Neural networks

STAT 4710

November 17, 2022

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

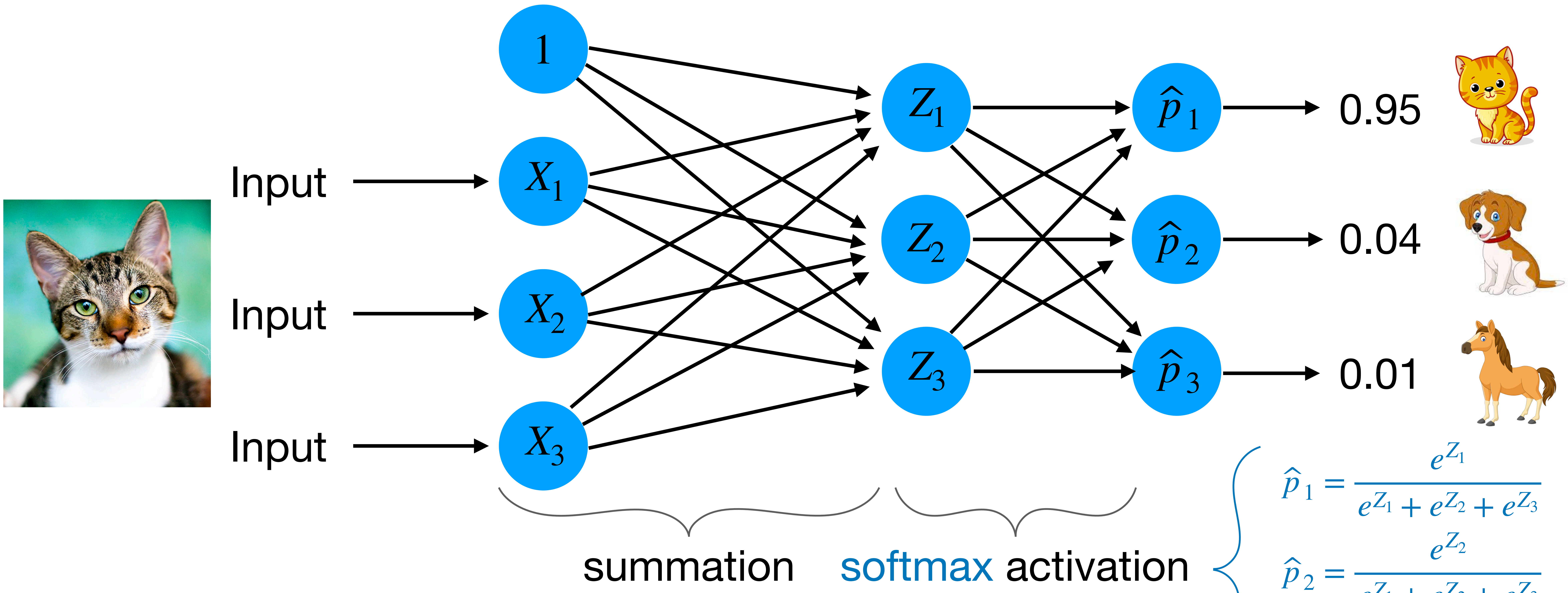
$\boxed{\textbf{Lecture 2: } \text{Neural networks}}$

Lecture 3: Deep learning for images

Lecture 4: Deep learning for text

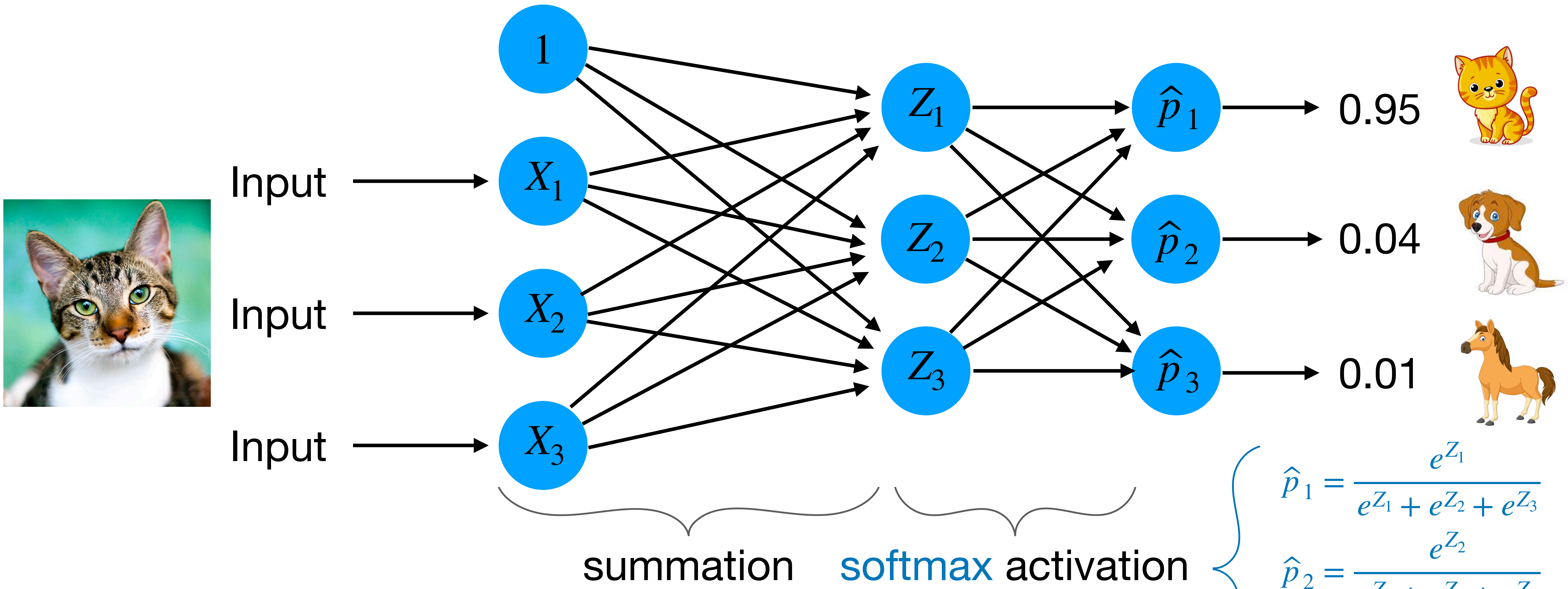
Lecture 5: Unit review and quiz in class

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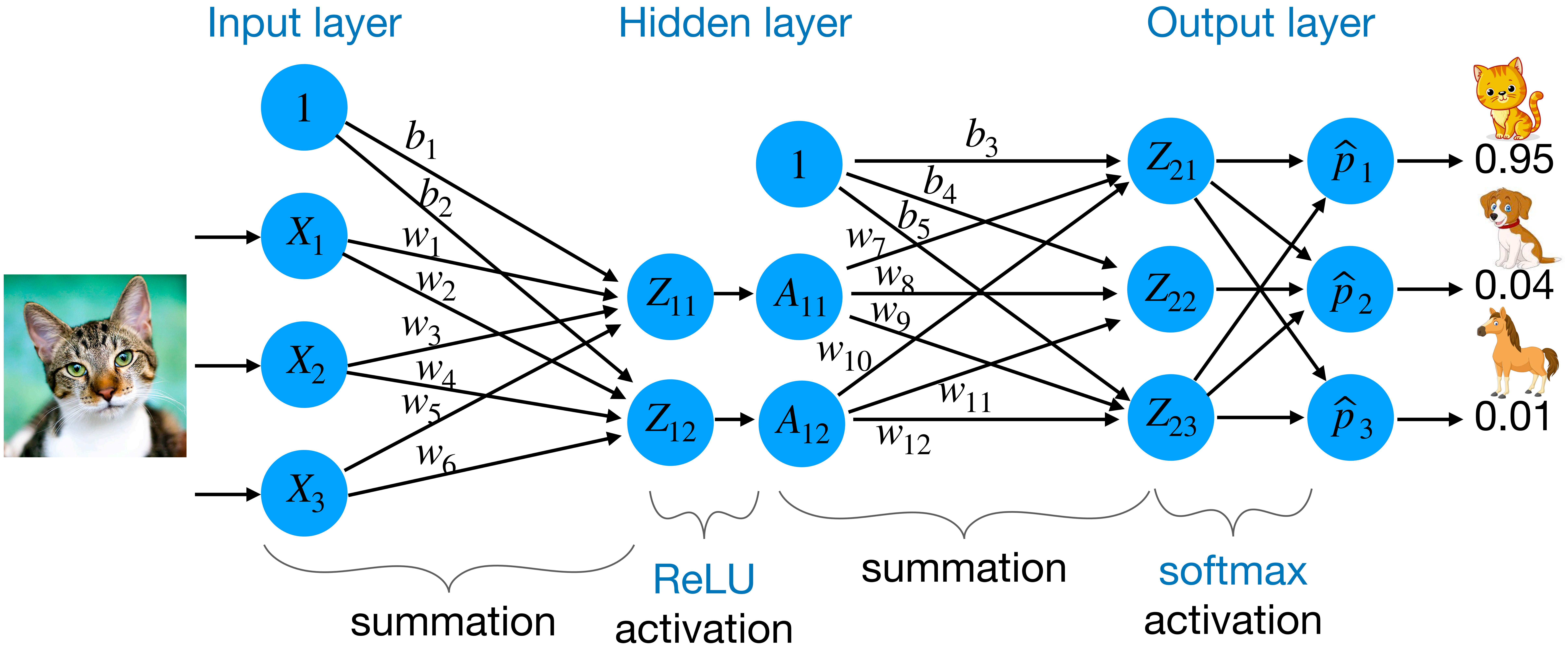
This simple architecture directly uses raw pixel features.
Intuitively, a good classifier would pick up on cat's eyes, ears, etc.

One-hidden-layer neural network



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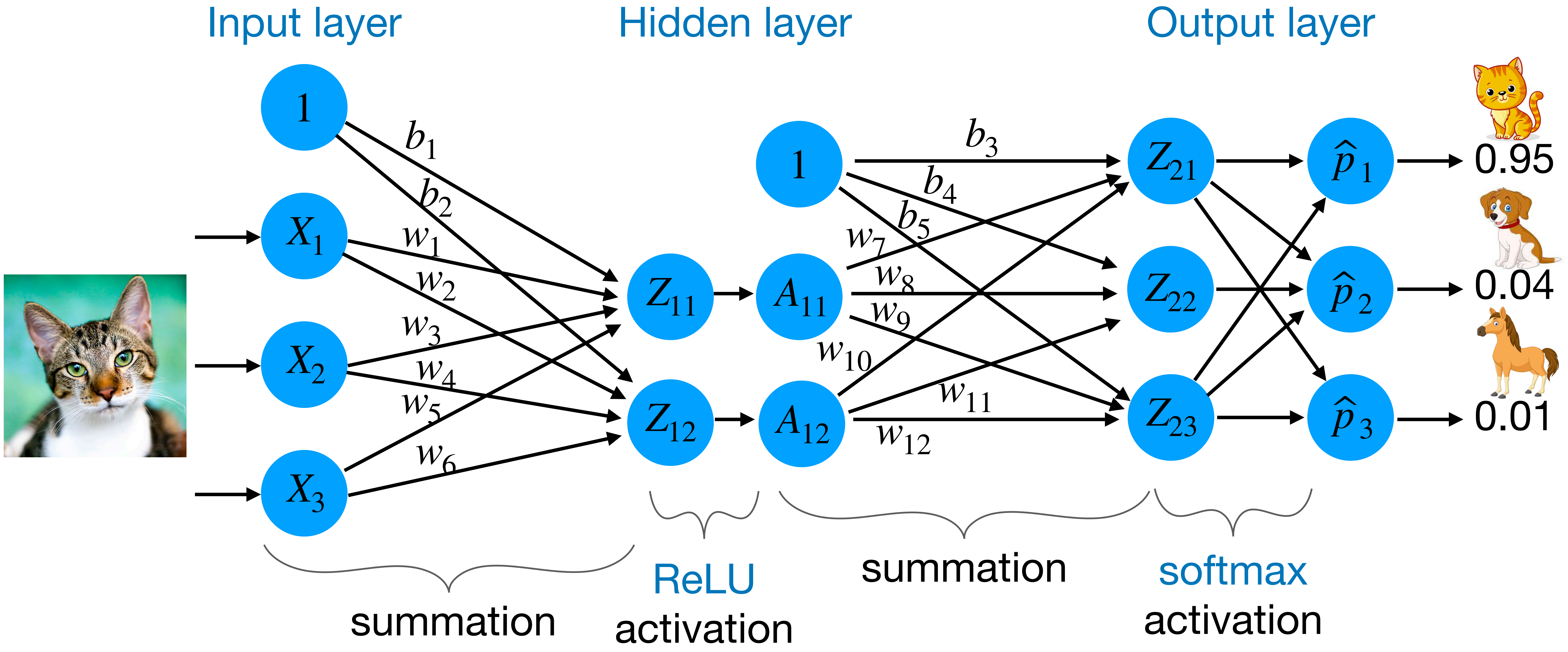

E.g., $Z_{12} = b_2 + w_2X_1 + w_4X_2 + w_6X_3$

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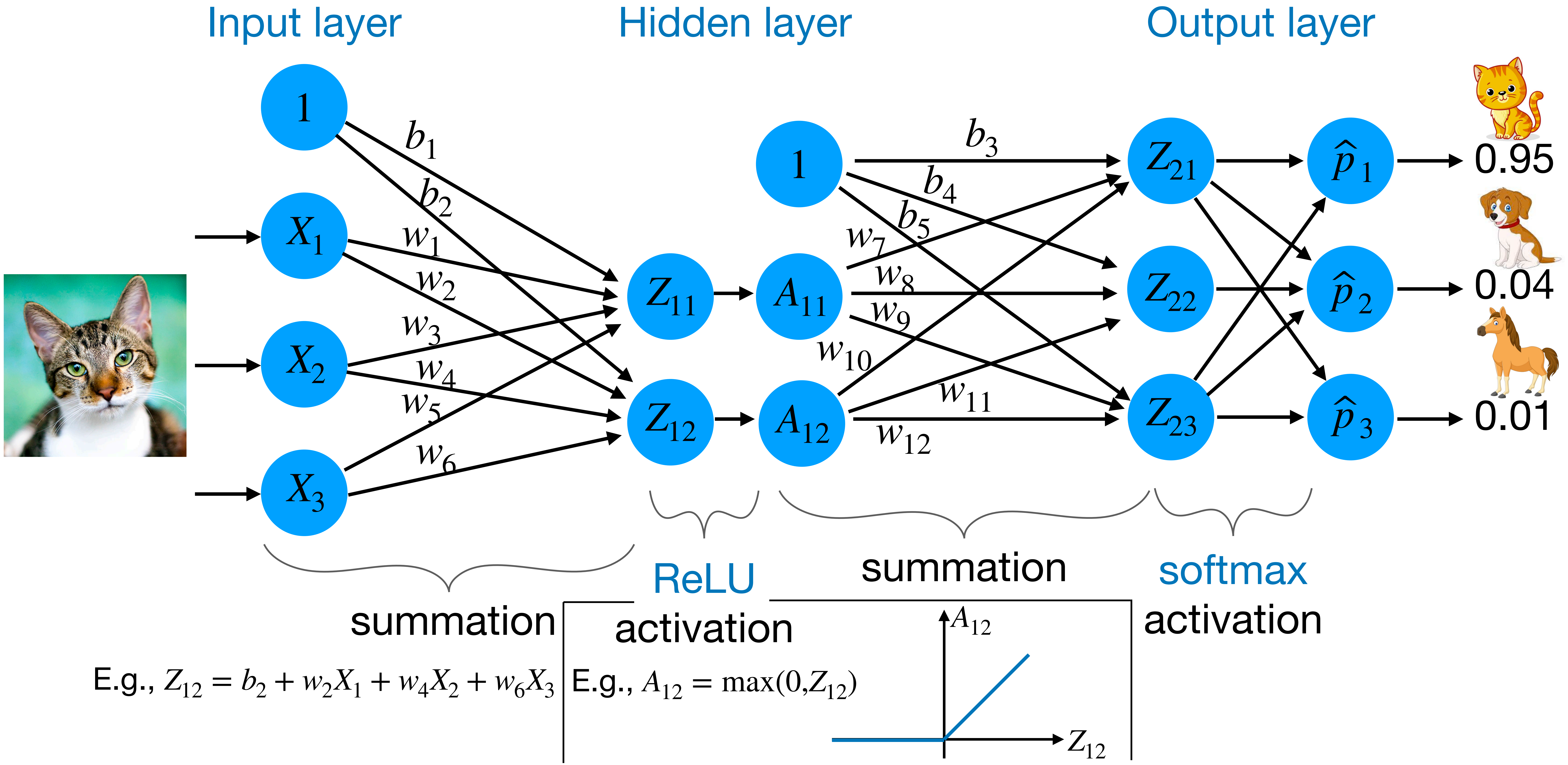

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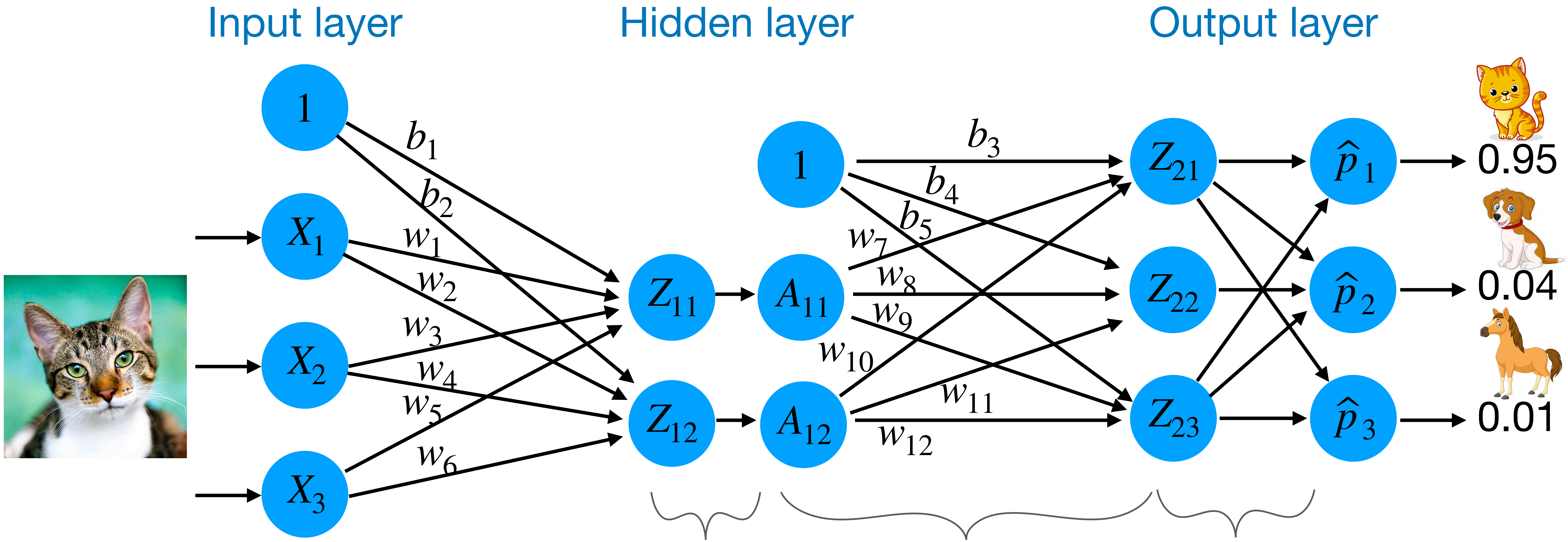
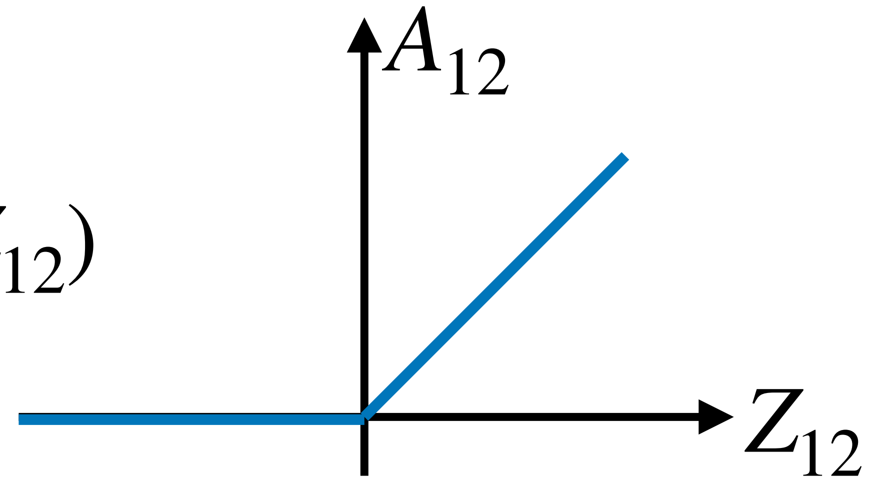


