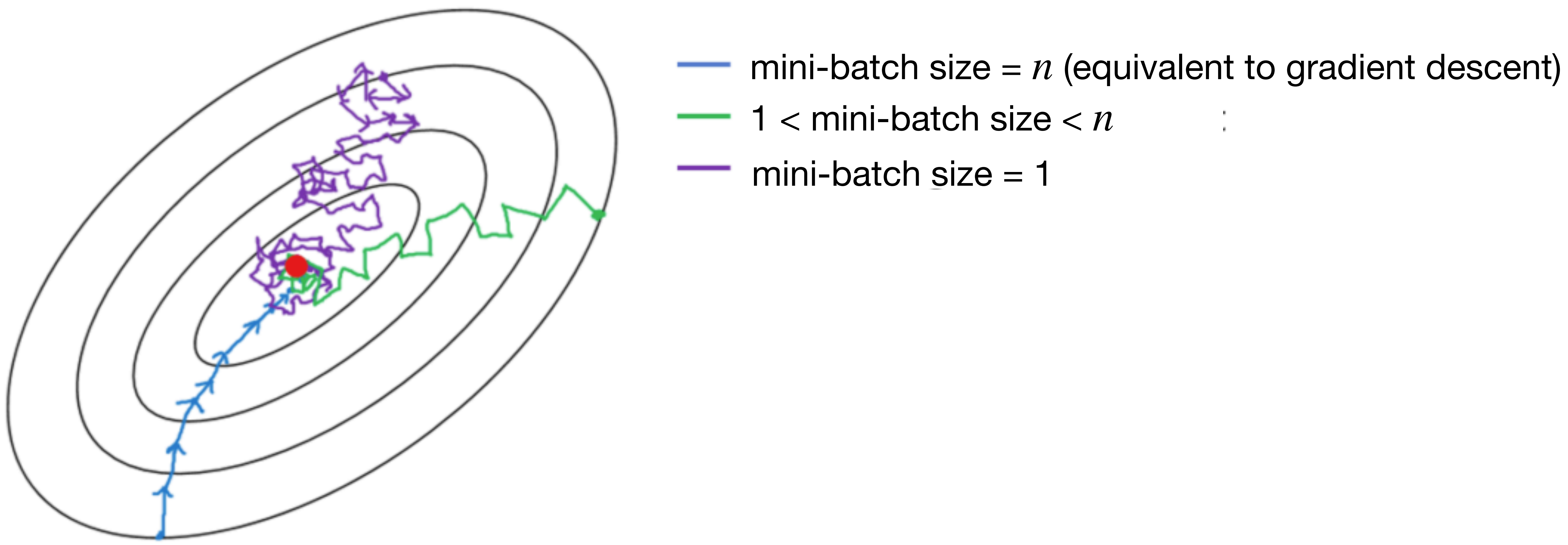
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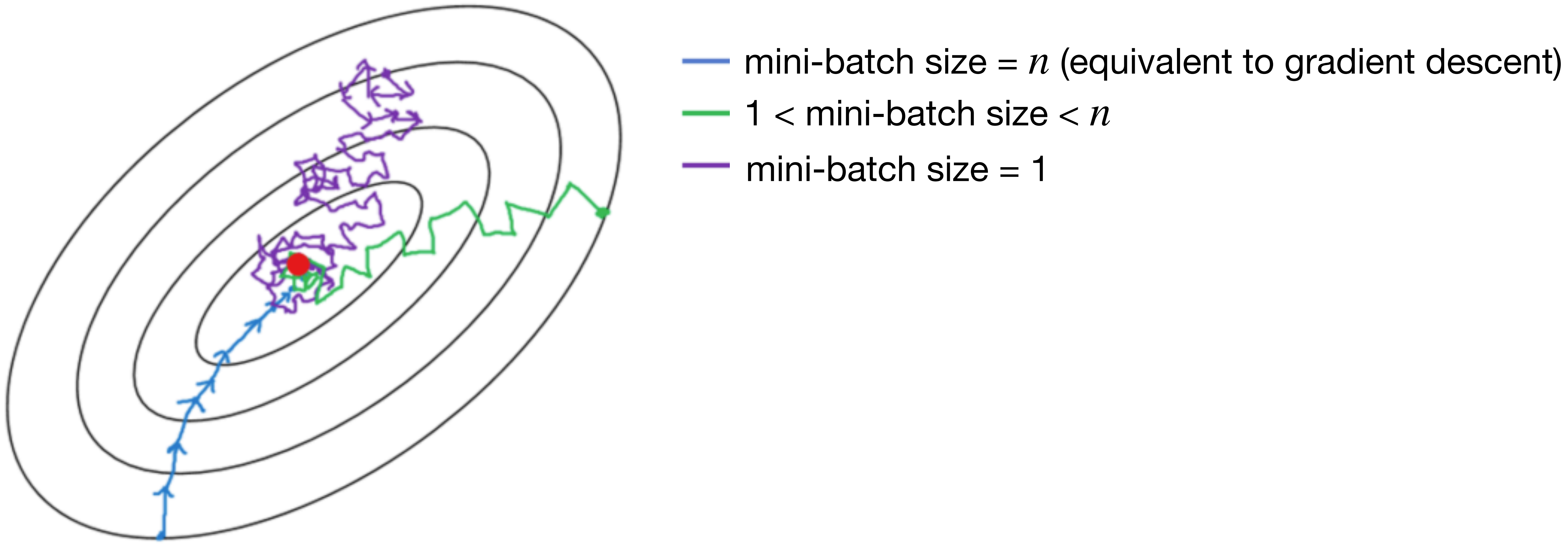
Bonus: The extra randomness sometimes allows SGD to wobble past local minima.