summation

E.g., $Z_{12} = b_2 + w_2 X_1 + w_4 X_2 + w_6 X_3$

ReLU activation

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



summation

softmax activation

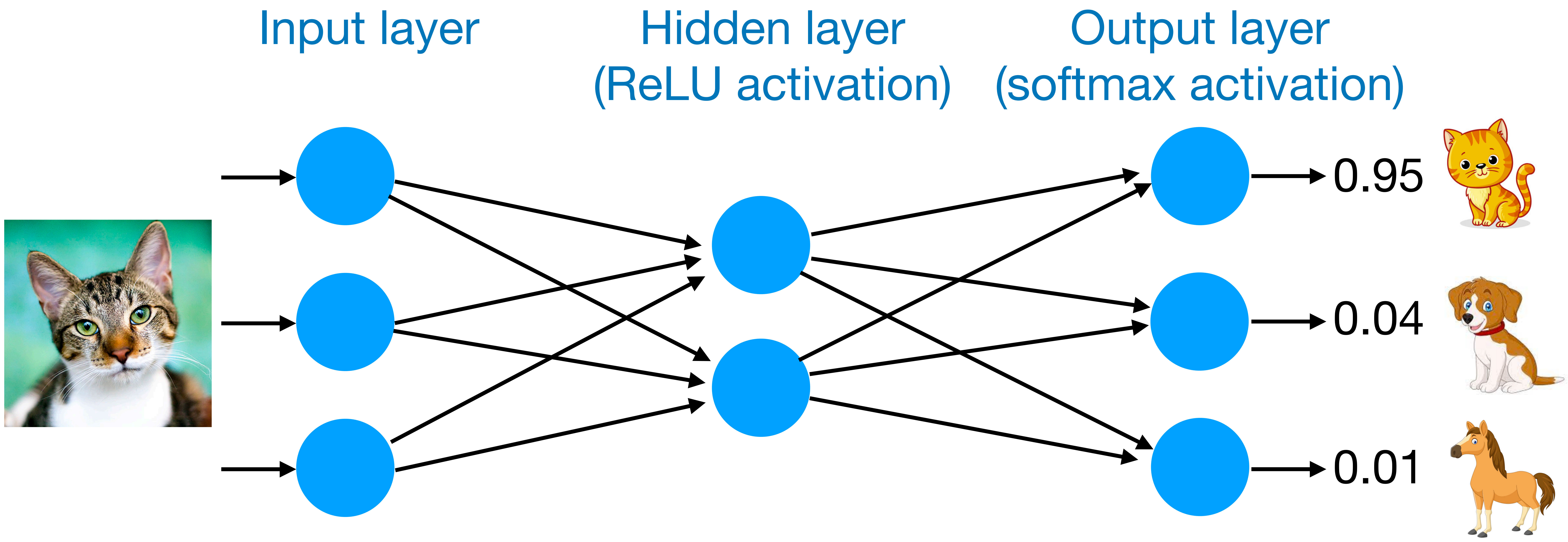
Terminology:

b_j: biases

w_j: weights

One-hidden-layer neural network

Concise representation



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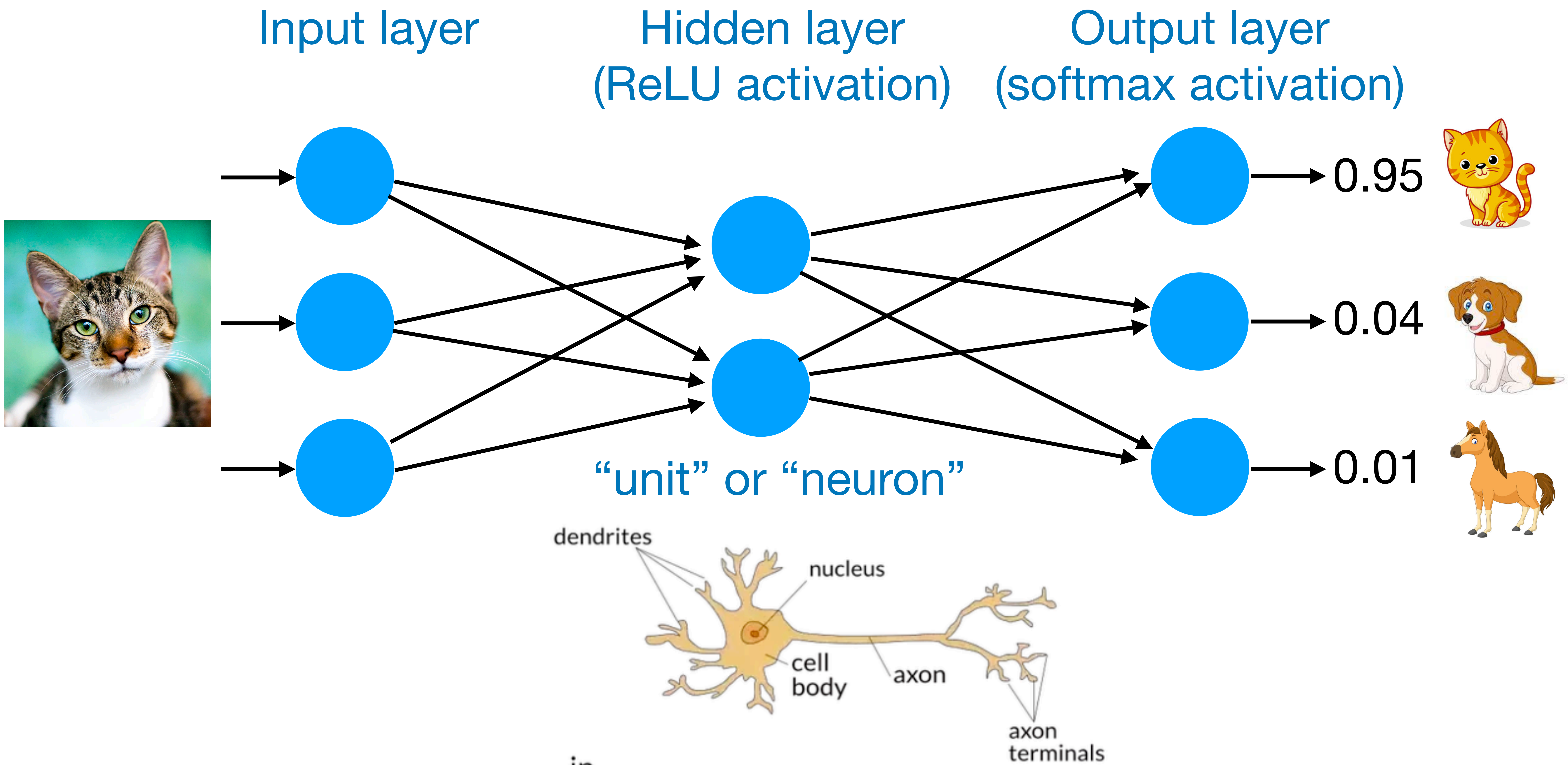

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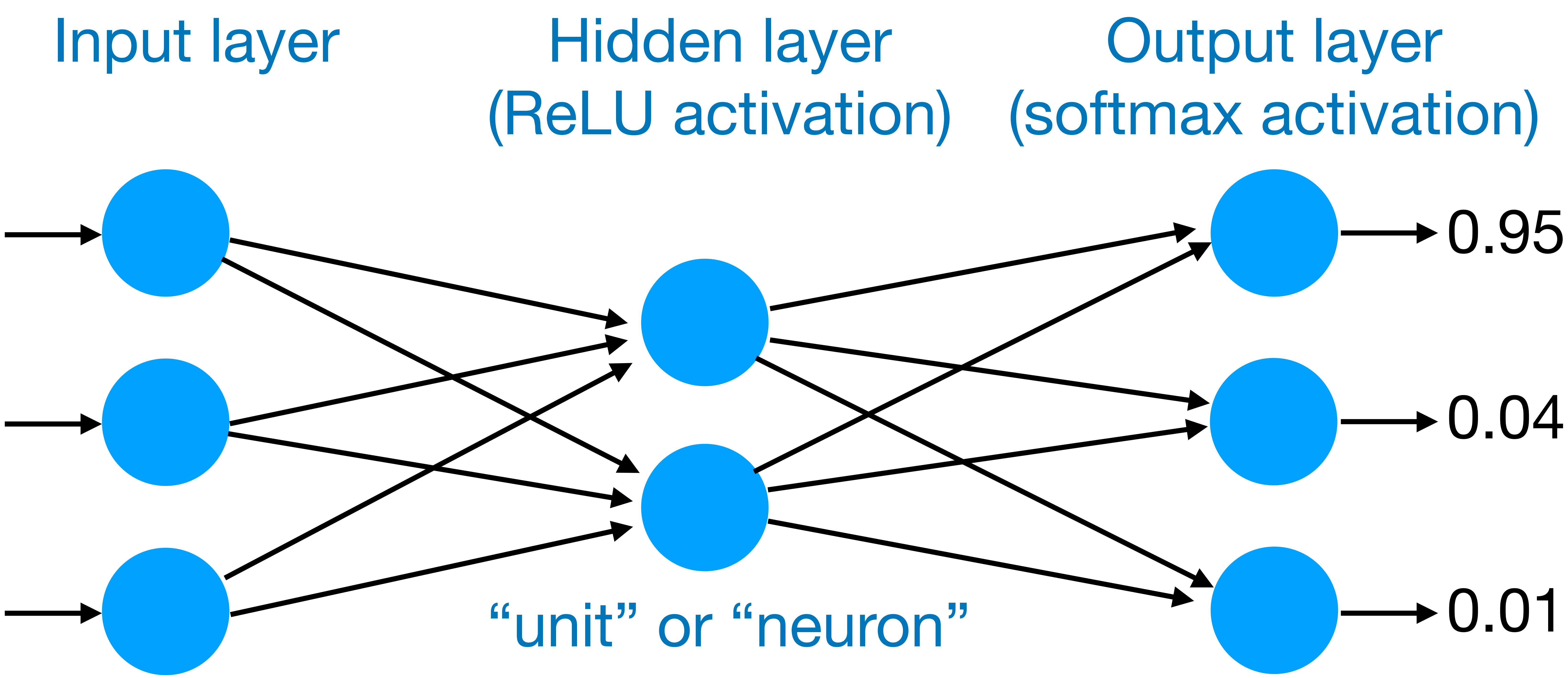
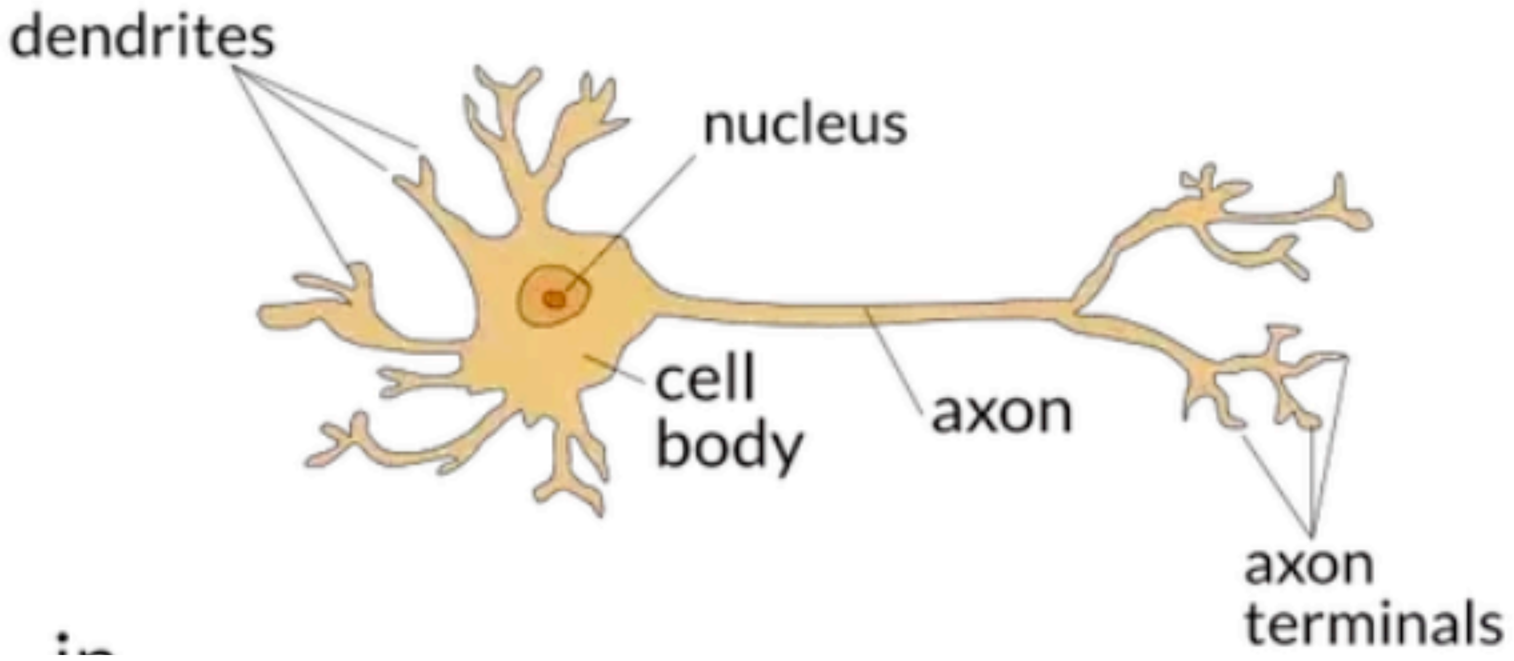


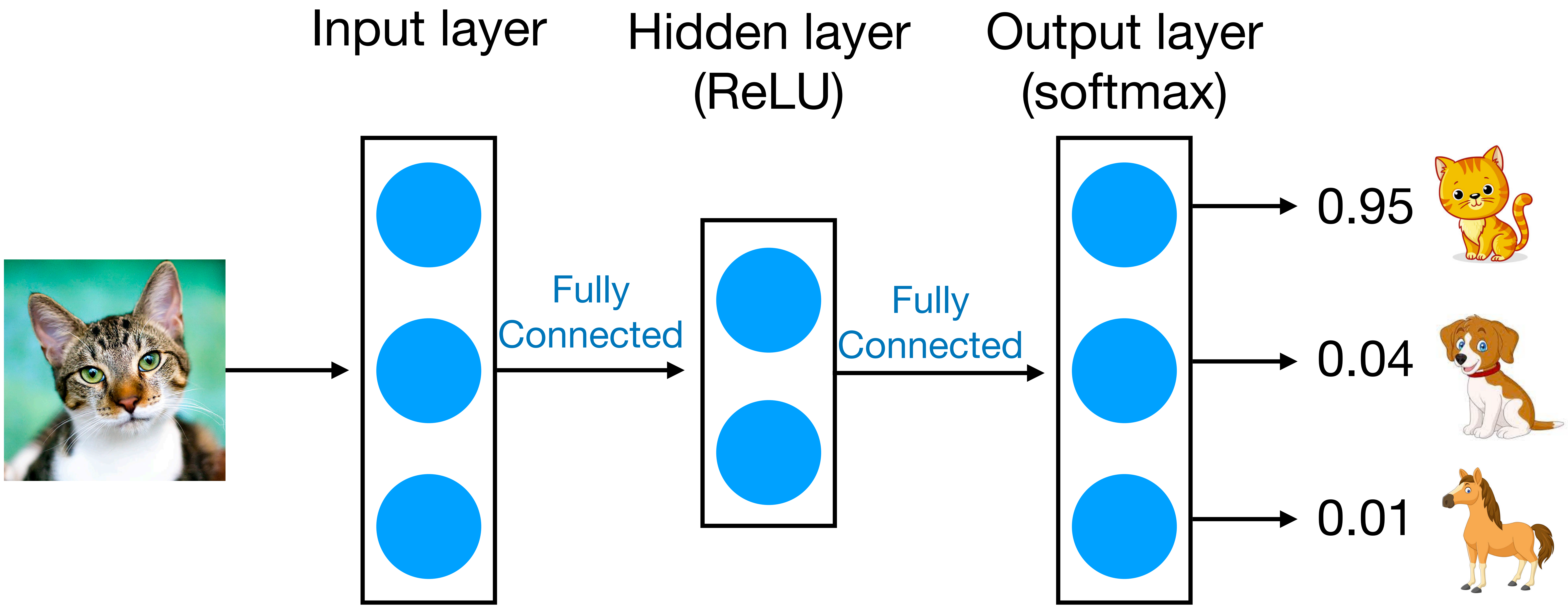


Notes:

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

One-hidden-layer neural network

Even more concise representation



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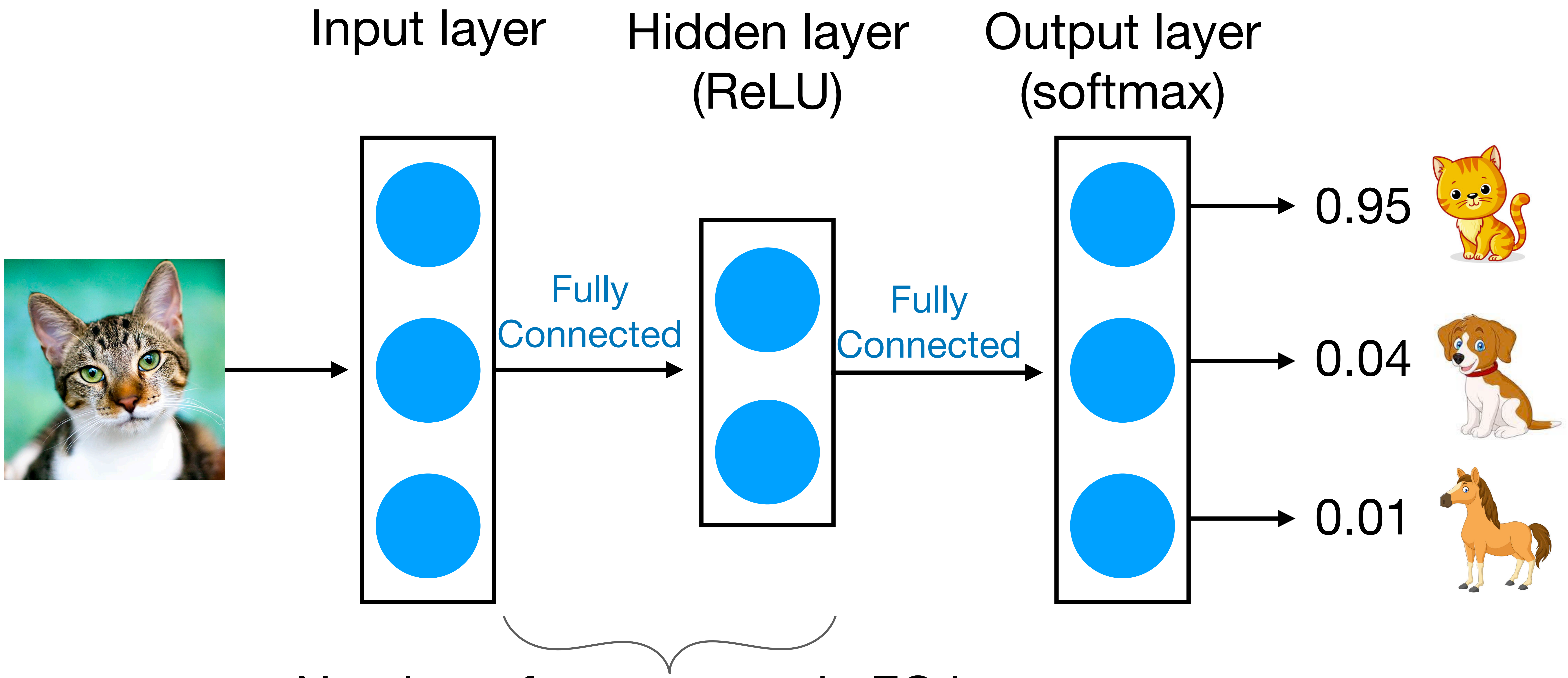
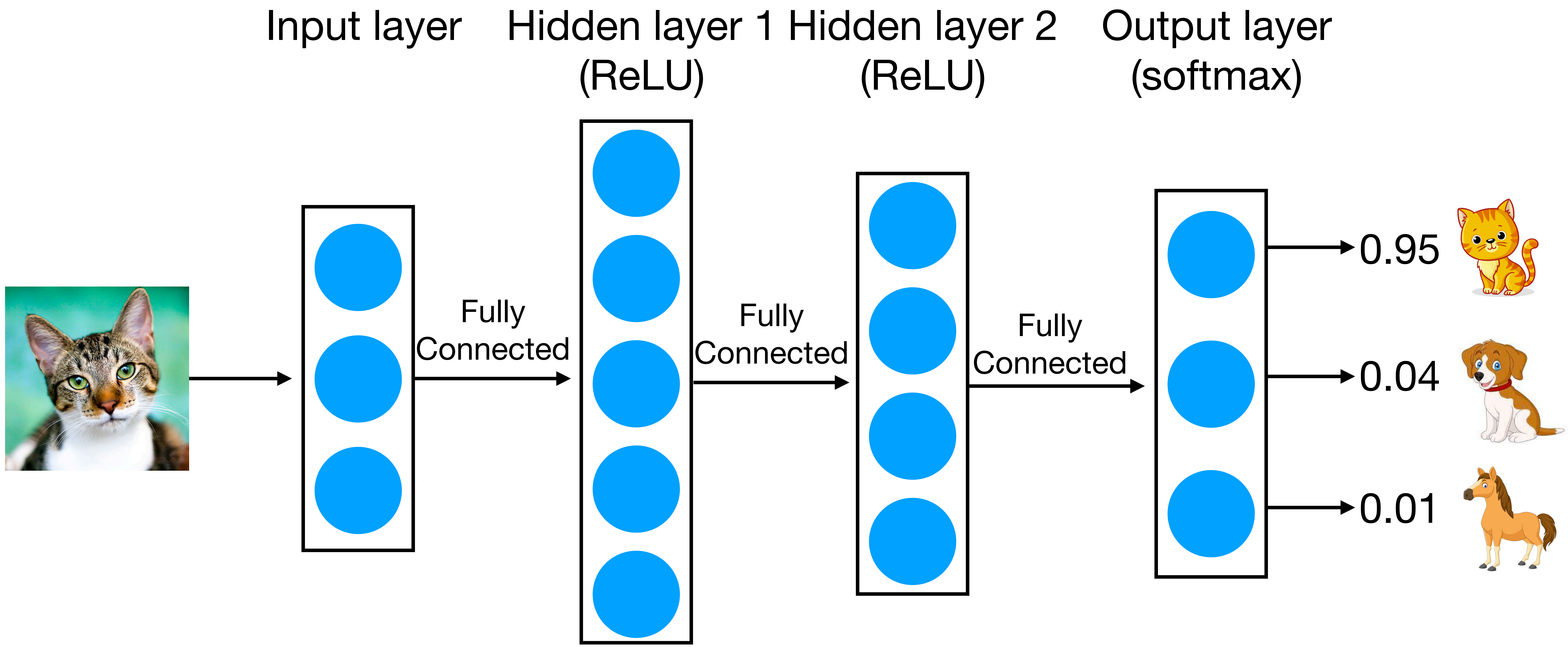


Number of parameters in FC layer =

(# units in previous layer + 1) $\times$ (# units in this layer)

Multi-layer fully connected neural networks



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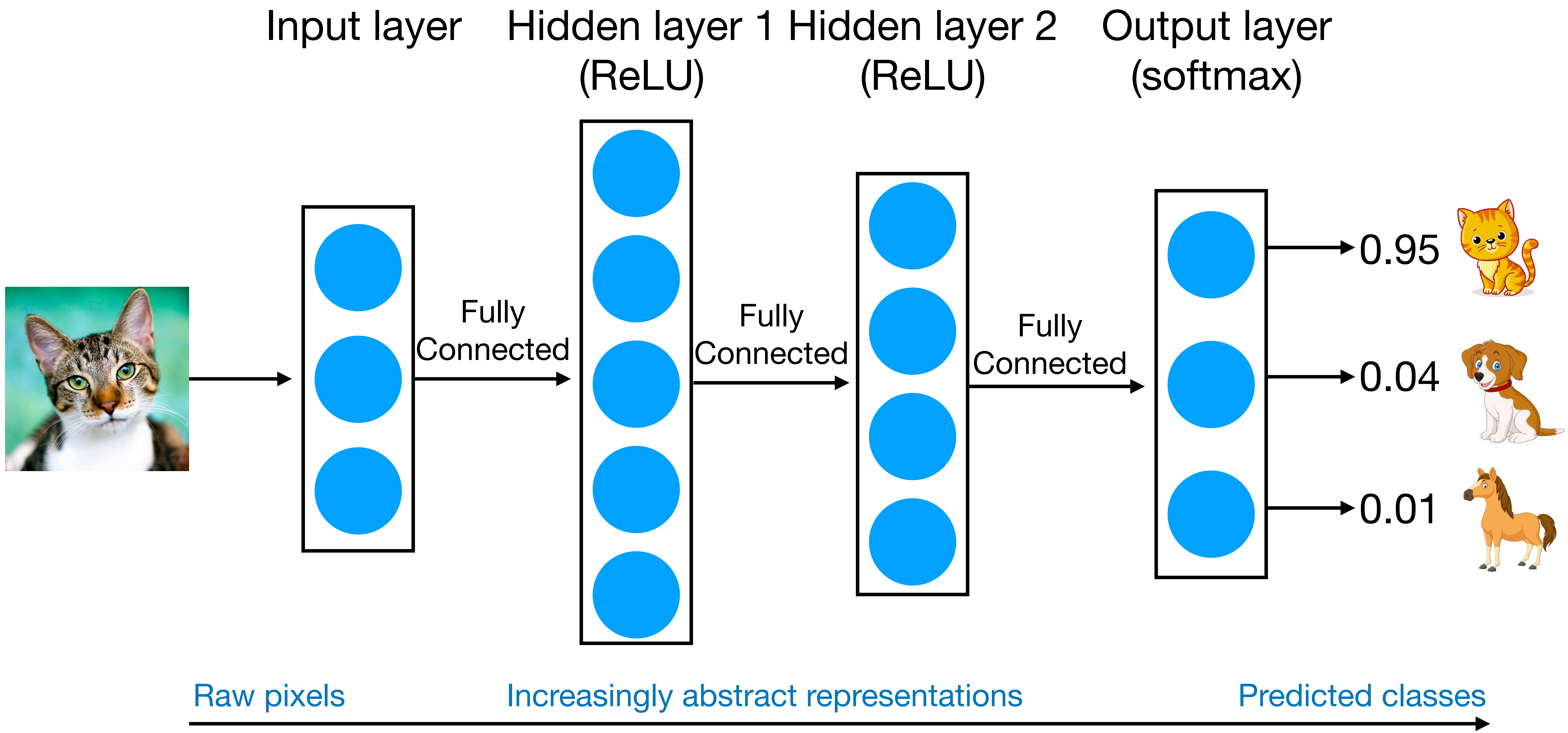

Training deep learning models

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

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

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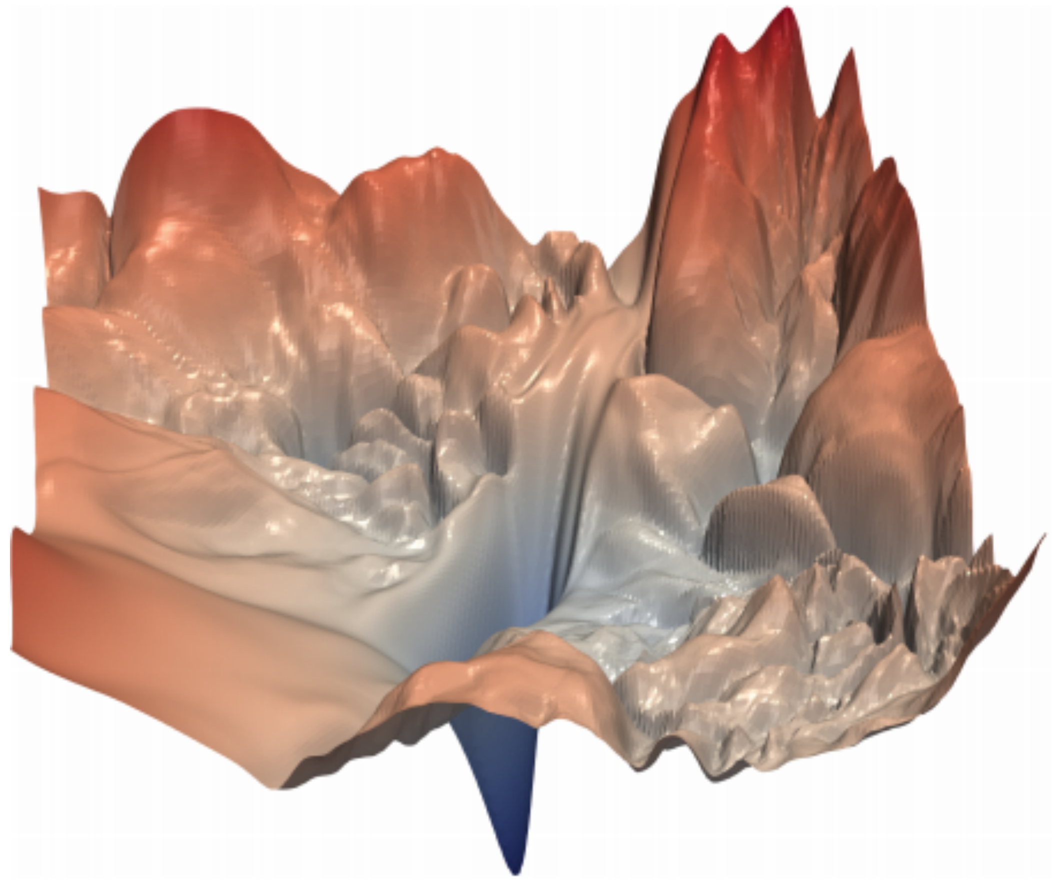

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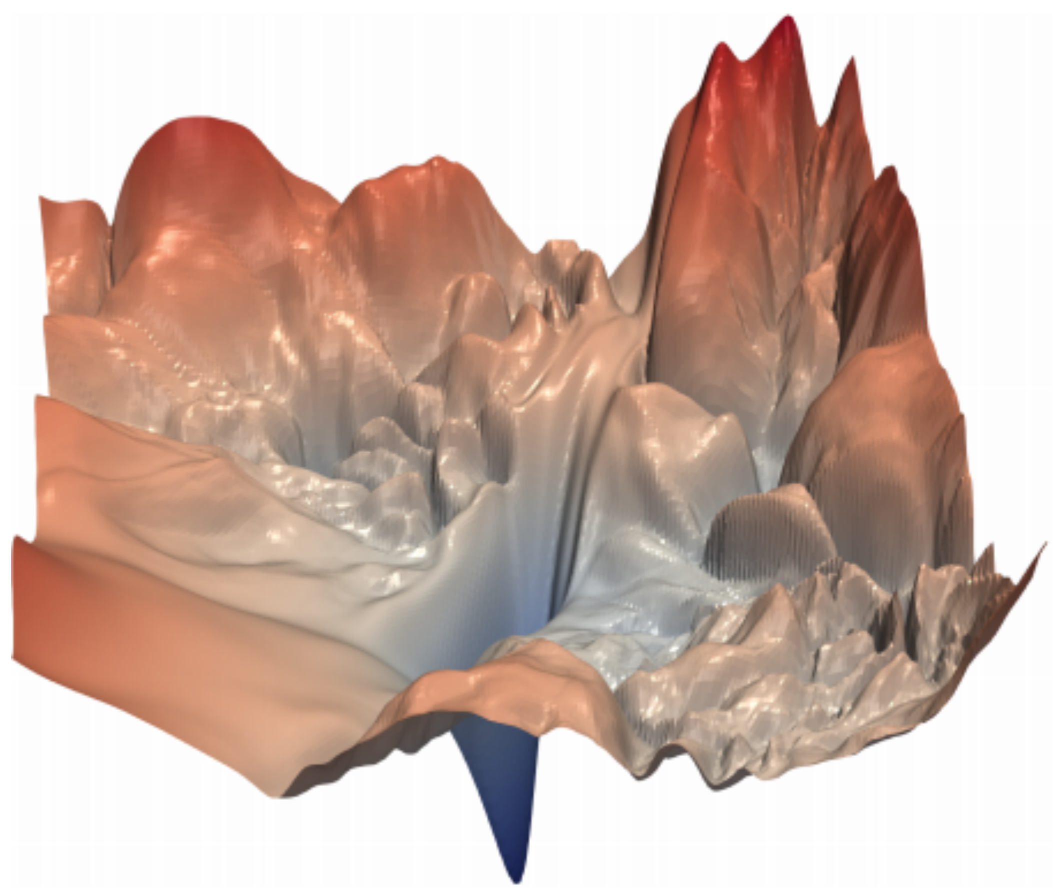

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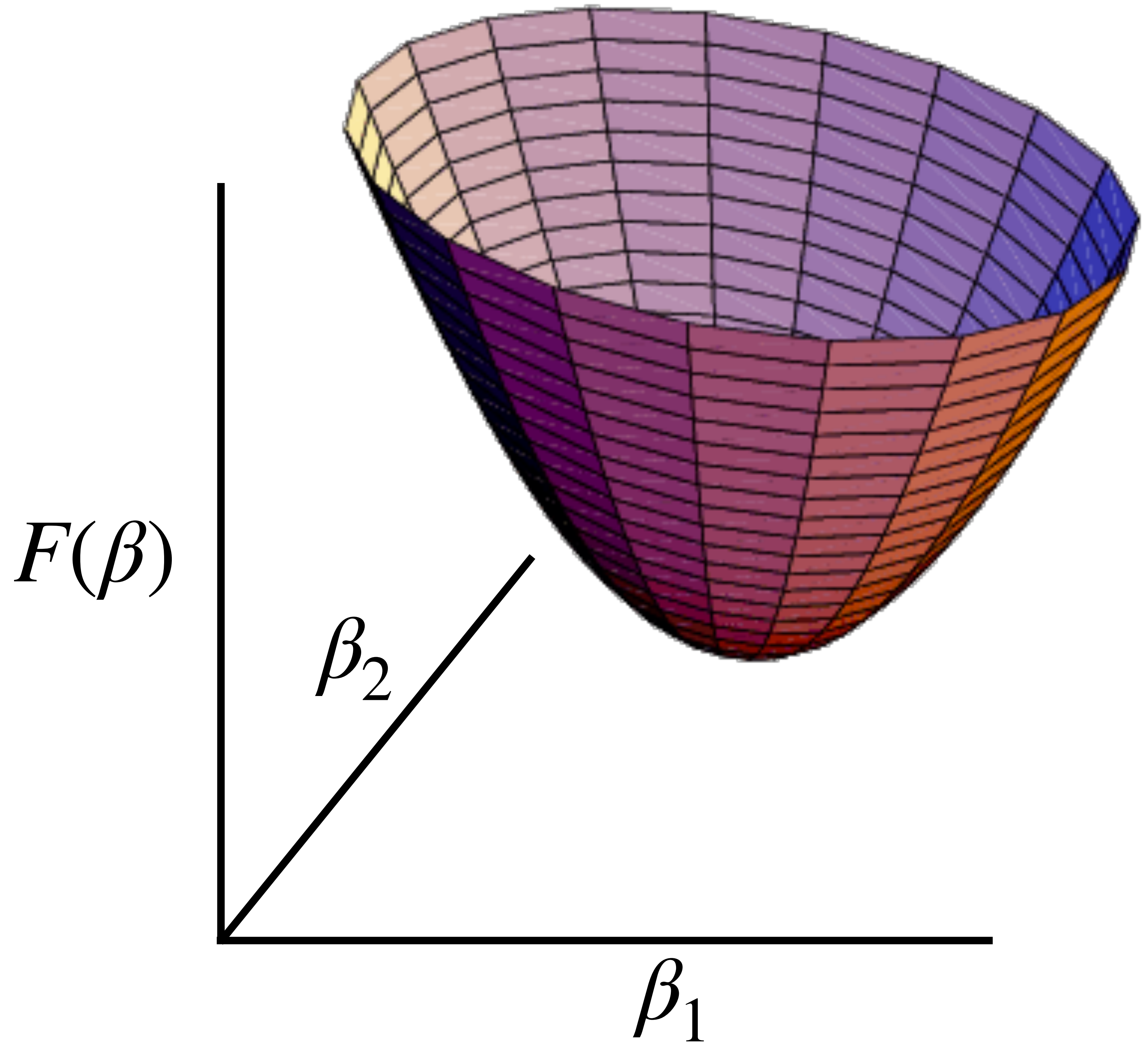

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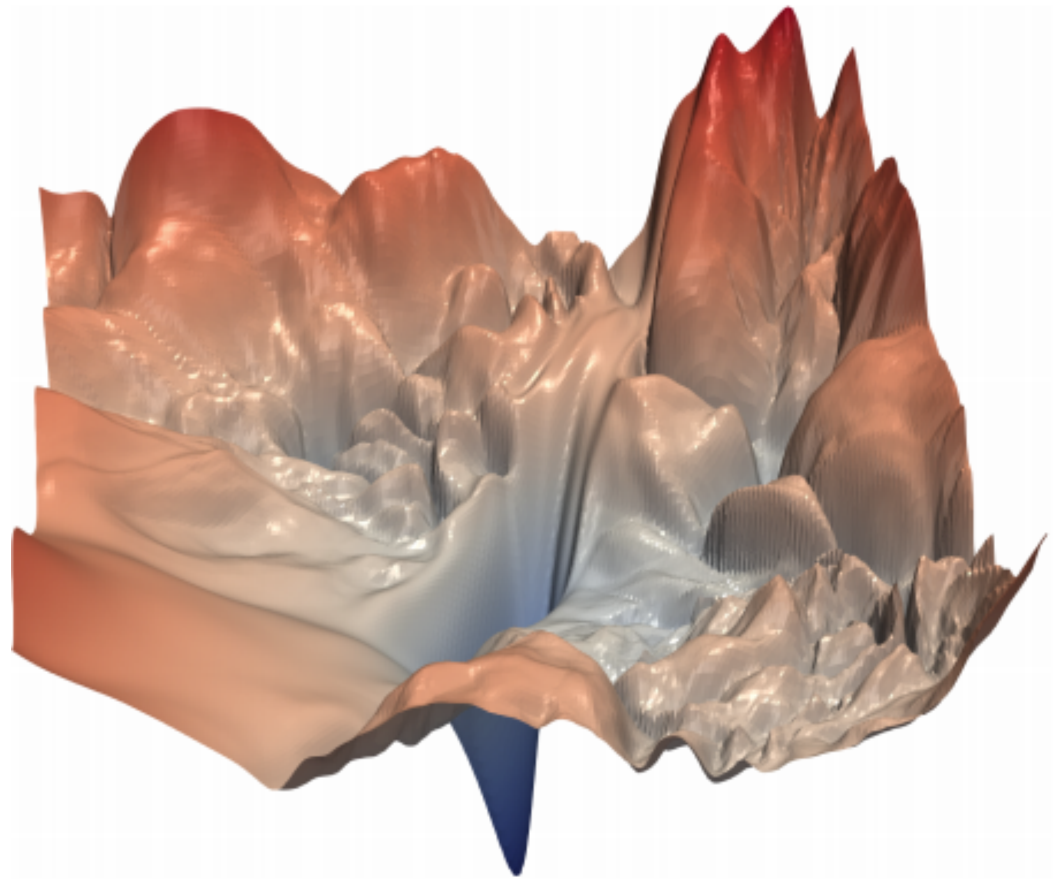