Stochastic gradient descent step versus epoch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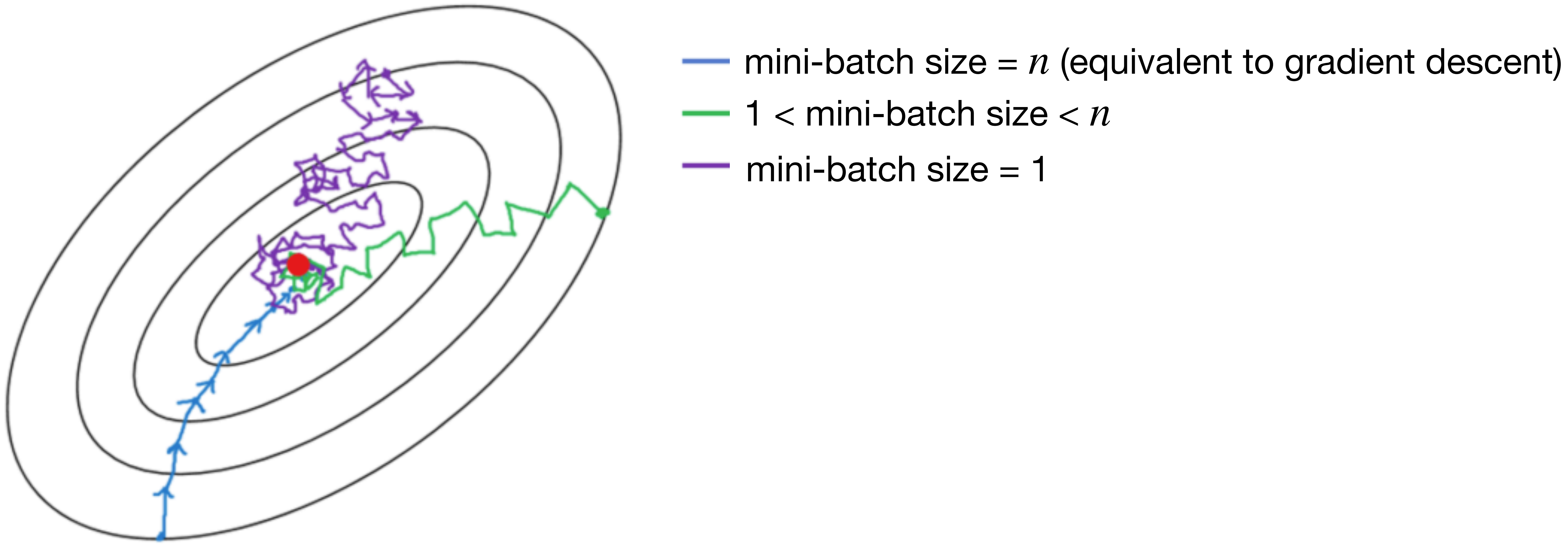
An epoch consists of SGD steps that cycle through all of the observations once.