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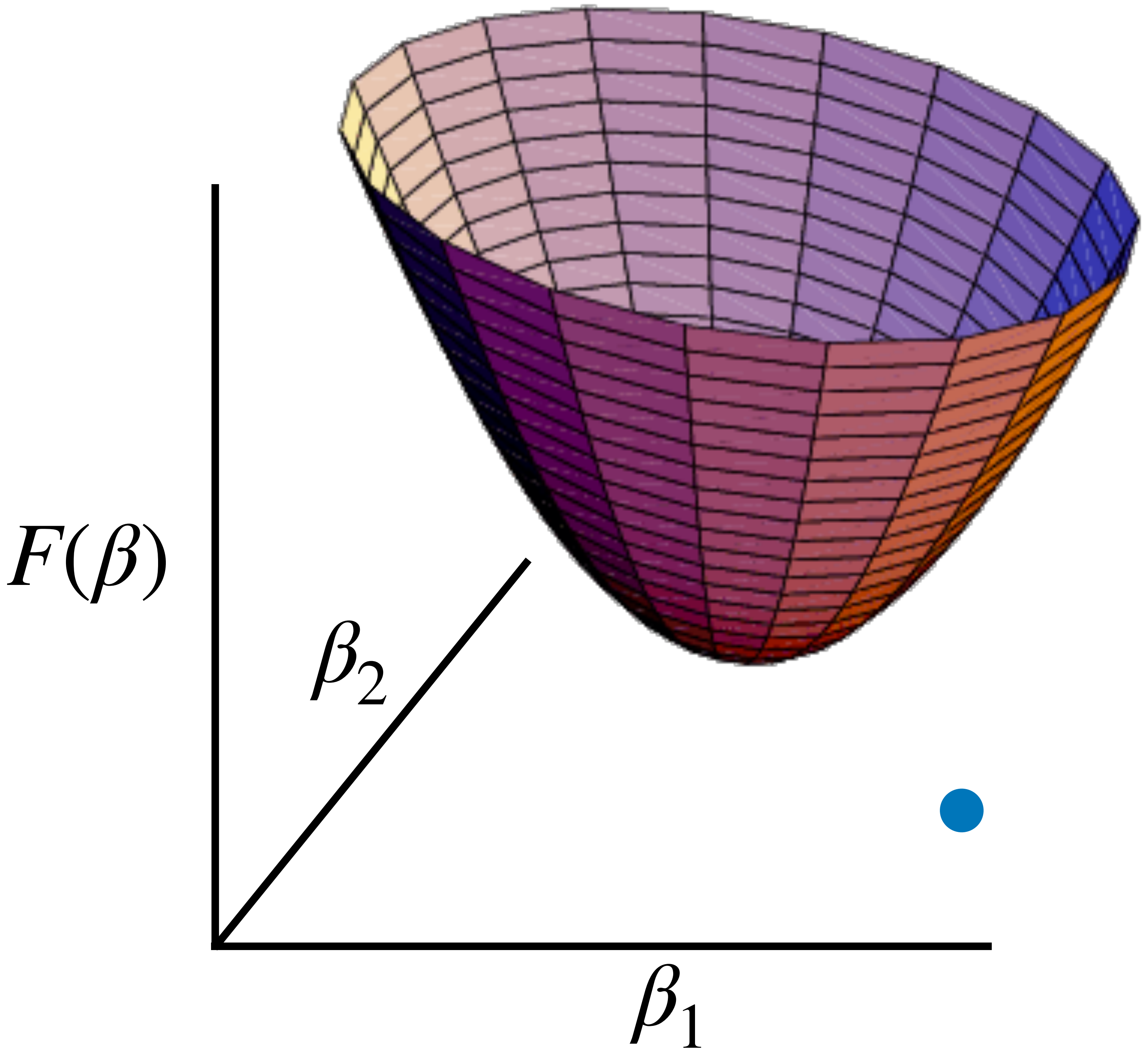

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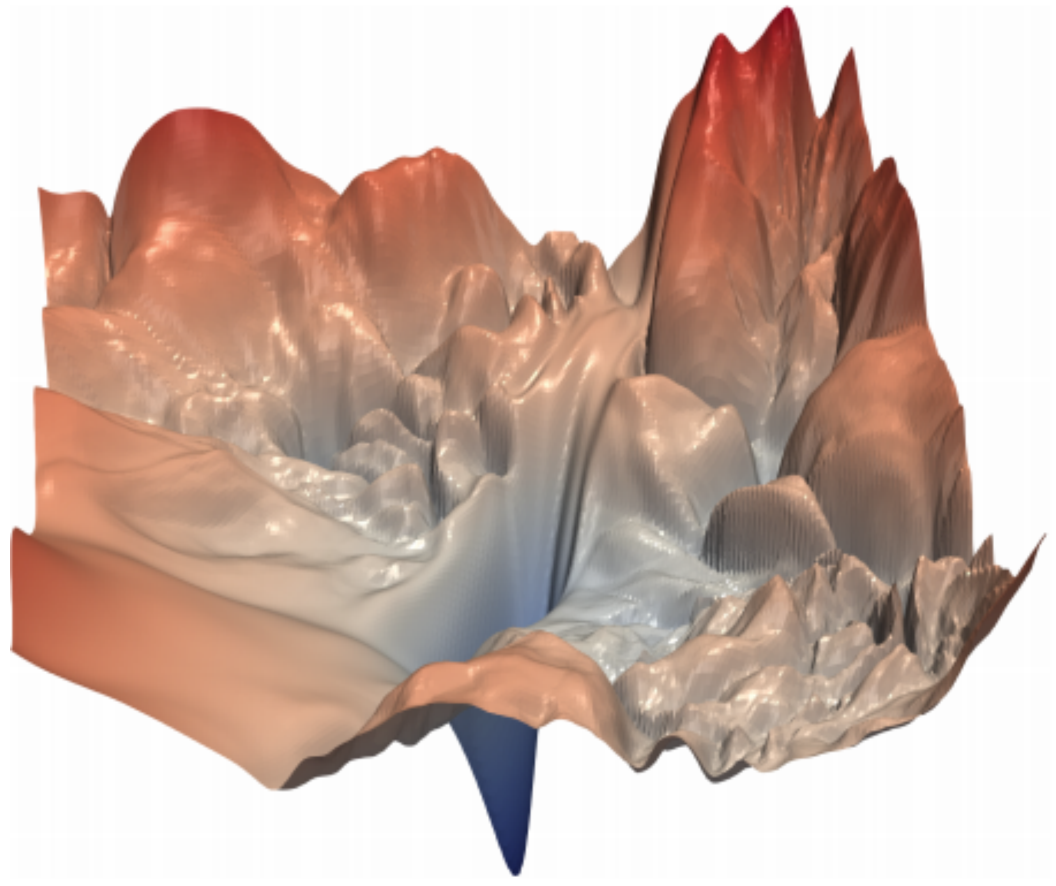

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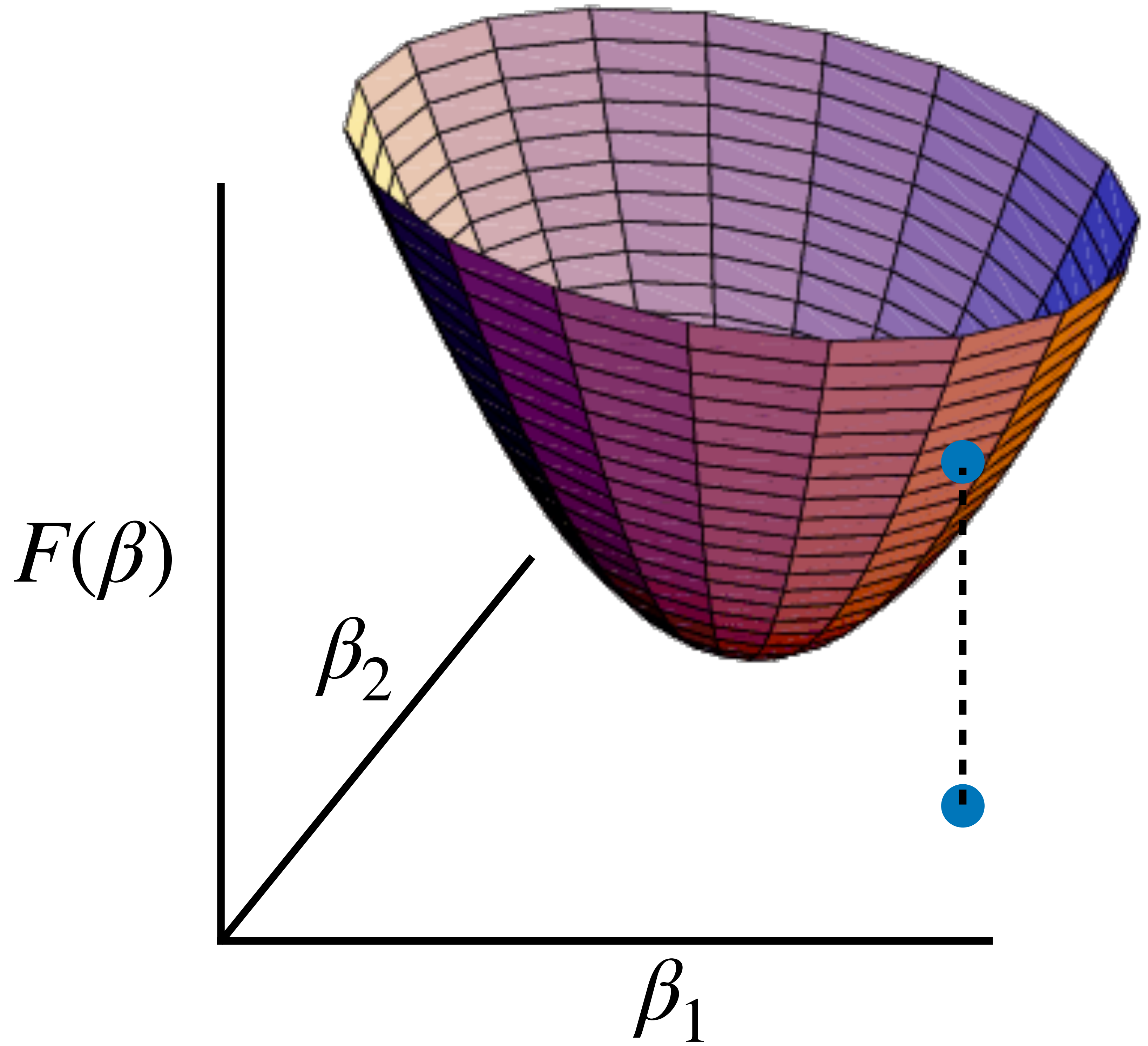

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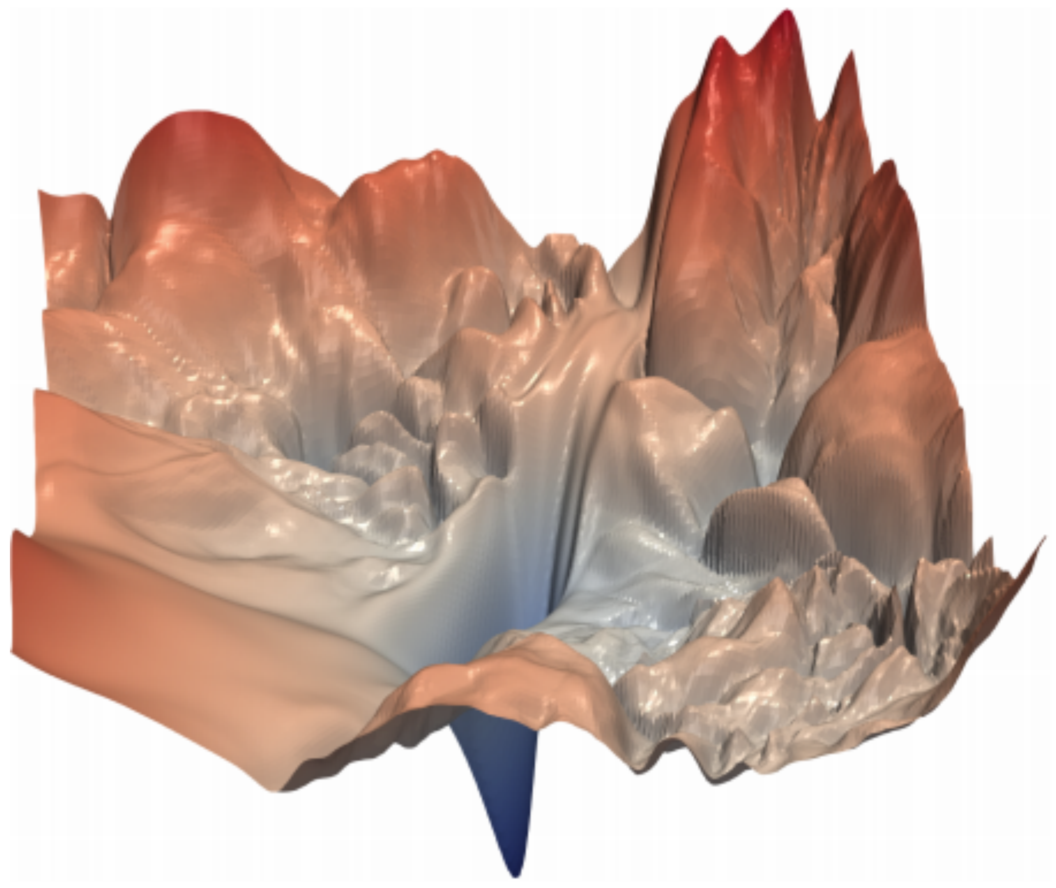

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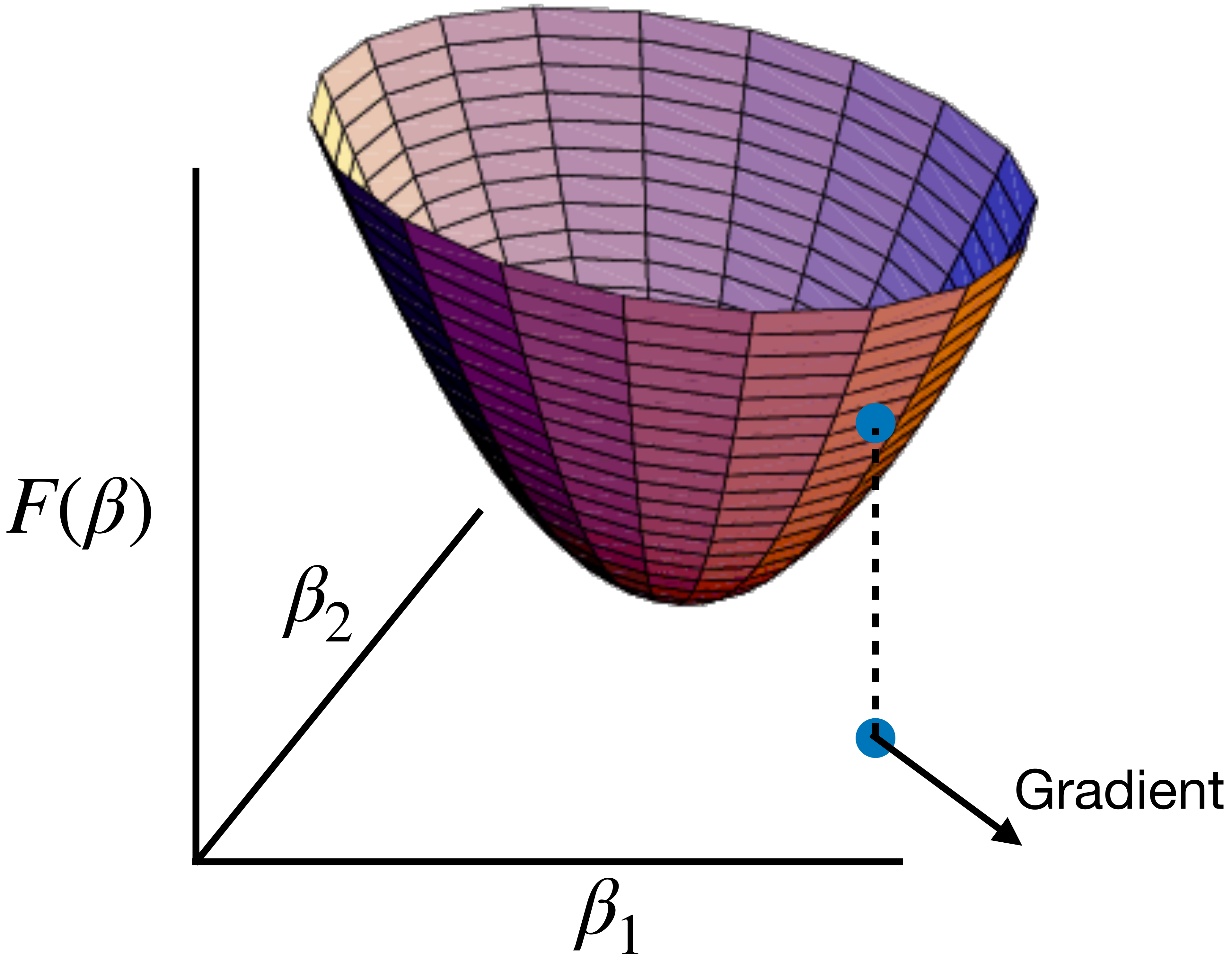

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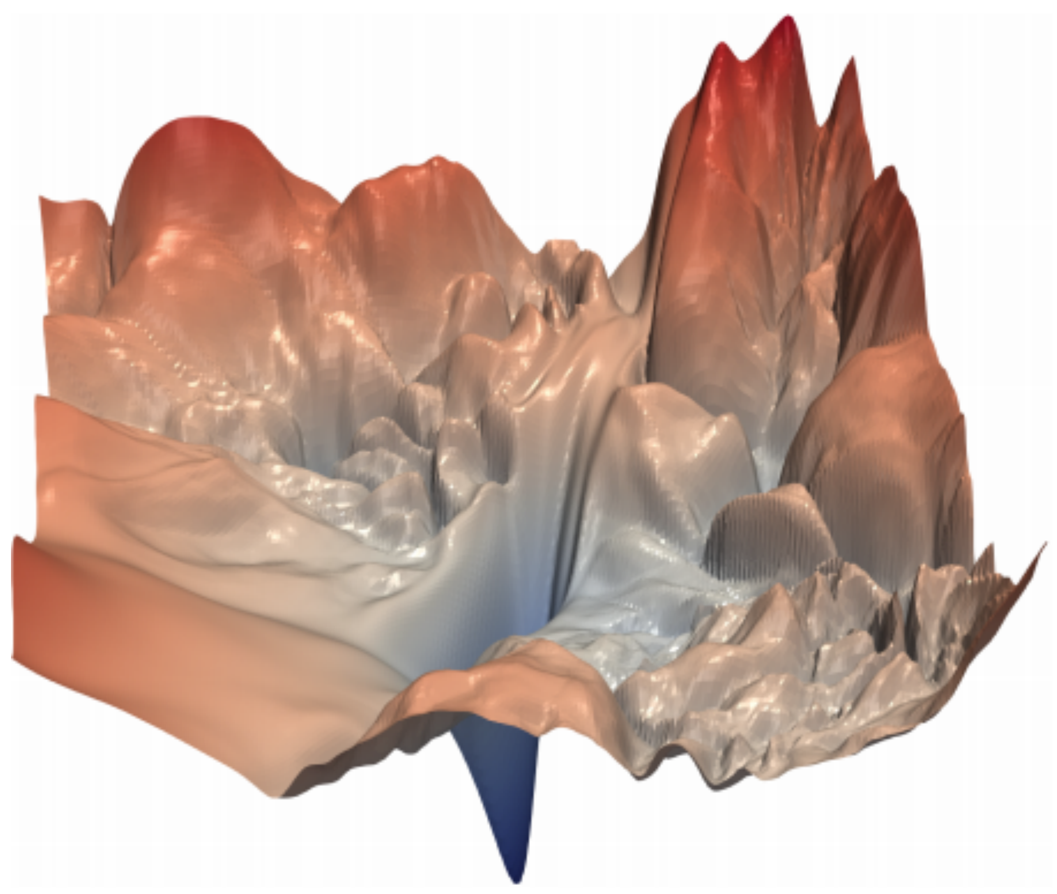

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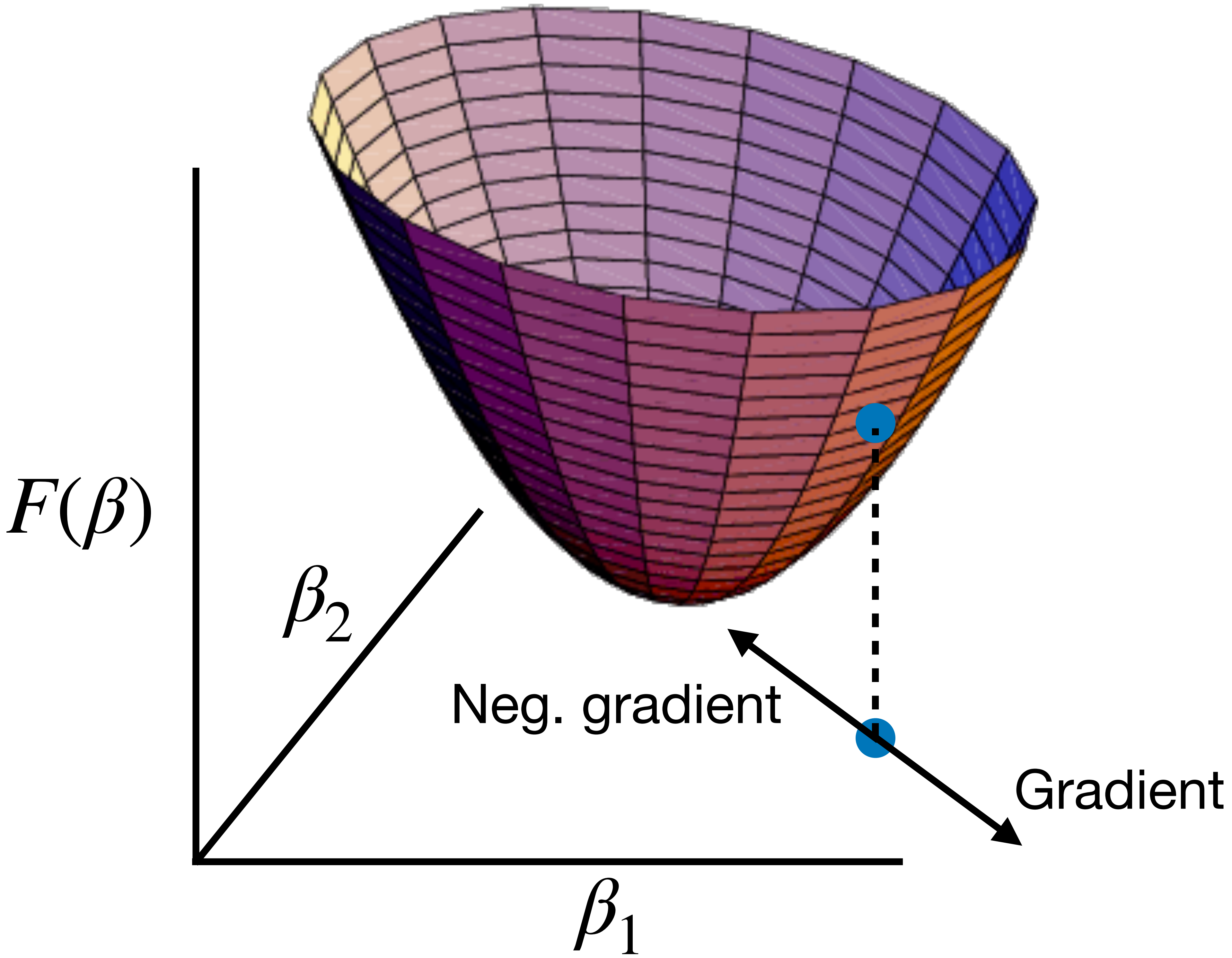

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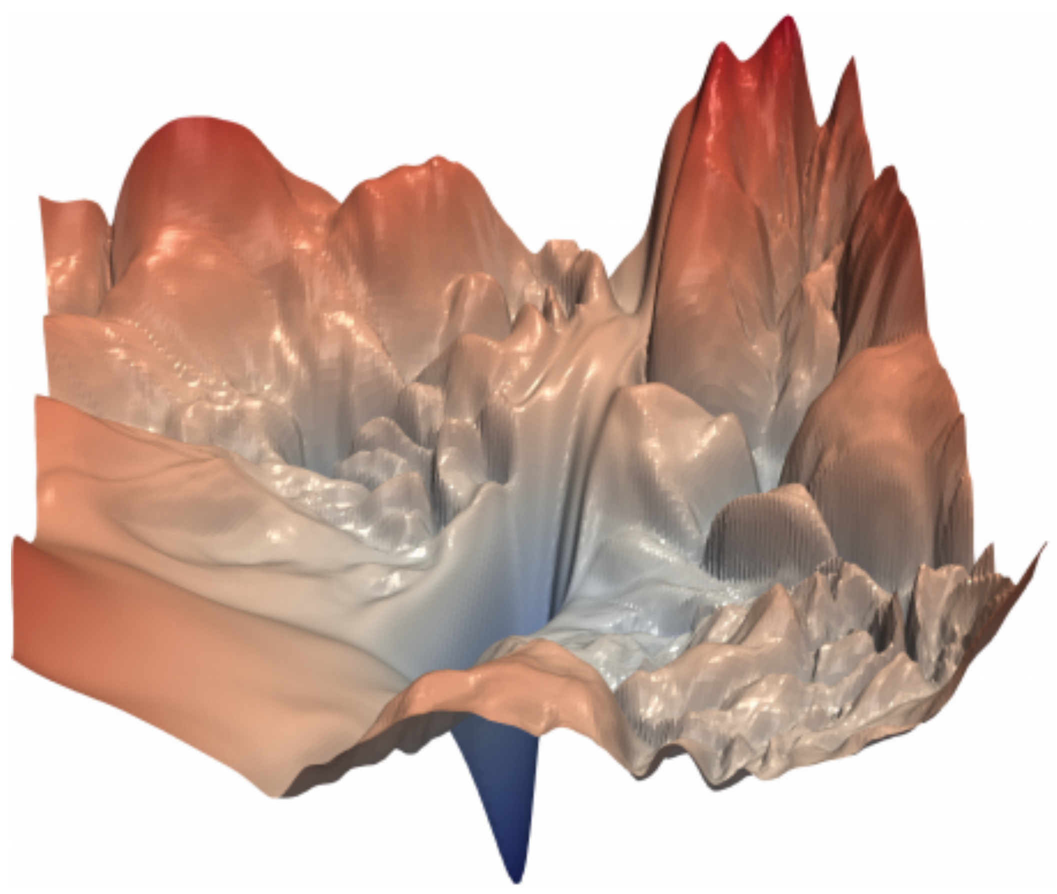

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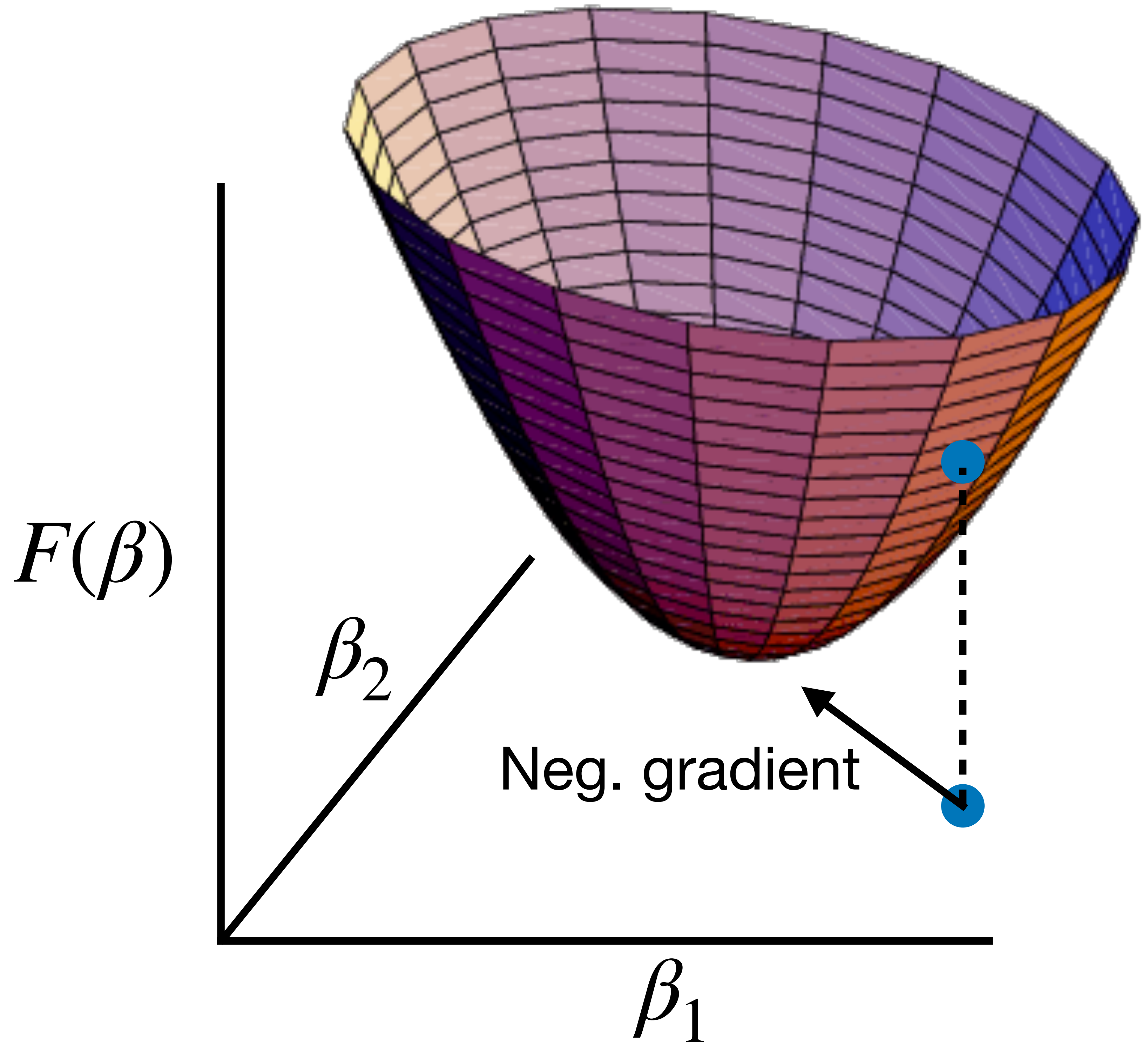

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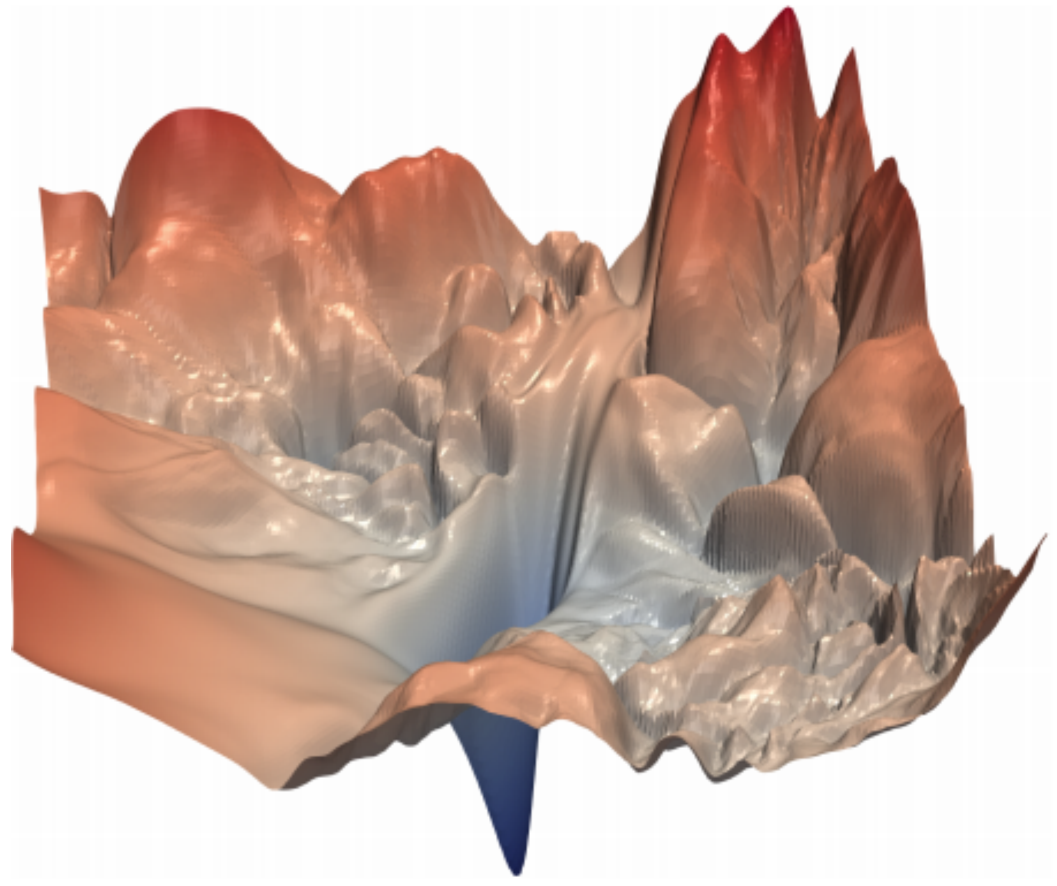

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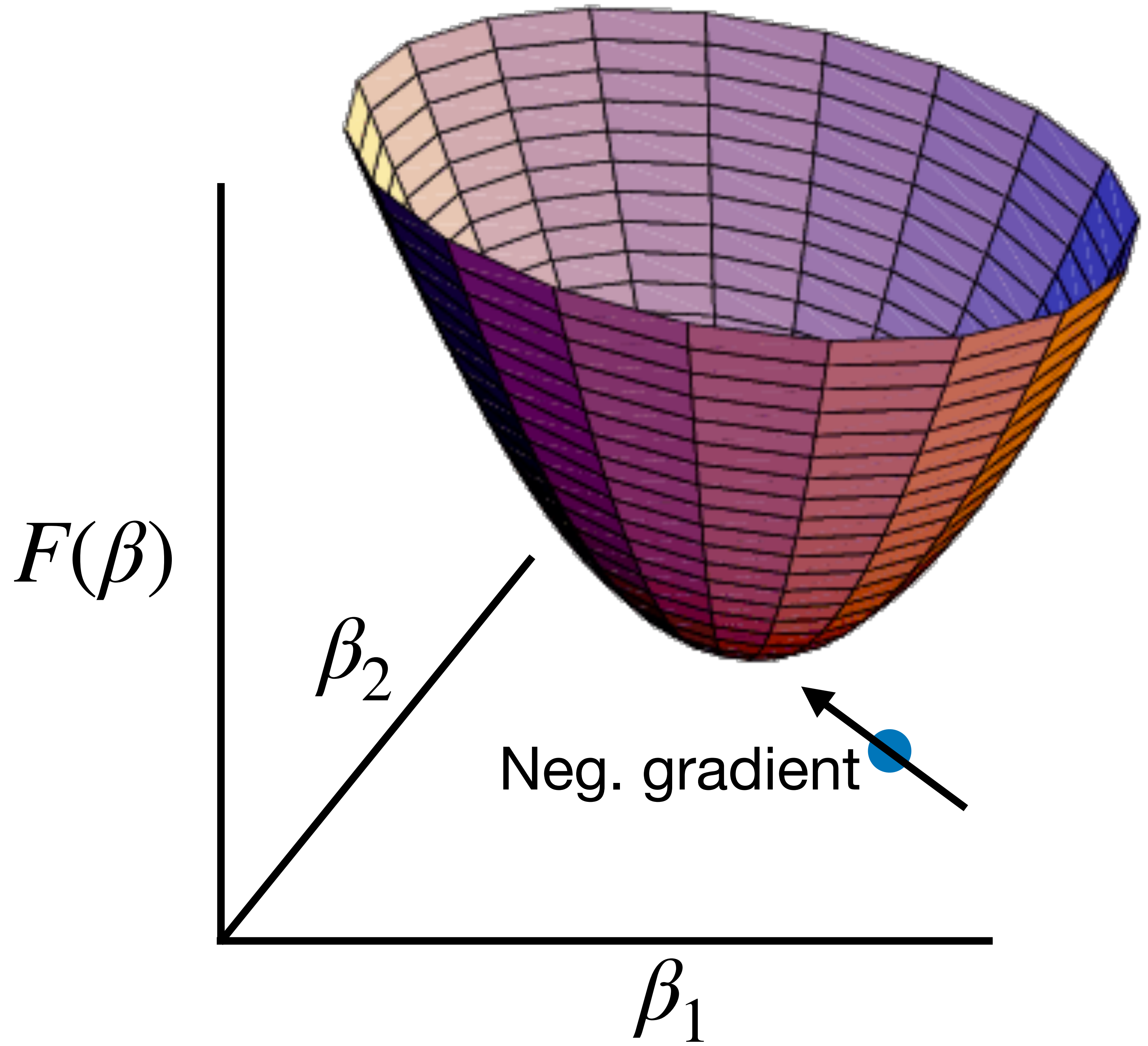

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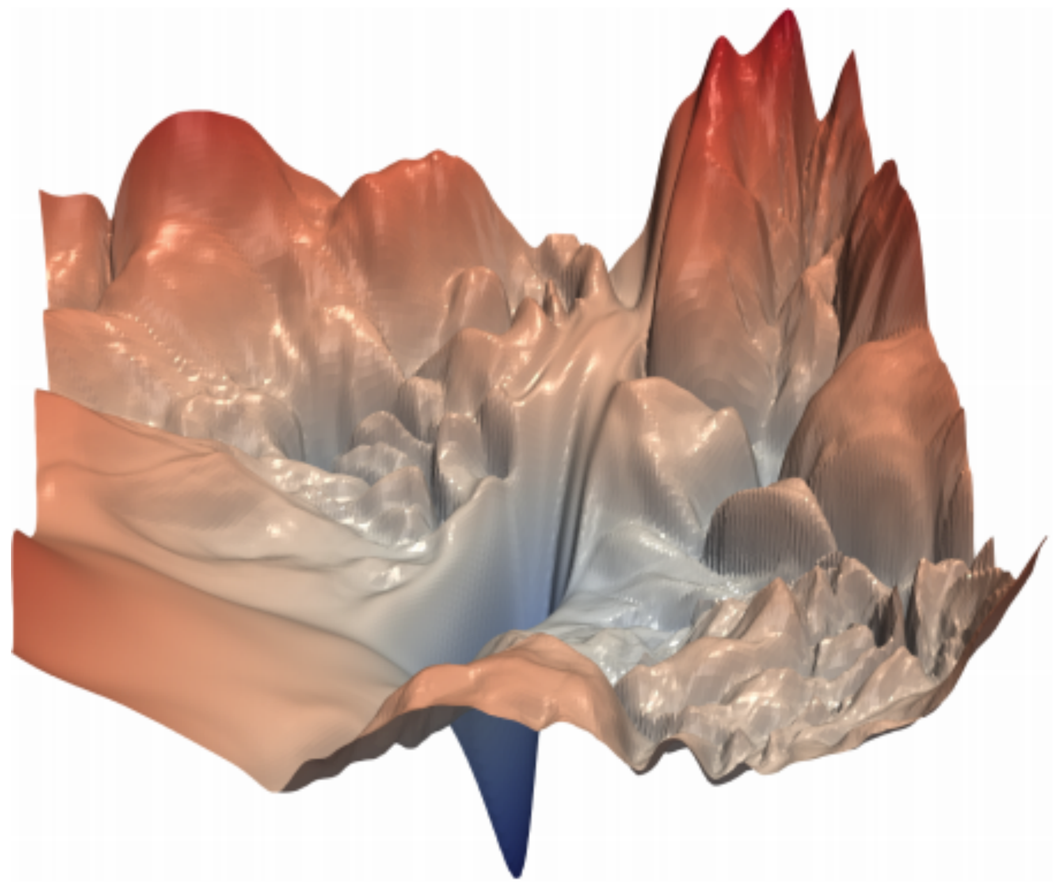