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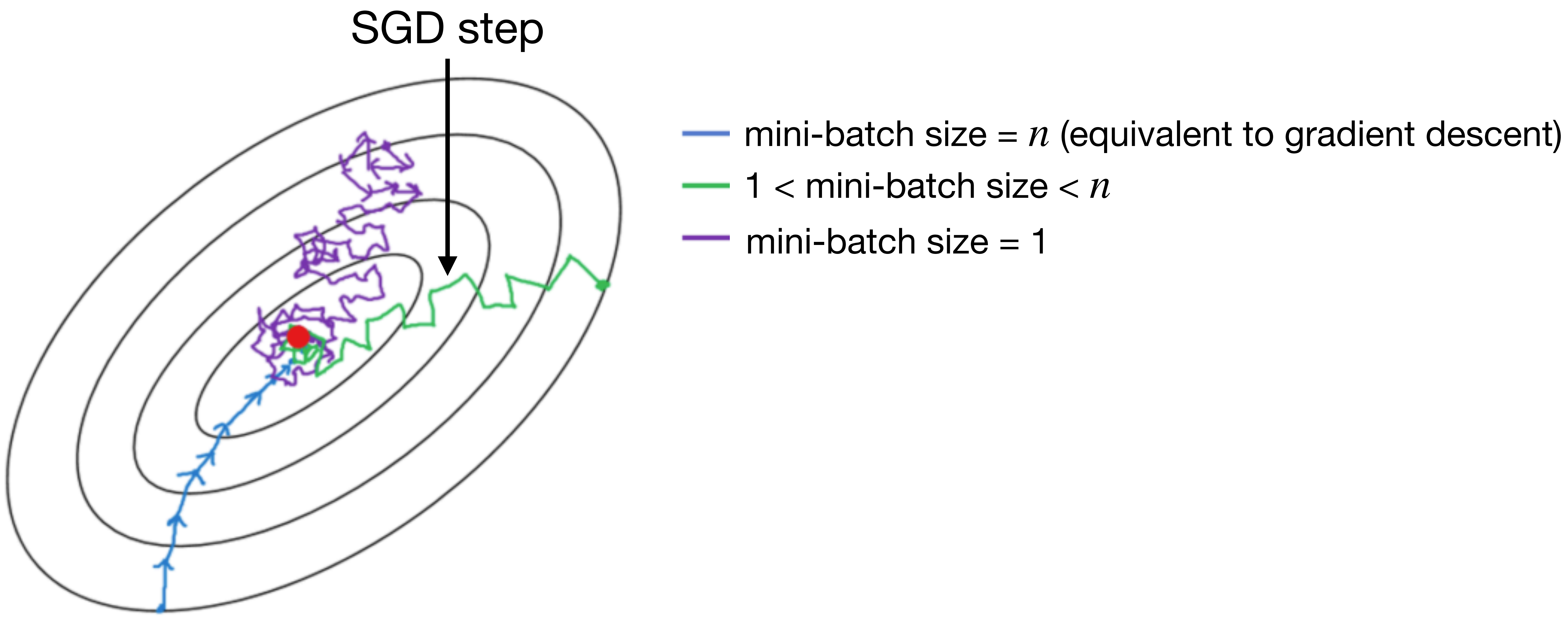
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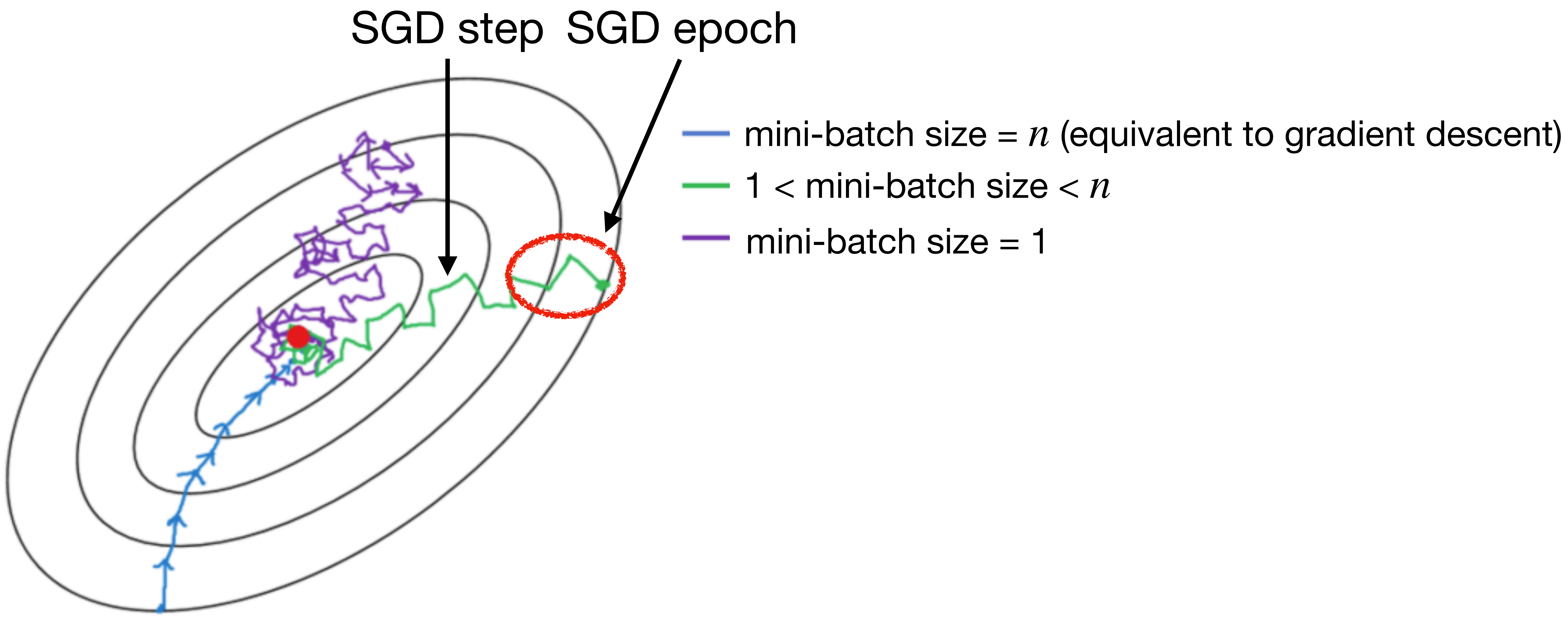
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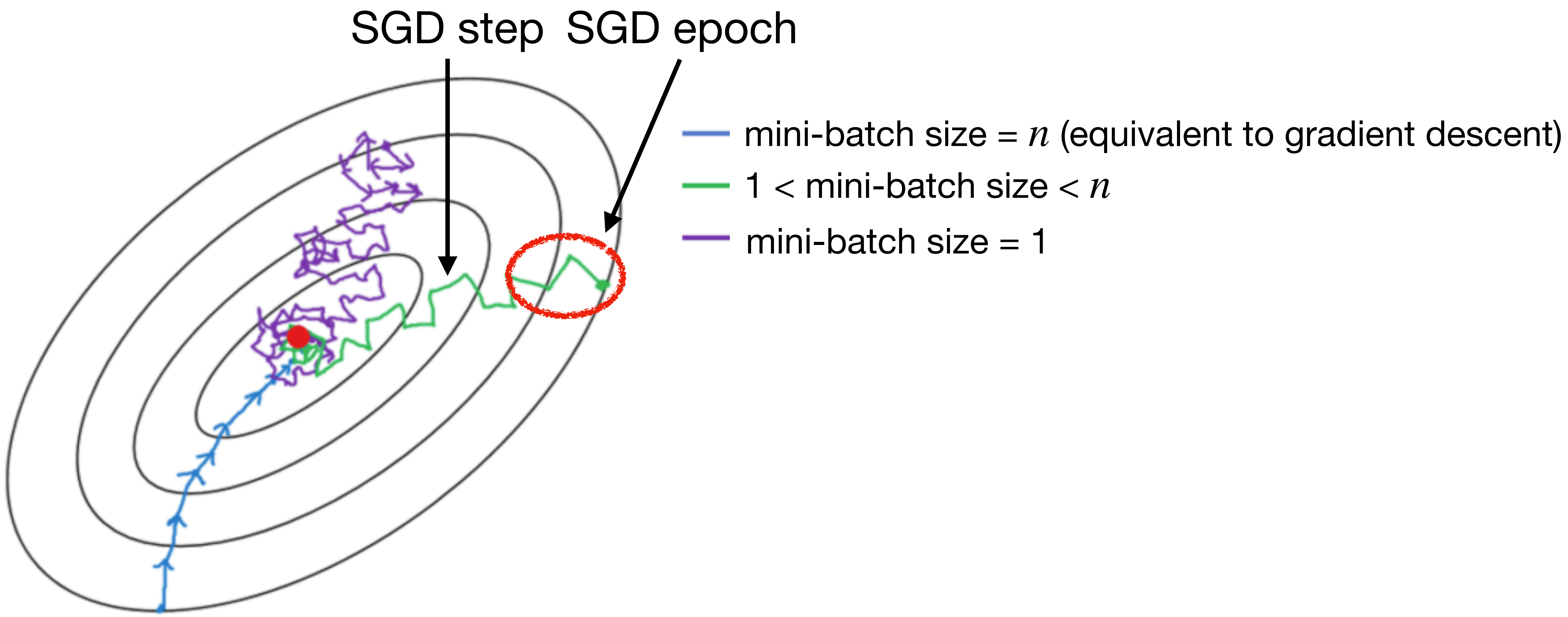

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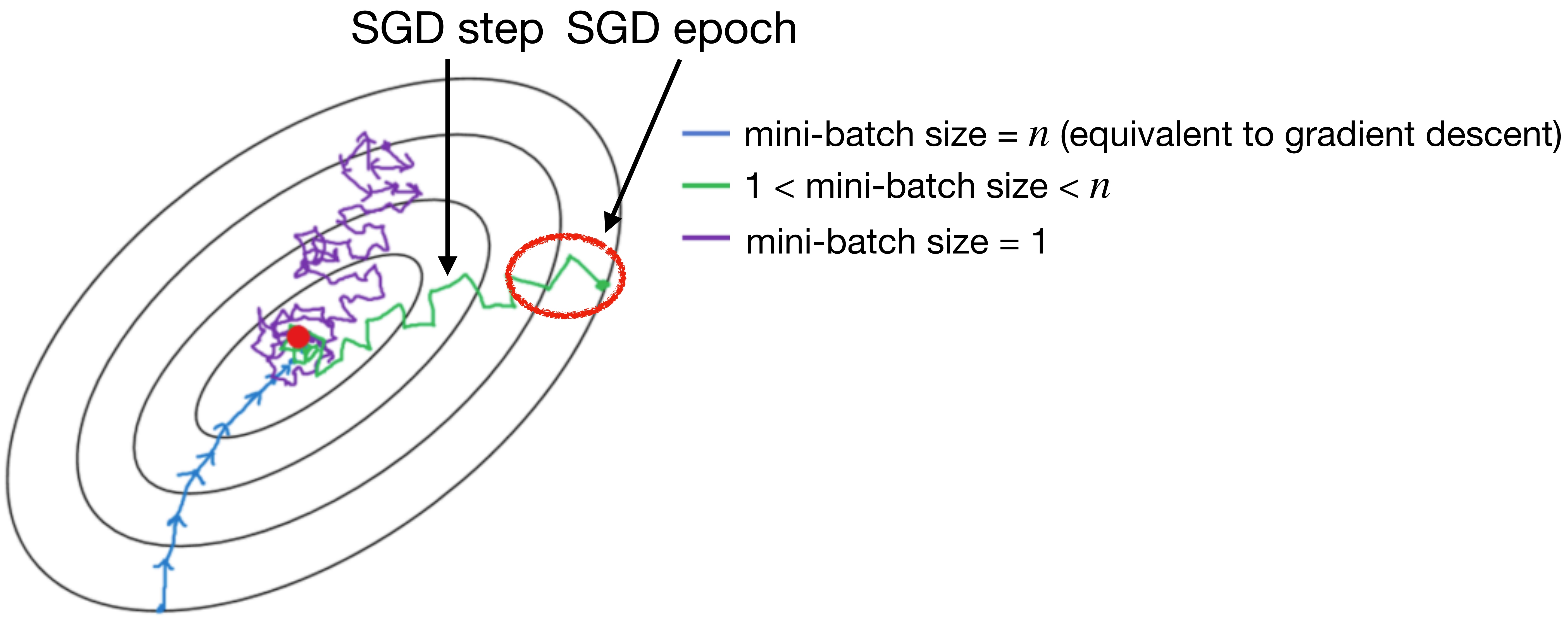
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Observation	1	2	3	4	5	6	7	8	9	1	2	3	4	5	6	7	8	9
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SGD step (mini-batch size 1)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18