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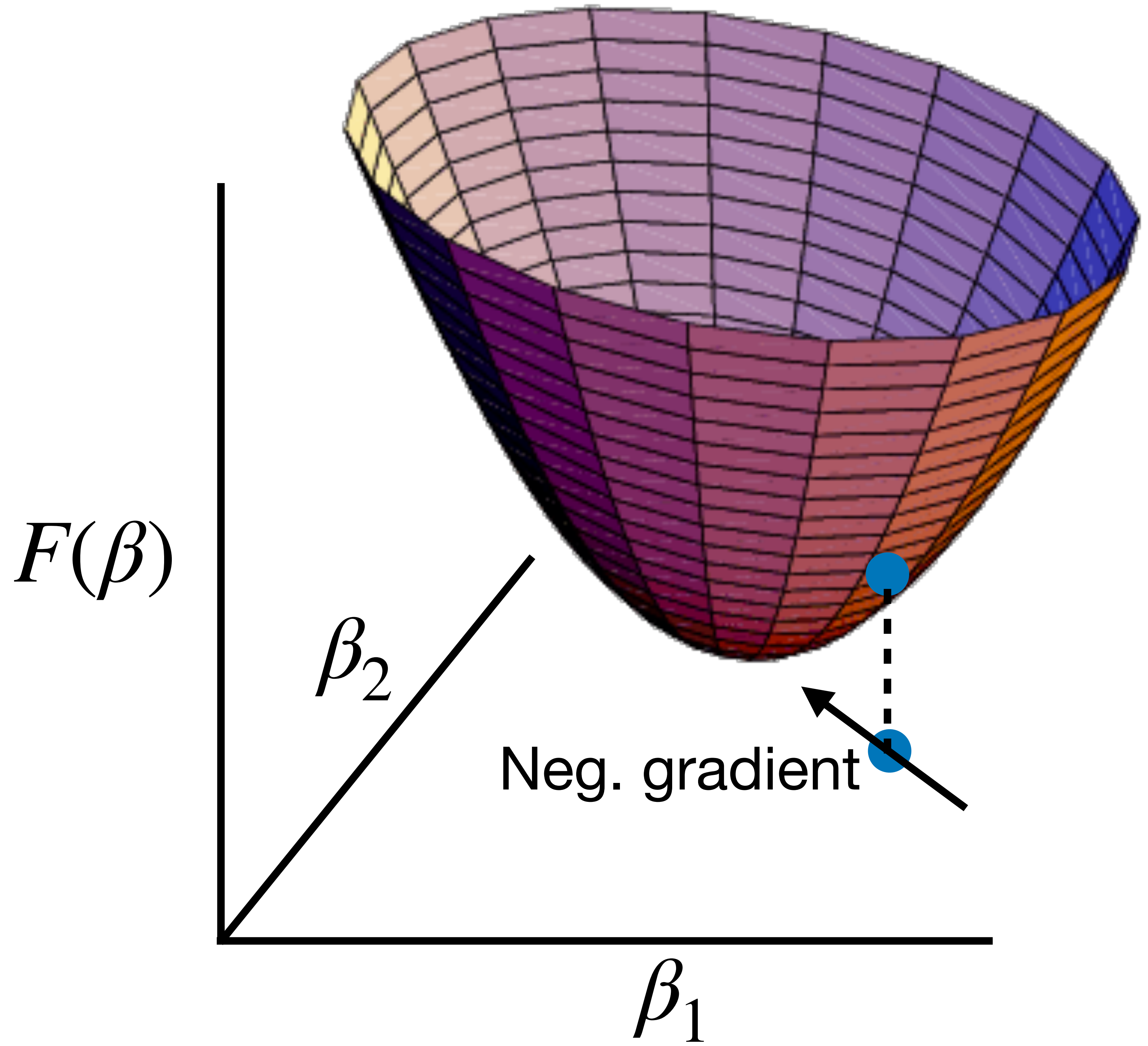

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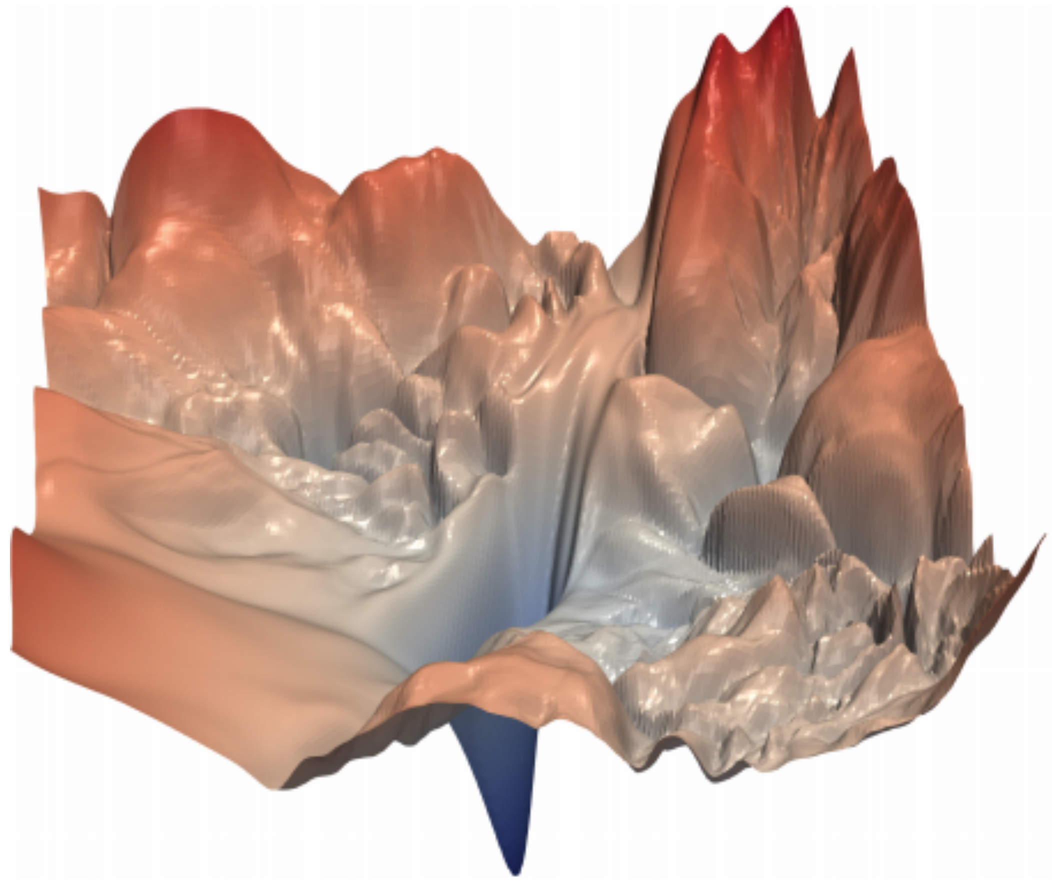

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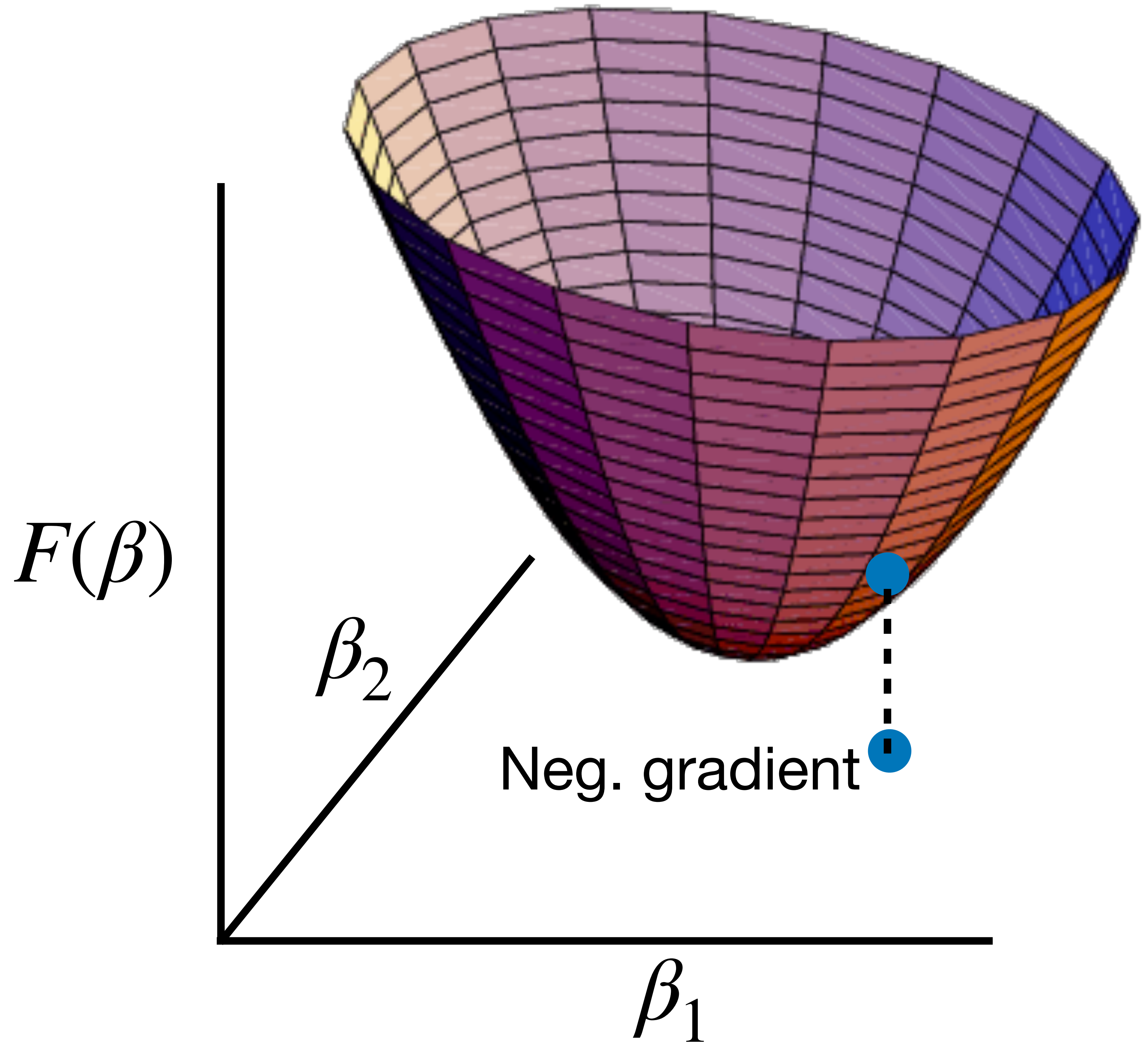

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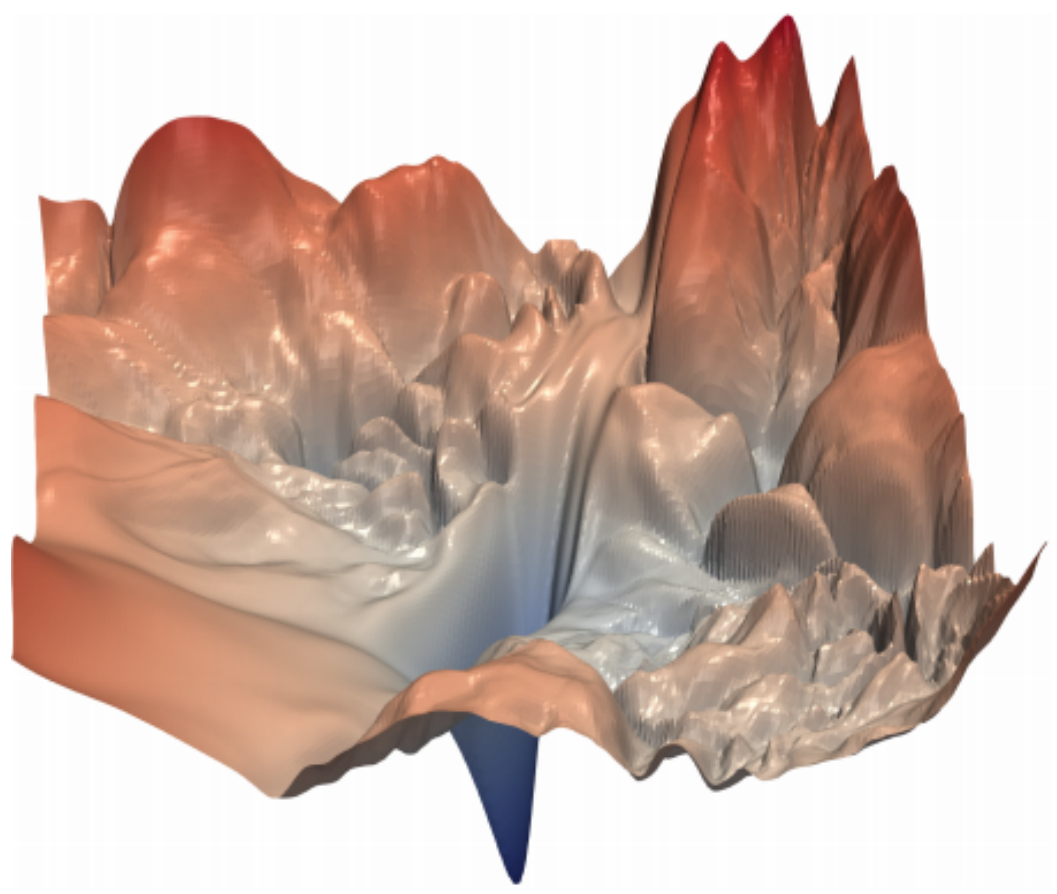

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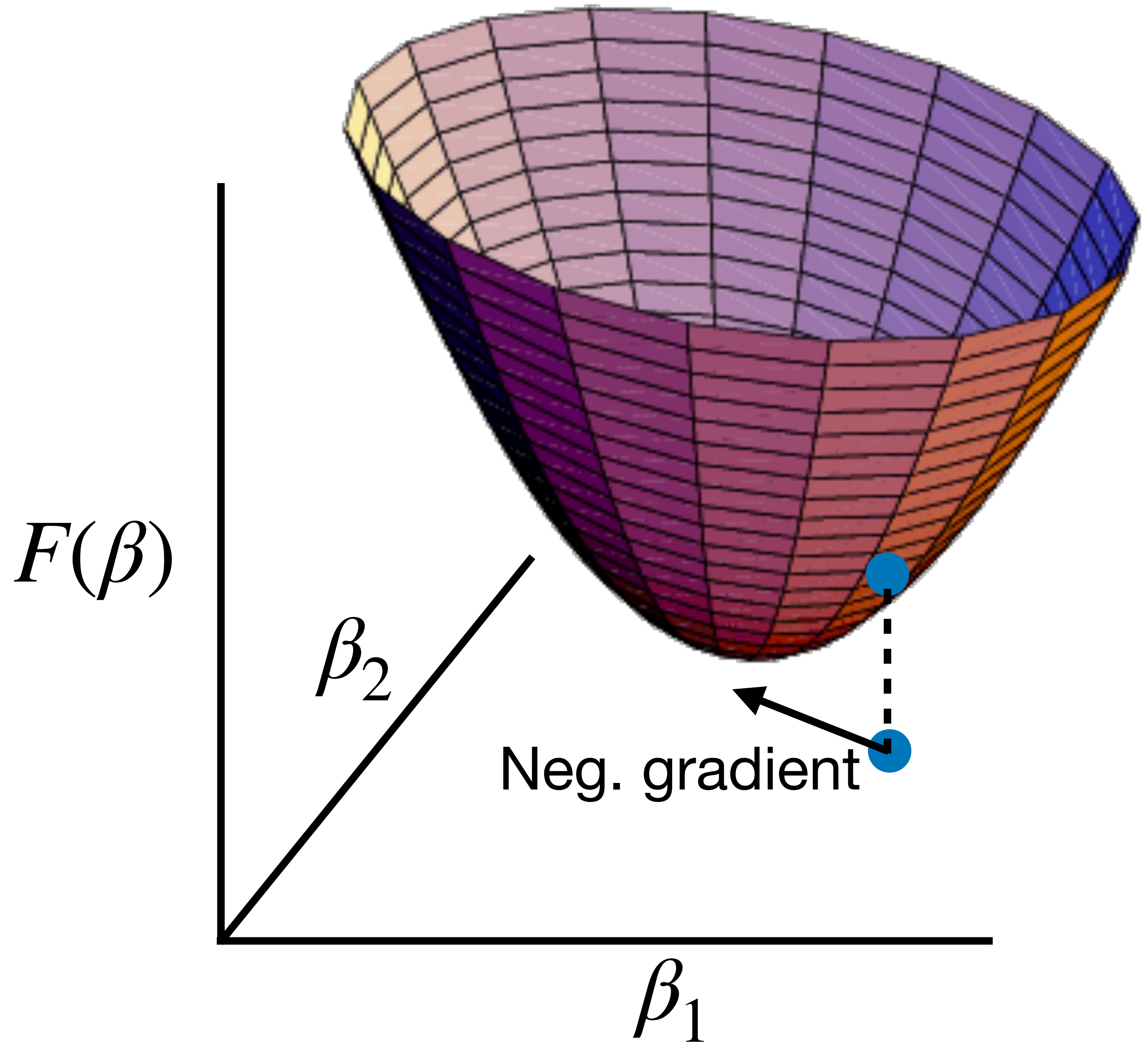

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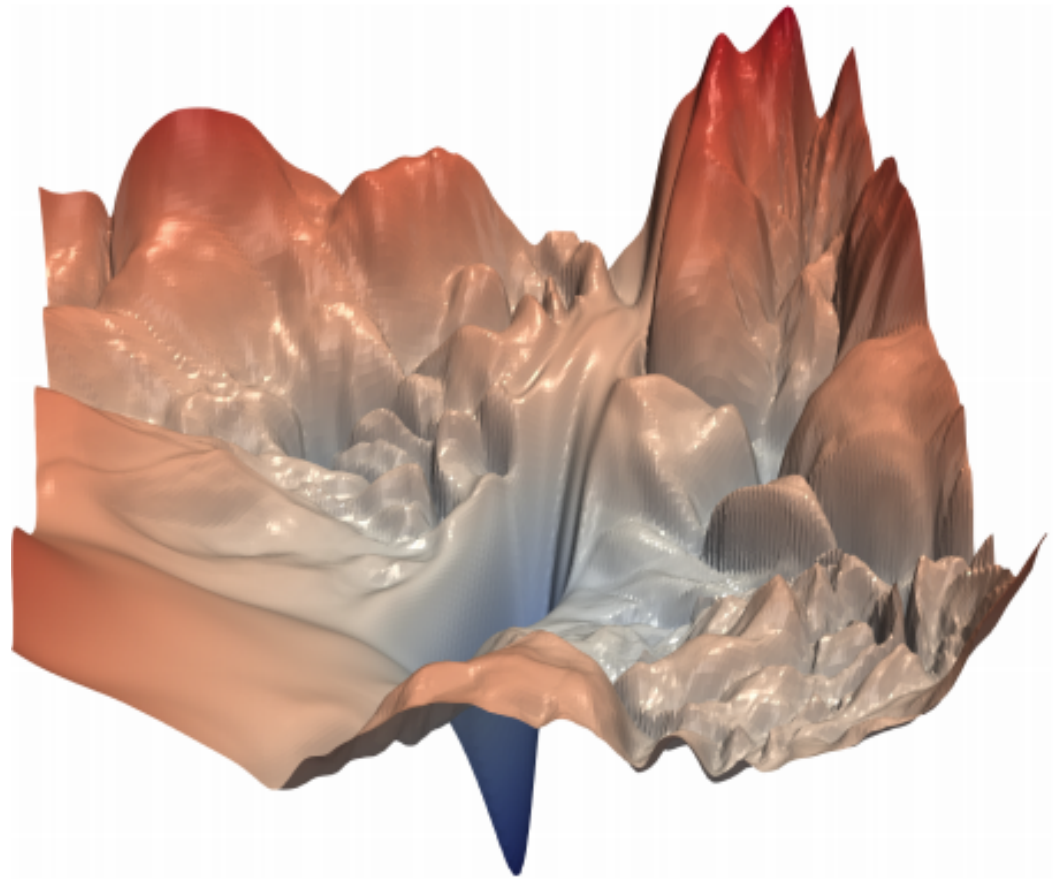