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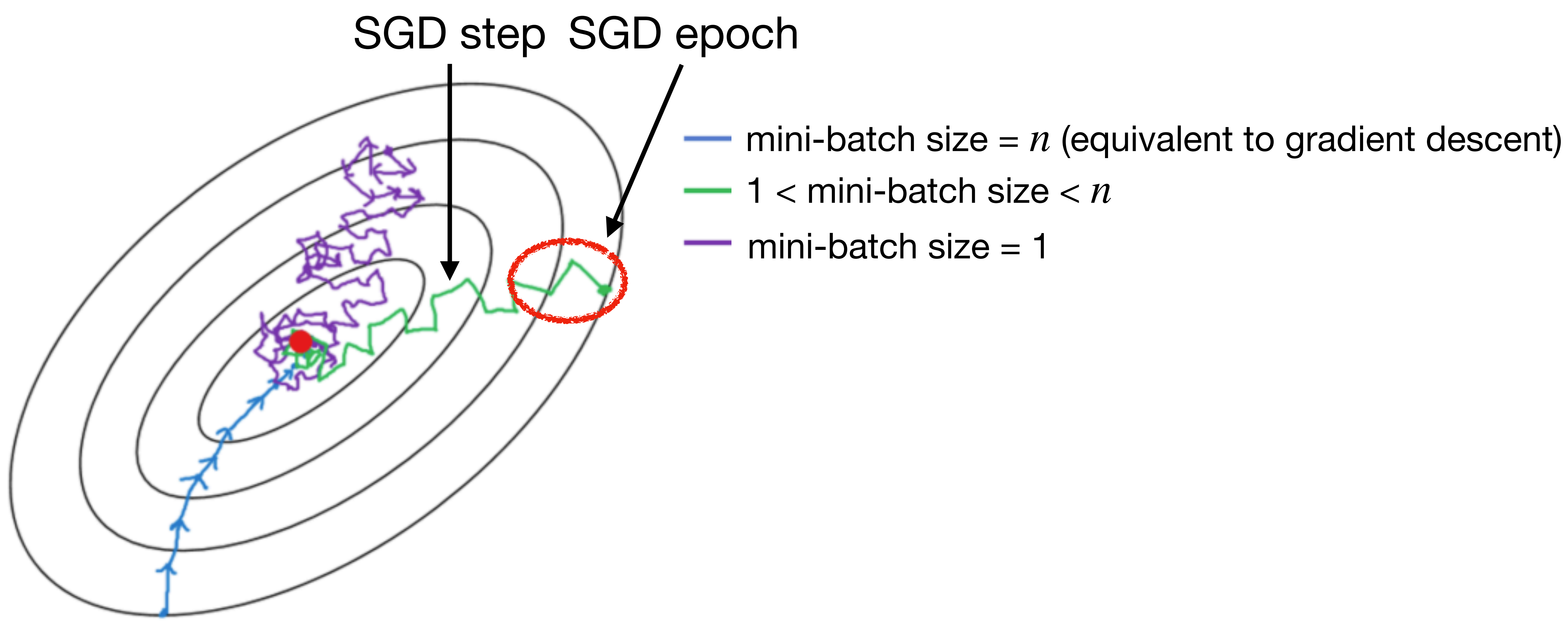
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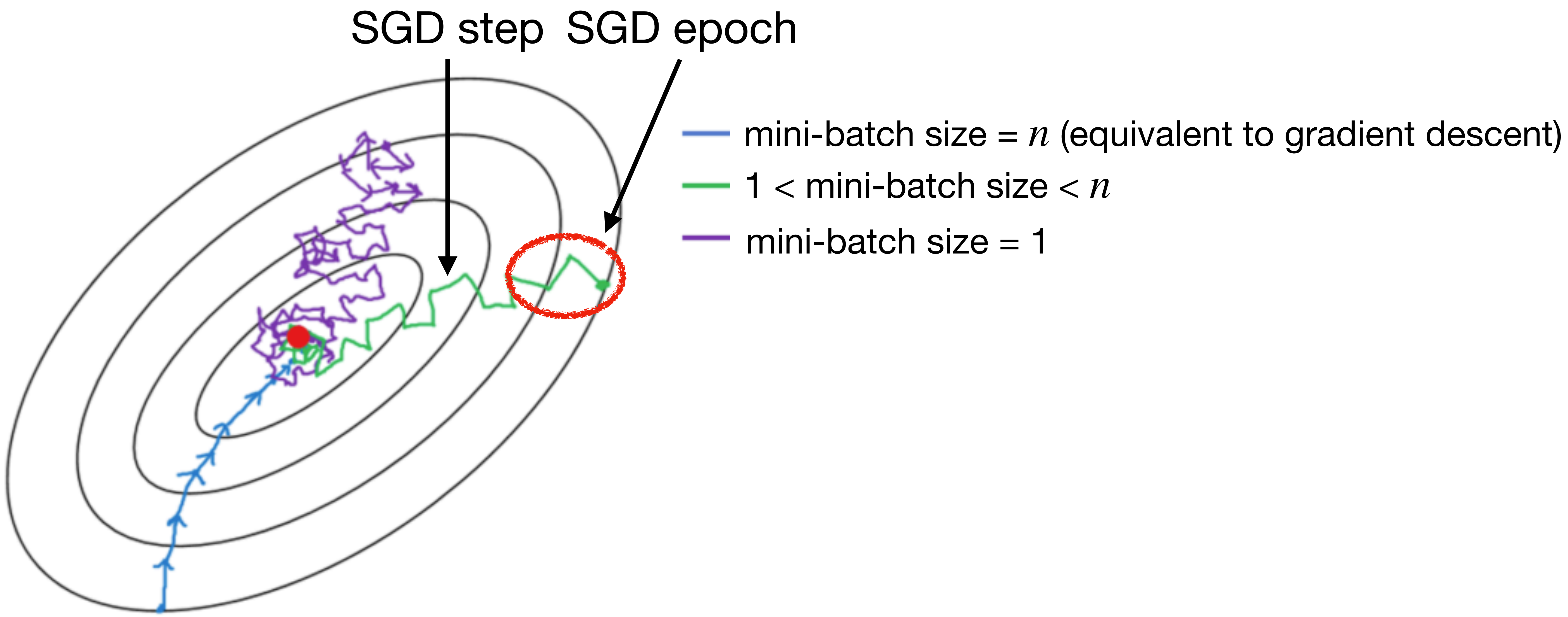
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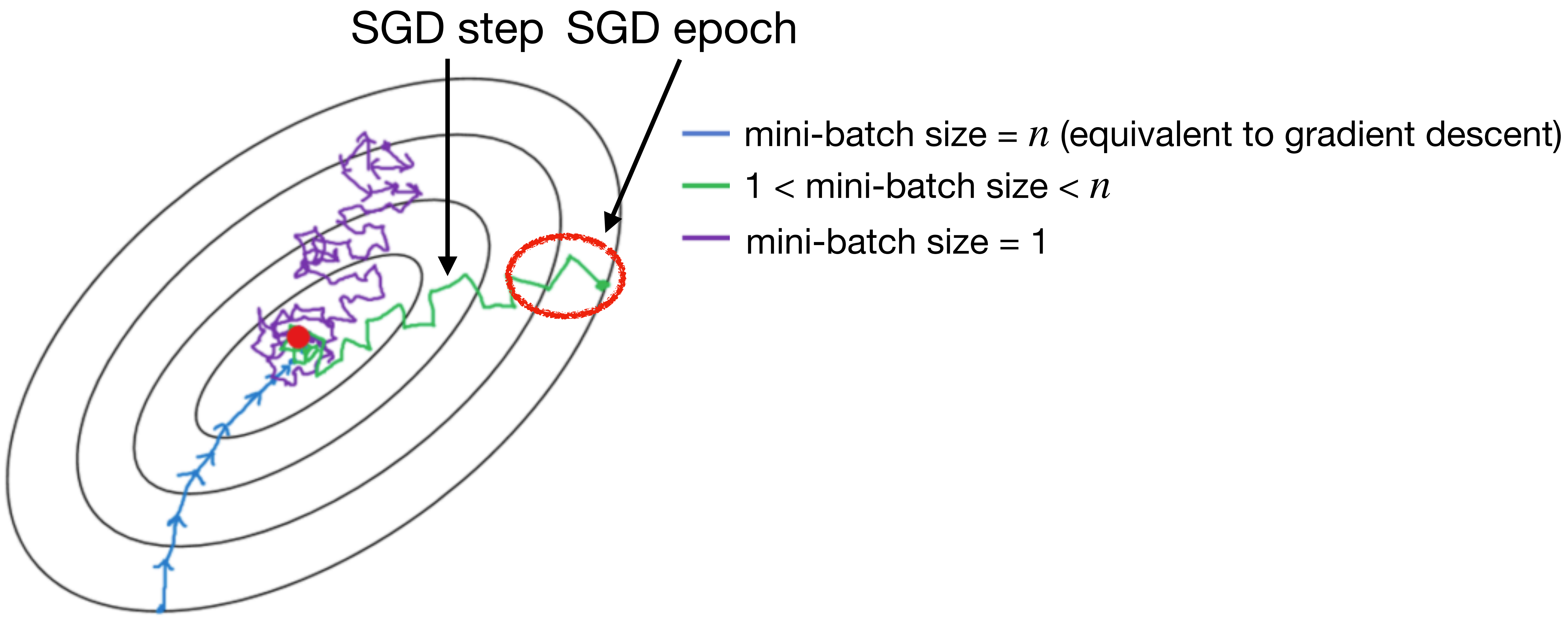
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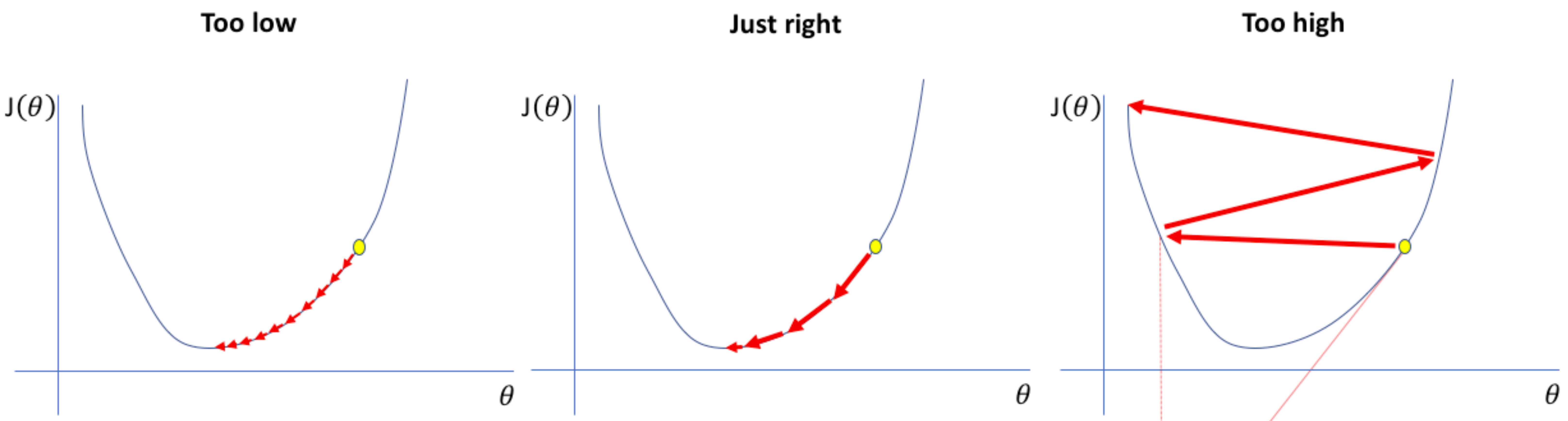
Gradient step	Step 1									Step 2								