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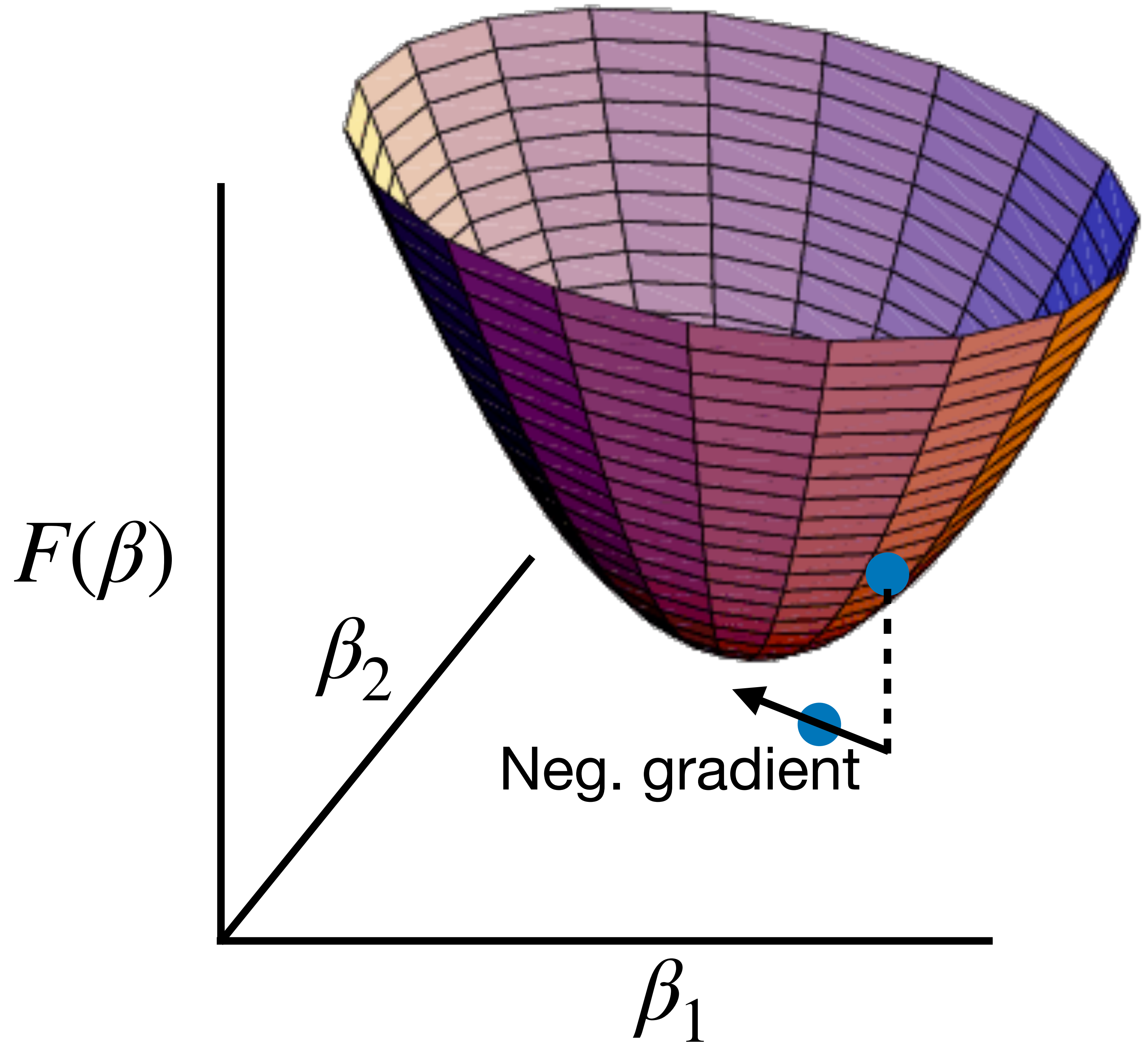

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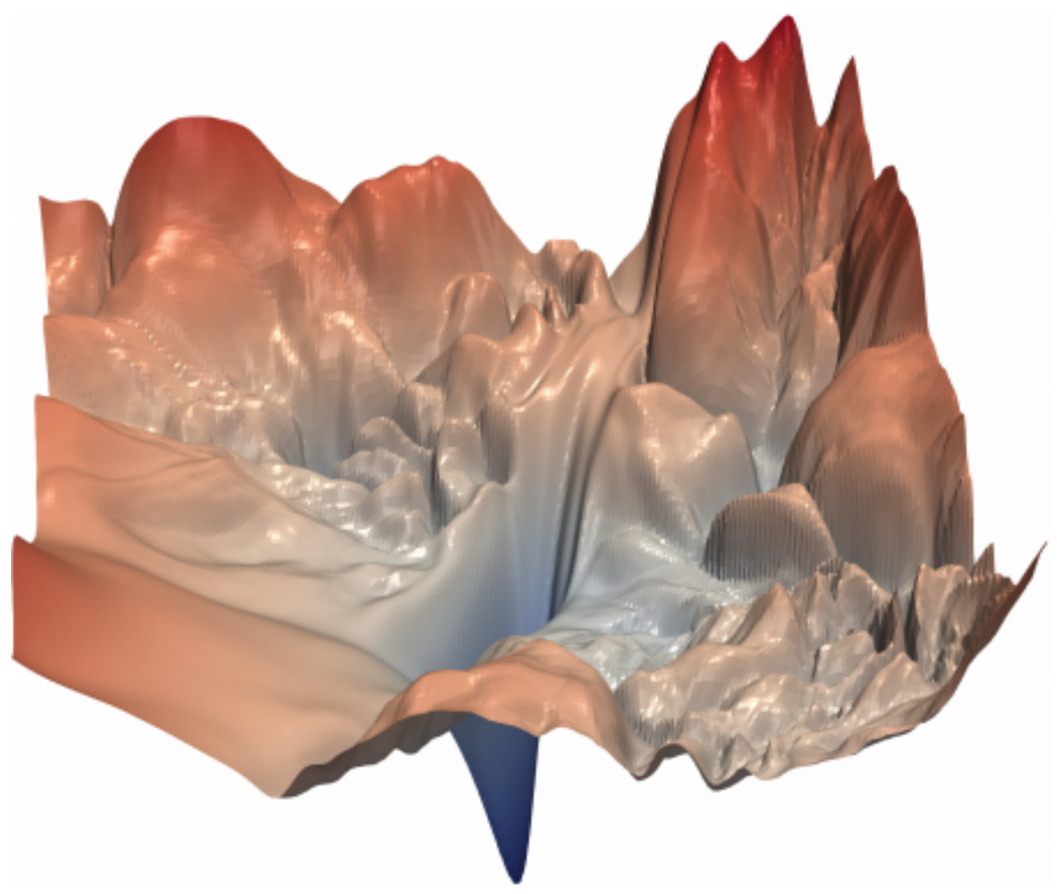

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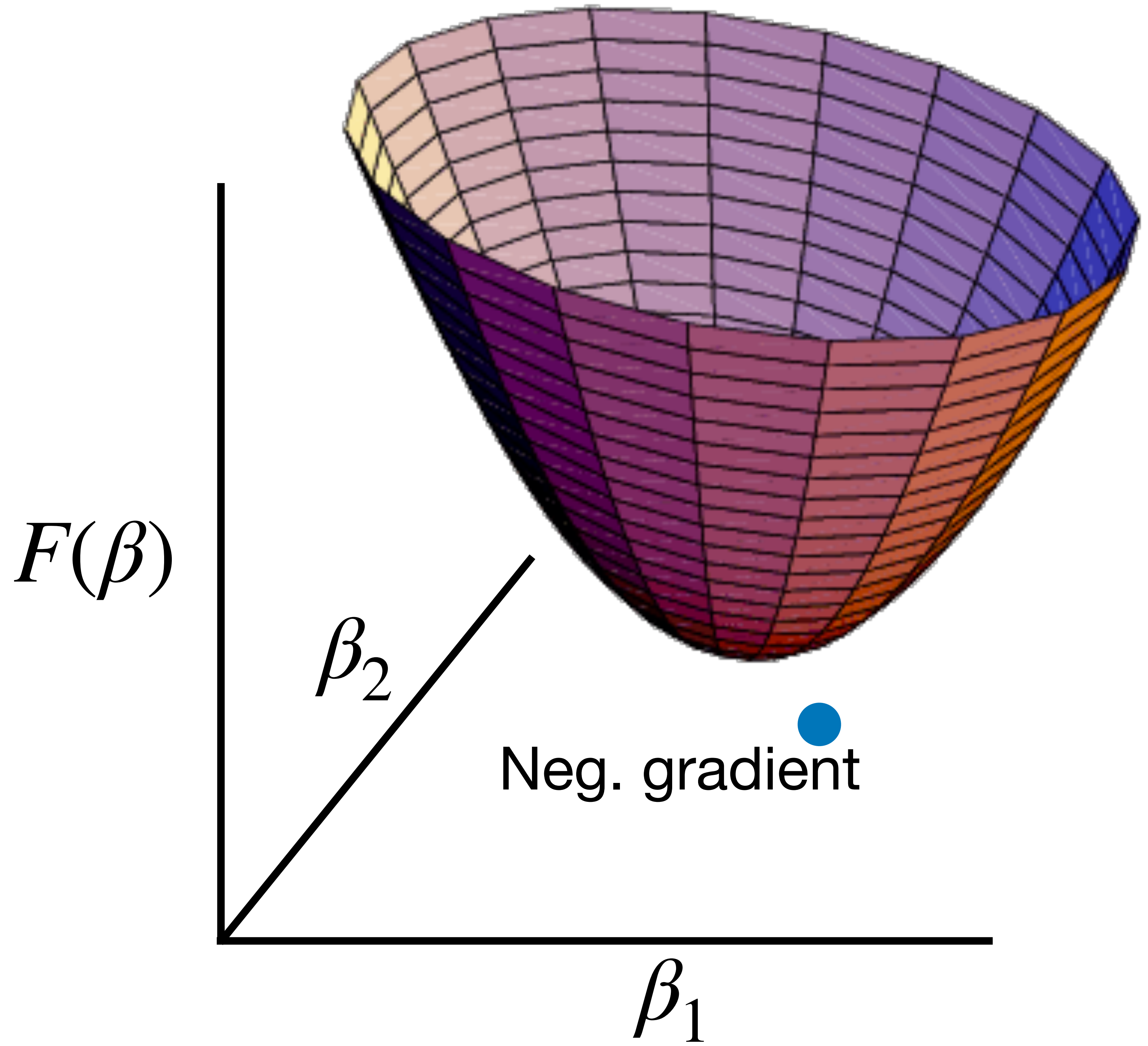

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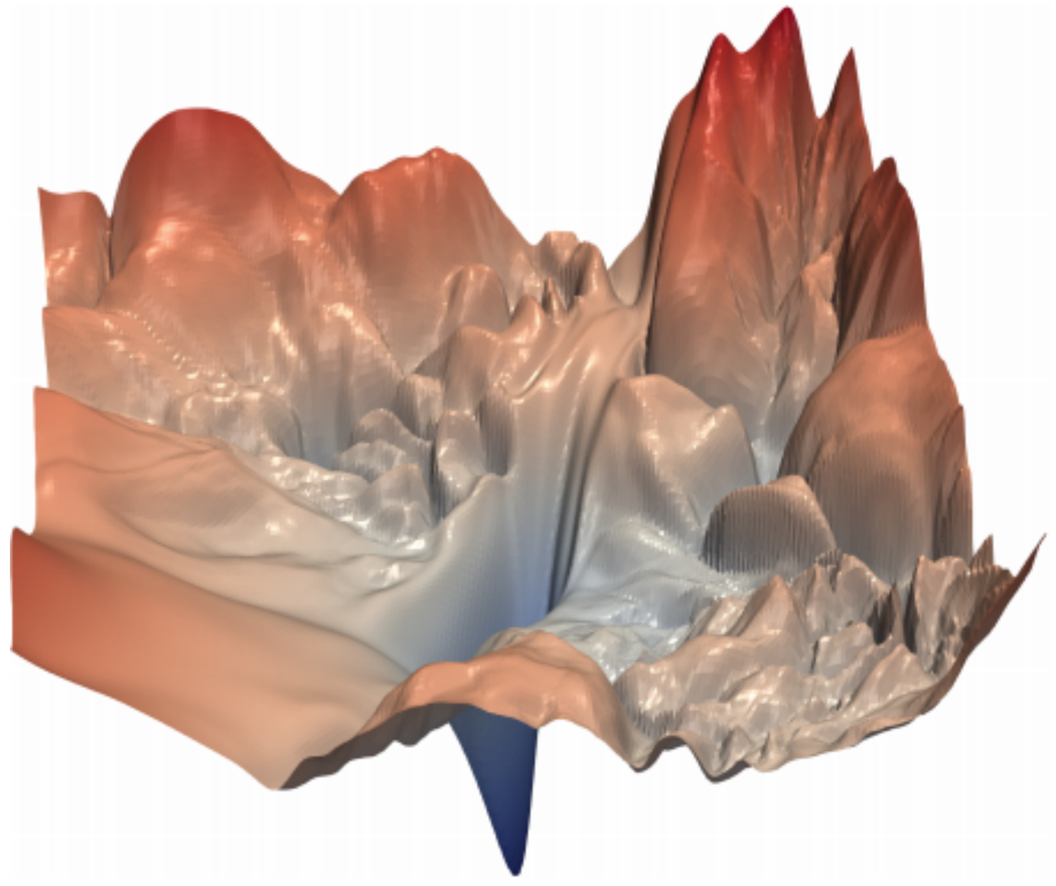

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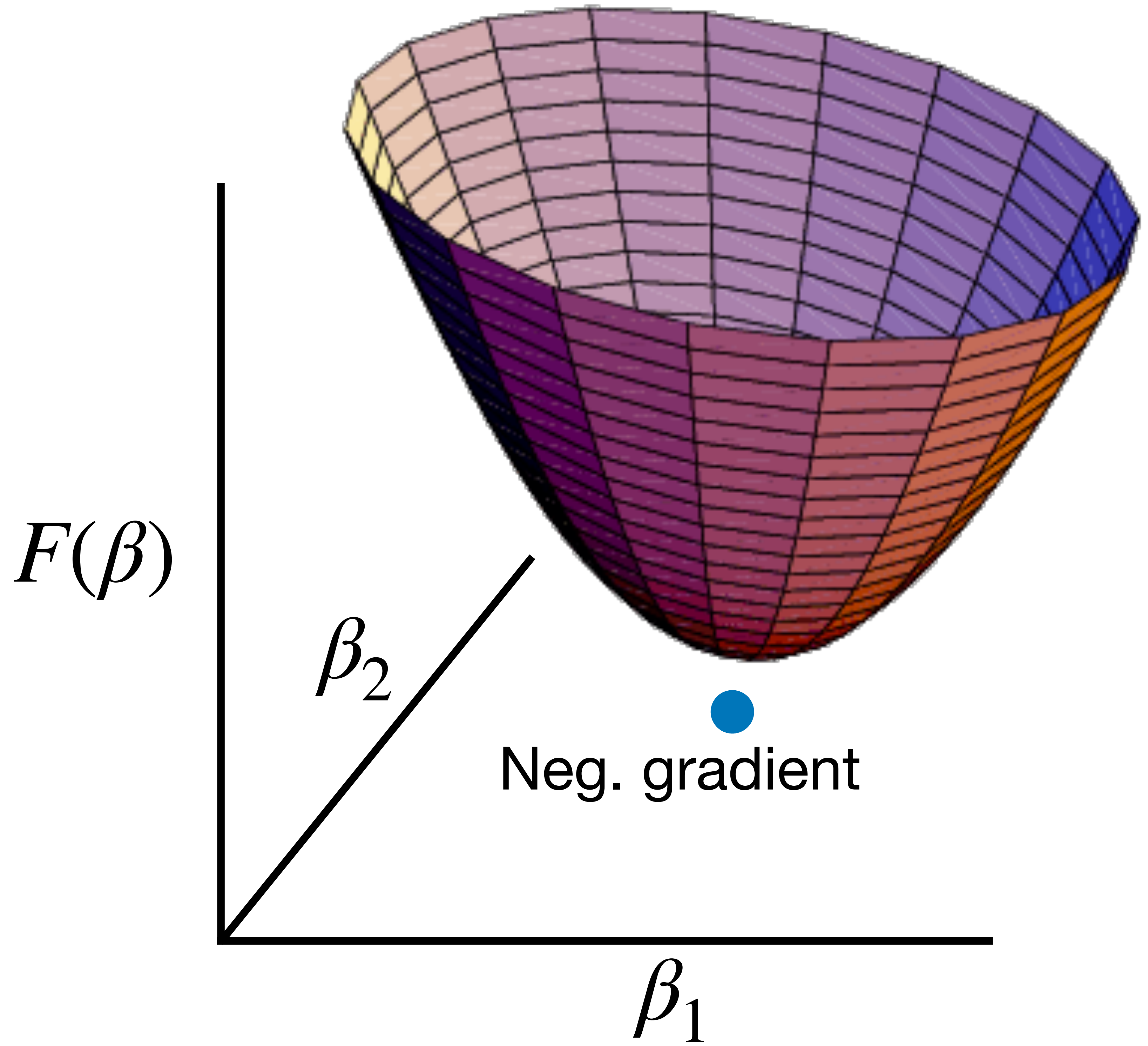

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If $F(\beta) = \frac{1}{n}\sum_{i=1}^{n} L(Y_i, f_\beta(X_i))$, then $\nabla F(\beta) = \frac{1}{n}\sum_{i=1}^{n} \nabla L(Y_i, f_\beta(X_i))$.