The learning rate for (stochastic) gradient descent



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A small learning rate requires many updates before reaching the minimum point

Just right

The optimal learning rate swiftly reaches the minimum point

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Too large of a learning rate causes drastic updates which lead to divergent behaviors

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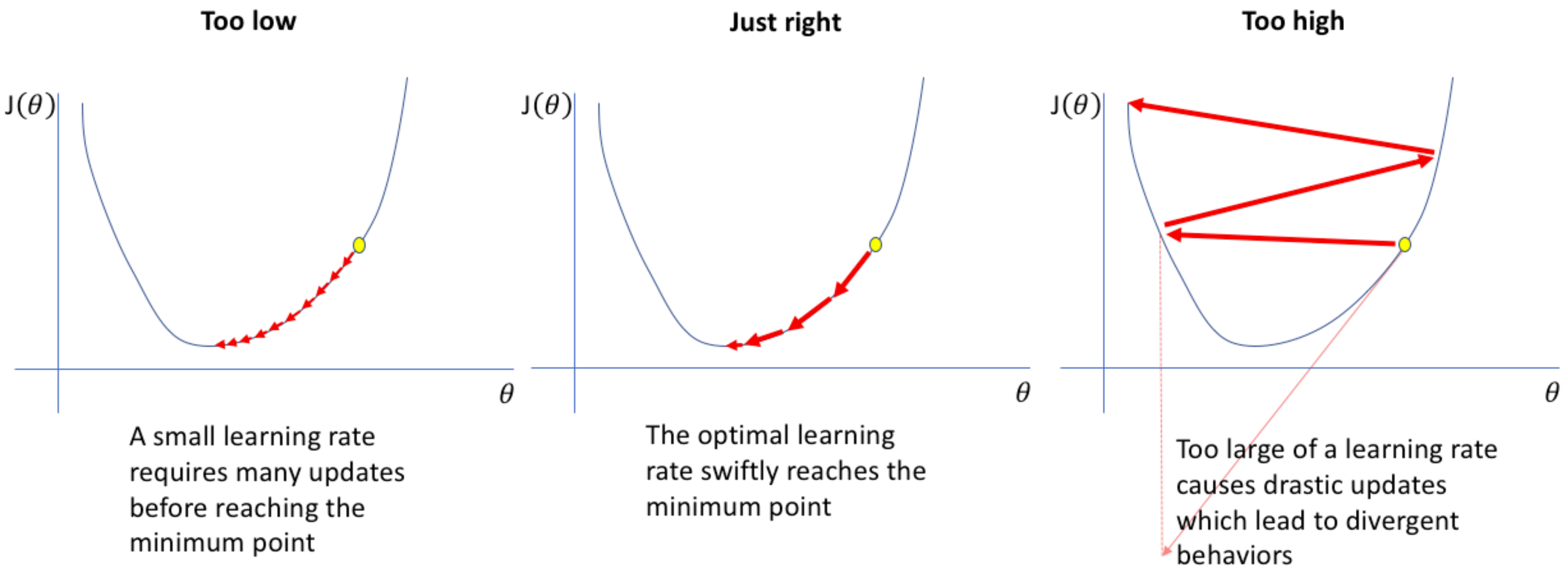

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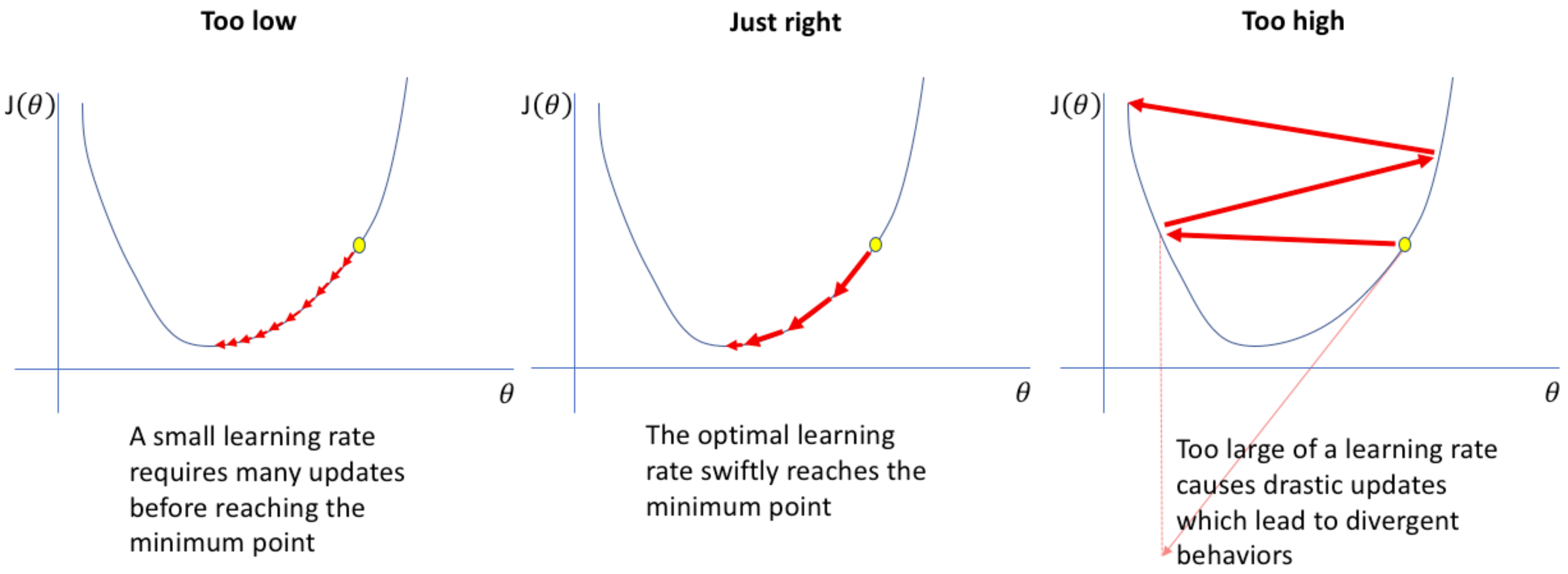

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- Especially for non-convex optimization, people come up with clever strategies like shrinking learning rates, cycling learning rates, adaptive learning rates, etc. (RMSprop, Adam, AdaGrad, AdaDelta, …)

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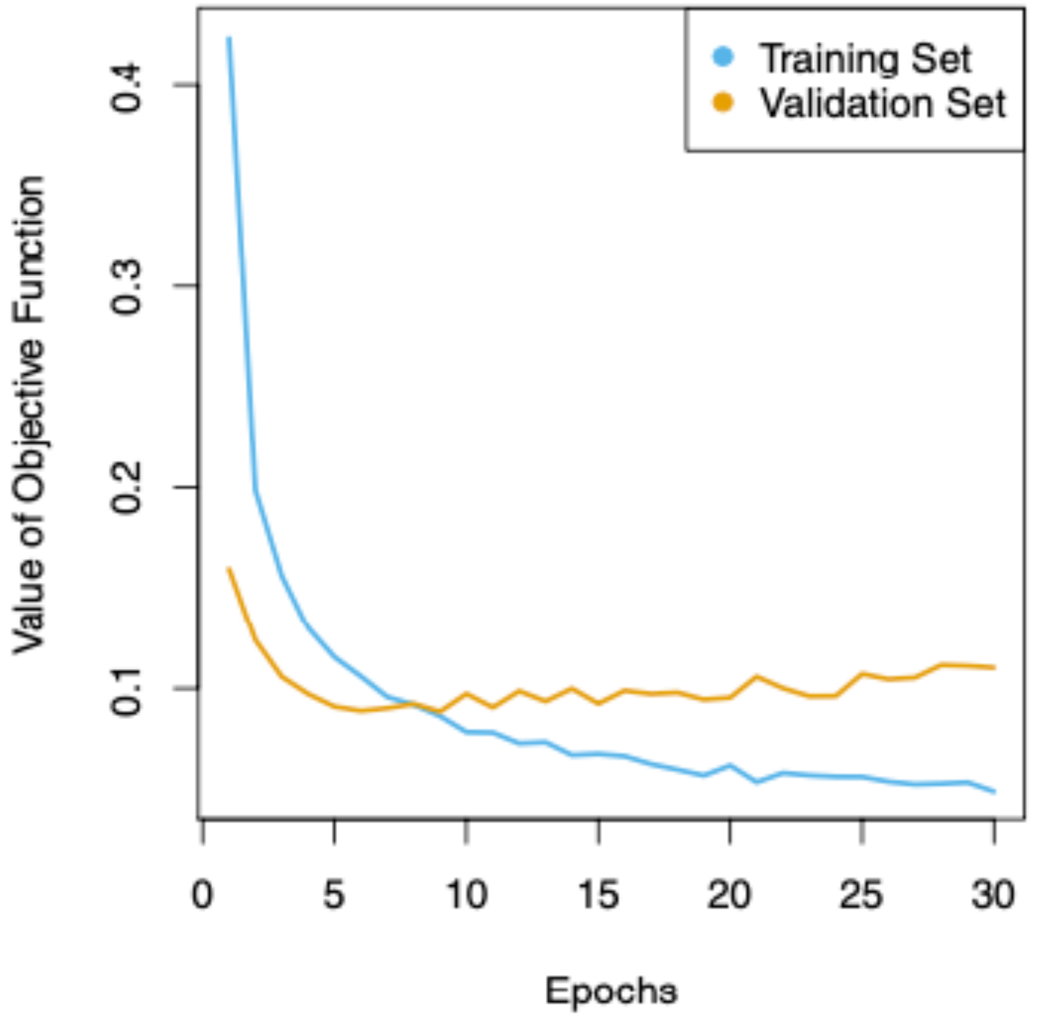

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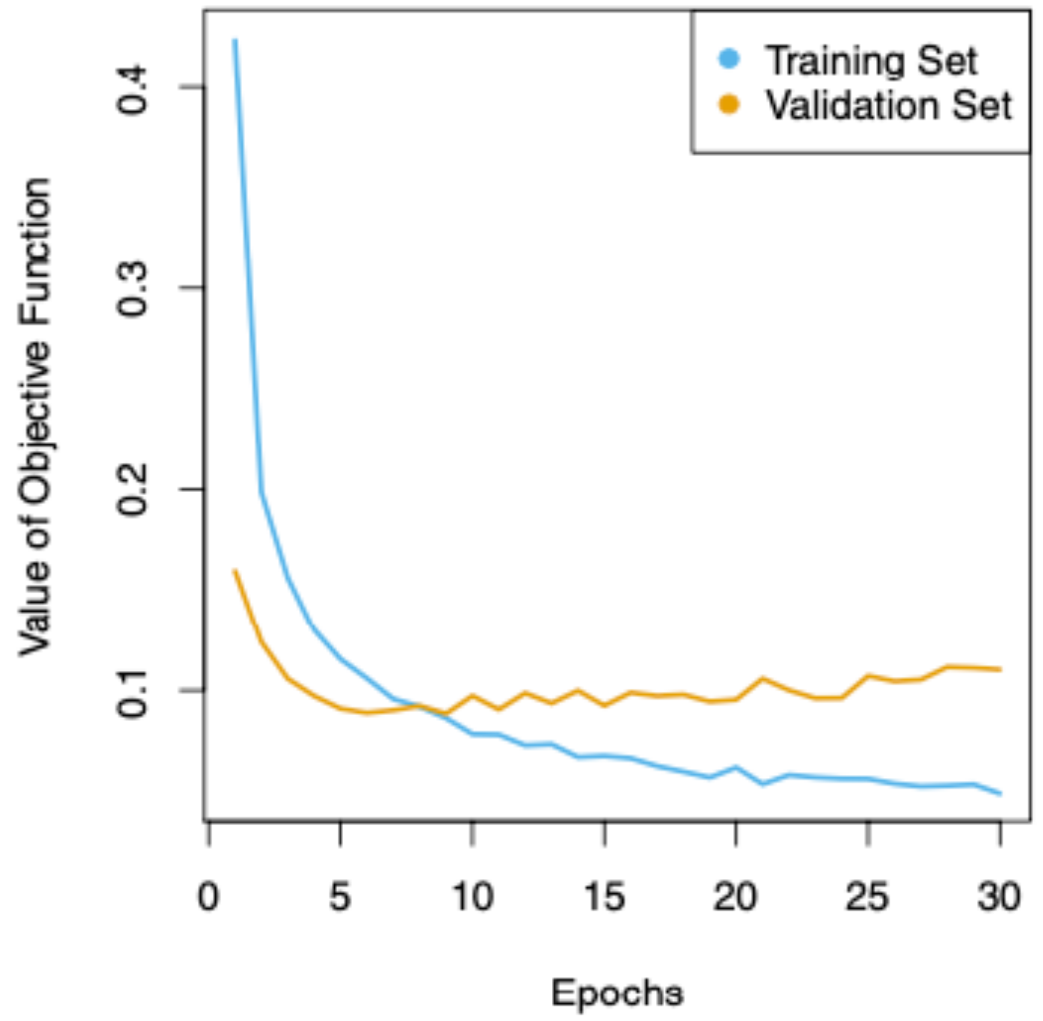

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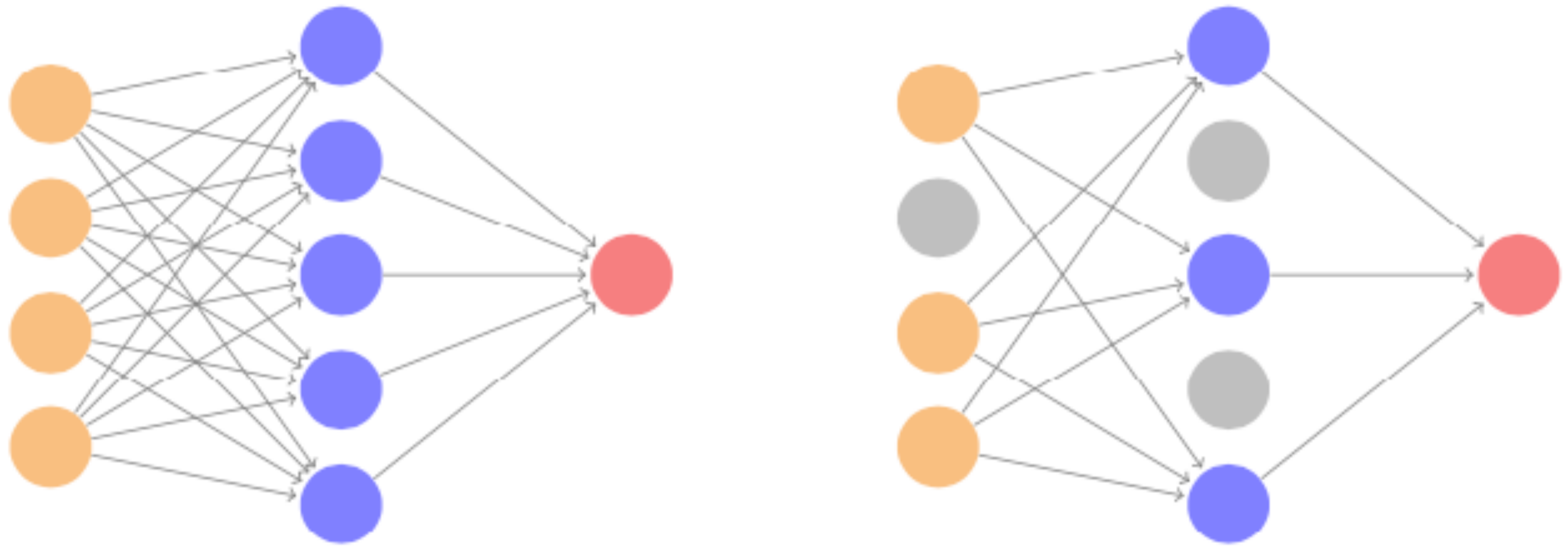
- Dropout: At each SGD iteration, remove a randomly selected set of nodes from the network (analogous to sub-sampling features for random forests).



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- Explicit and implicit regularization are used to control model complexity, the latter including early stopping and dropout.
- Neural networks come with a smorgasbord of tuning parameters, which often require considerable effort to tune.