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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:

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

Stochastic gradient descent

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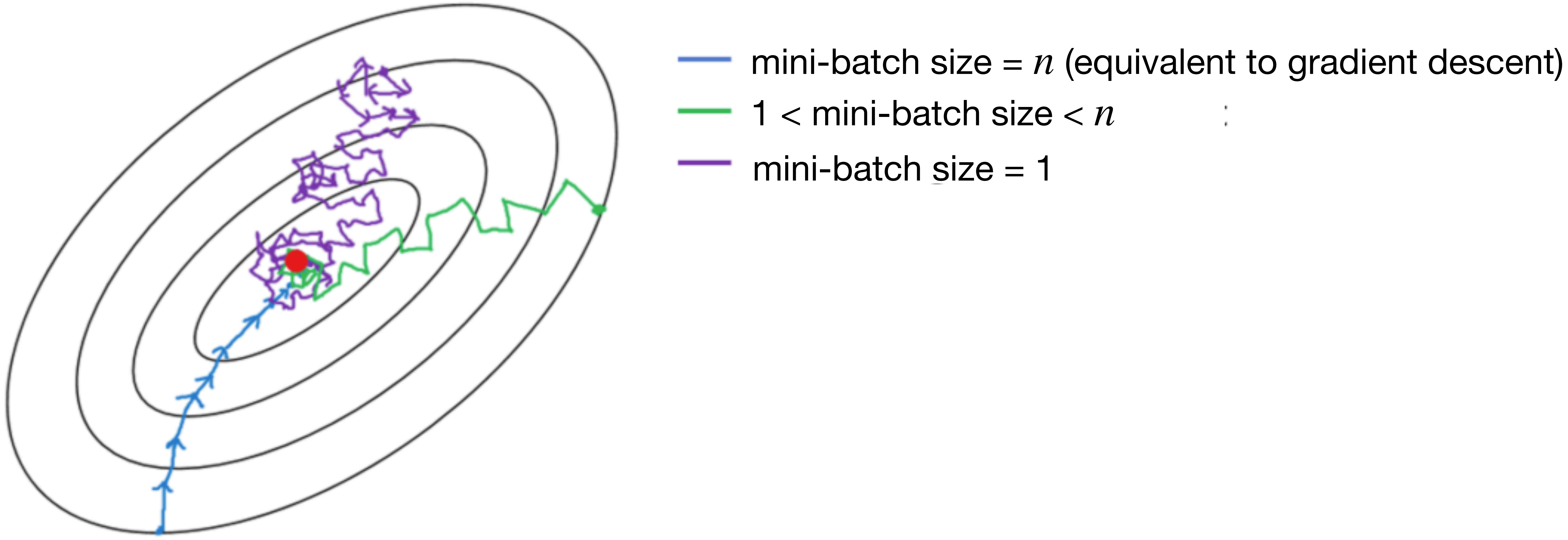
Backpropagation: An efficient algorithm to compute $\nabla L(Y_i, f_\beta(X_i))$

Behavior of stochastic gradient descent

Stochastic gradient descent wobbles toward decreasing values of the objective:

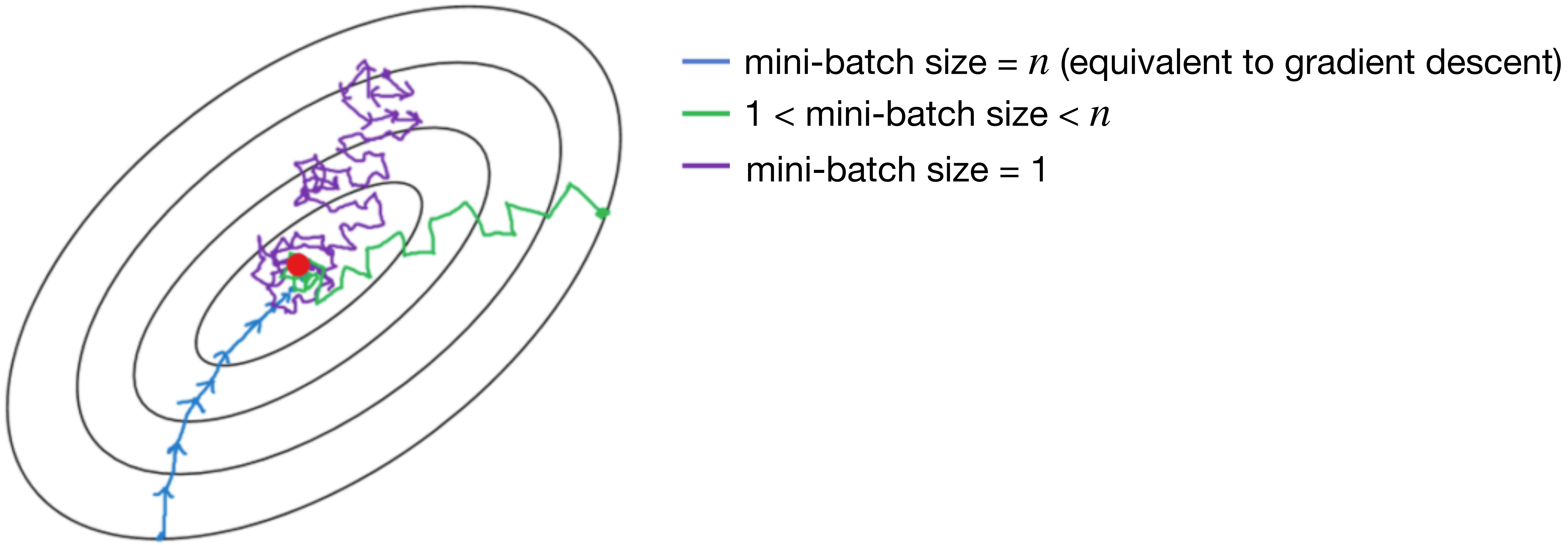


Source: https://medium.com/analytics-vidhya/gradient-descent-vs-stochastic-gd-vs-mini-batch-sgd-fbd3a2cb4ba4

The smaller the mini-batch, the cheaper and more wobbly each step is;
Intermediate mini-batch sizes tend to work well, e.g. mini-batch size = 32.

Bonus: The extra randomness sometimes allows SGD to wobble past local minima.

Stochastic gradient descent step versus epoch



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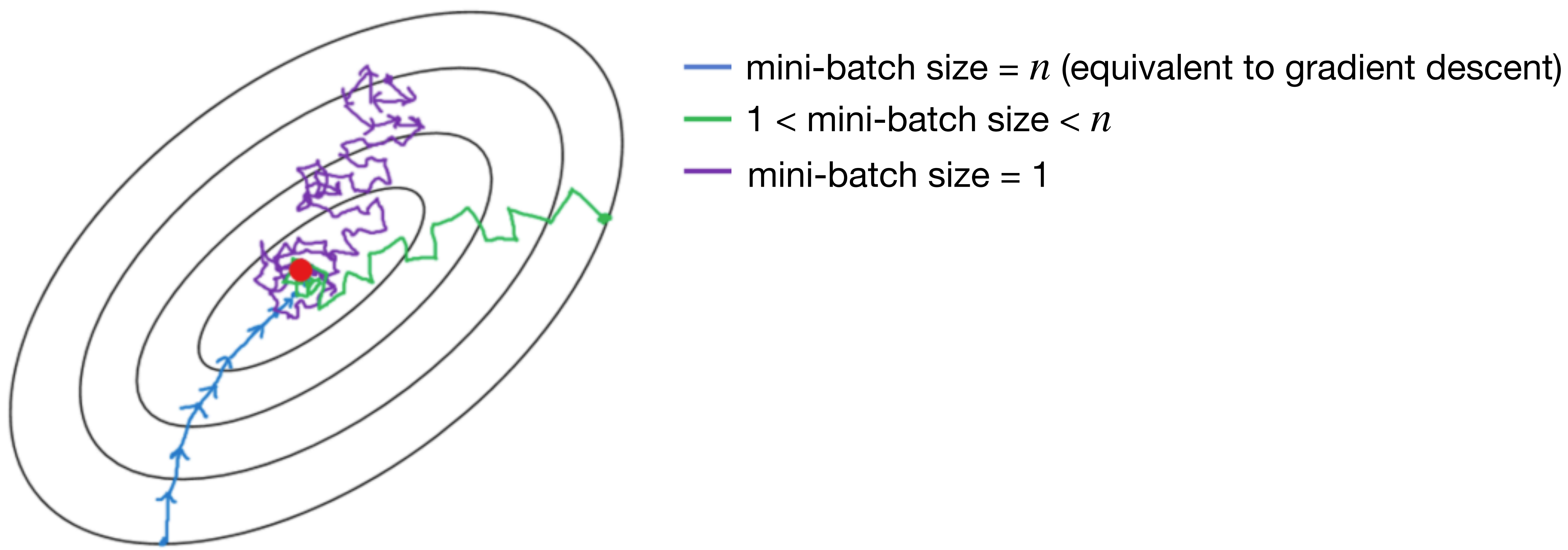
Stochastic gradient descent step versus epoch

An epoch consists of SGD steps that cycle through all of the observations once.



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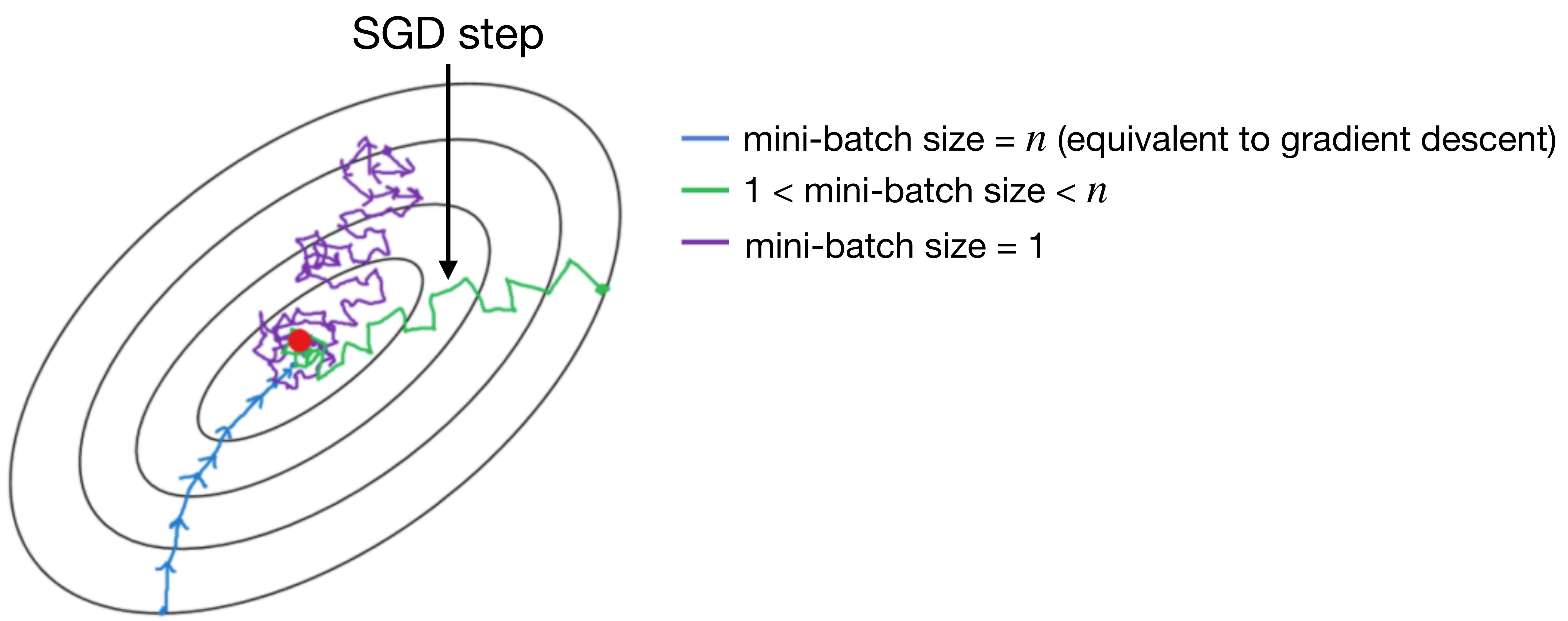

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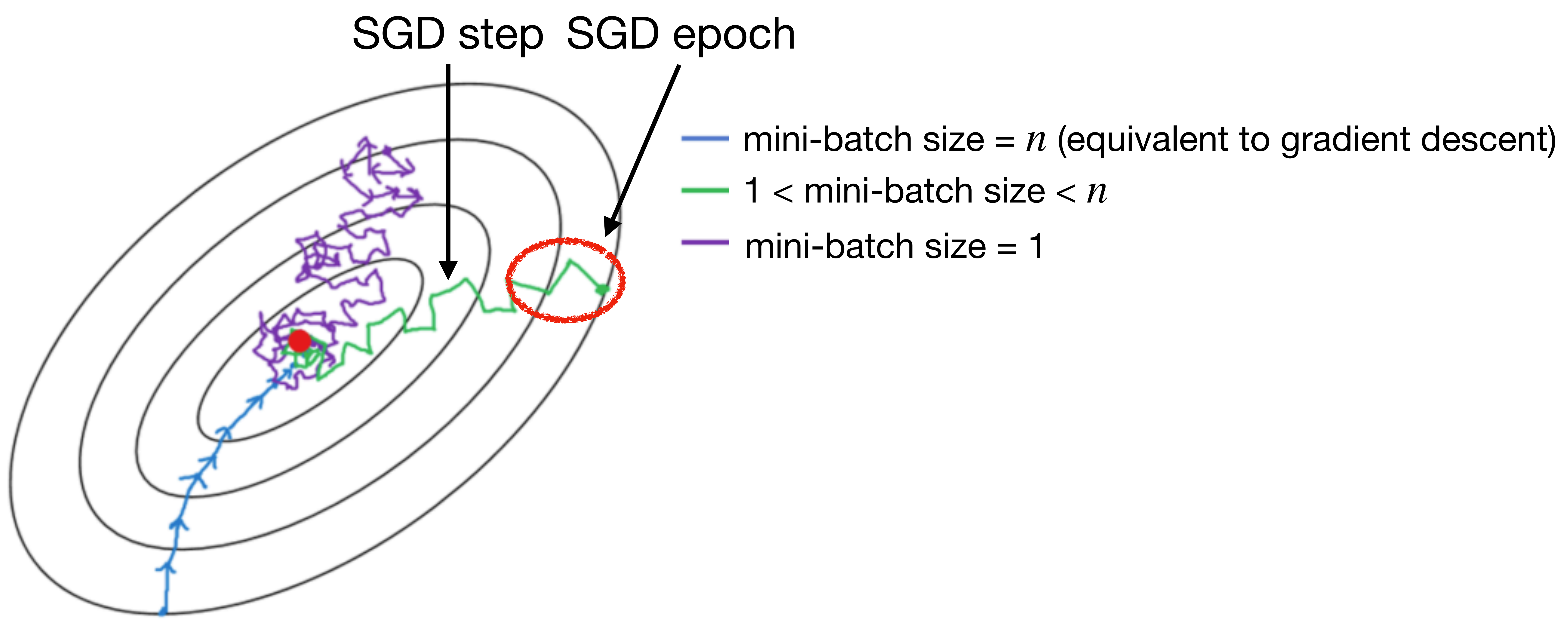

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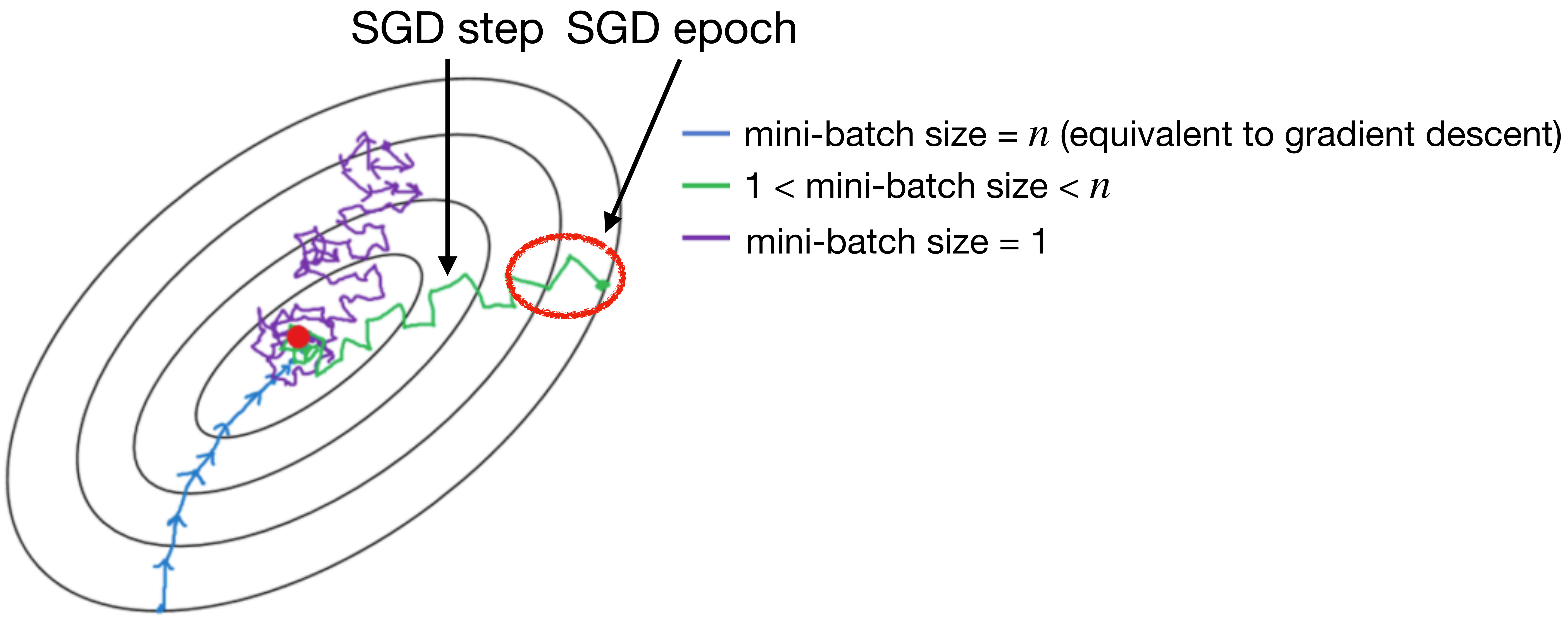

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Observation	1	2	3	4	5	6	7	8	9	1	2	3	4	5	6	7	8	9
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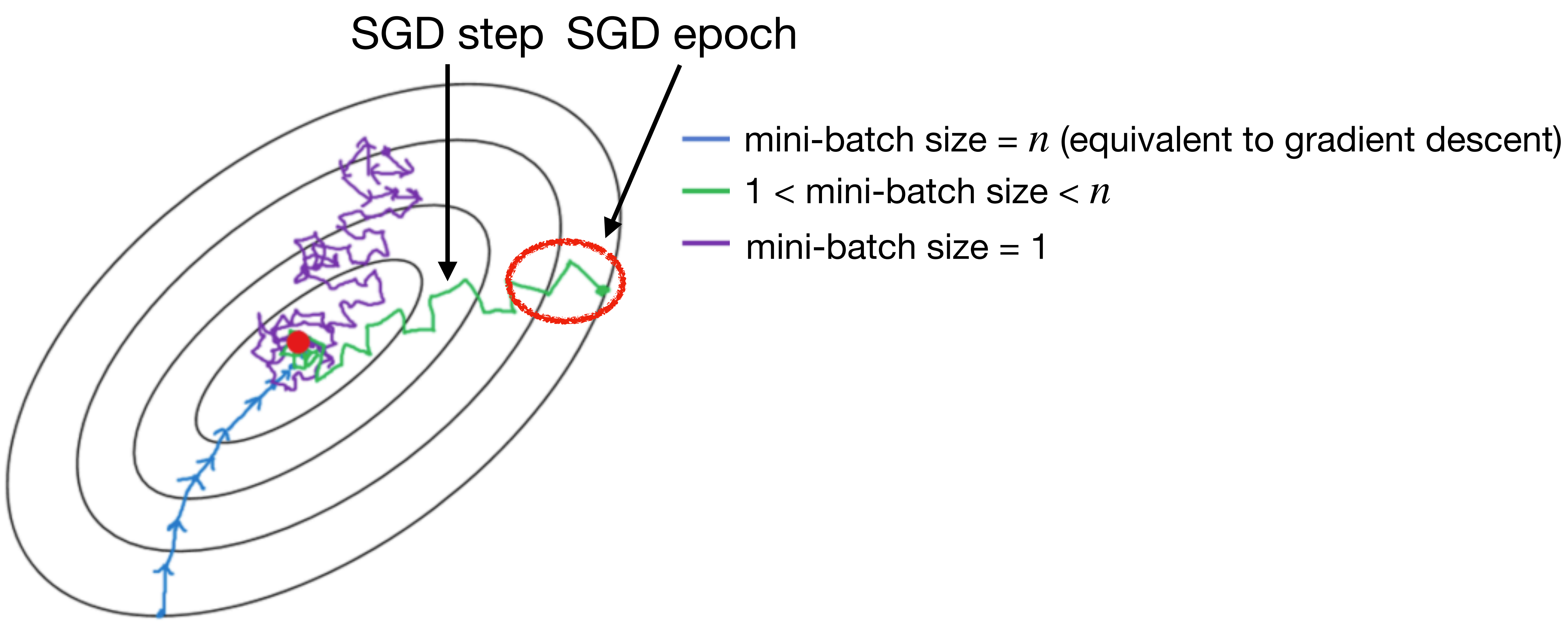

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Observation	1	2	3	4	5	6	7	8	9	1	2	3	4	5	6	7	8	9
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SGD step (mini-batch size 1)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18

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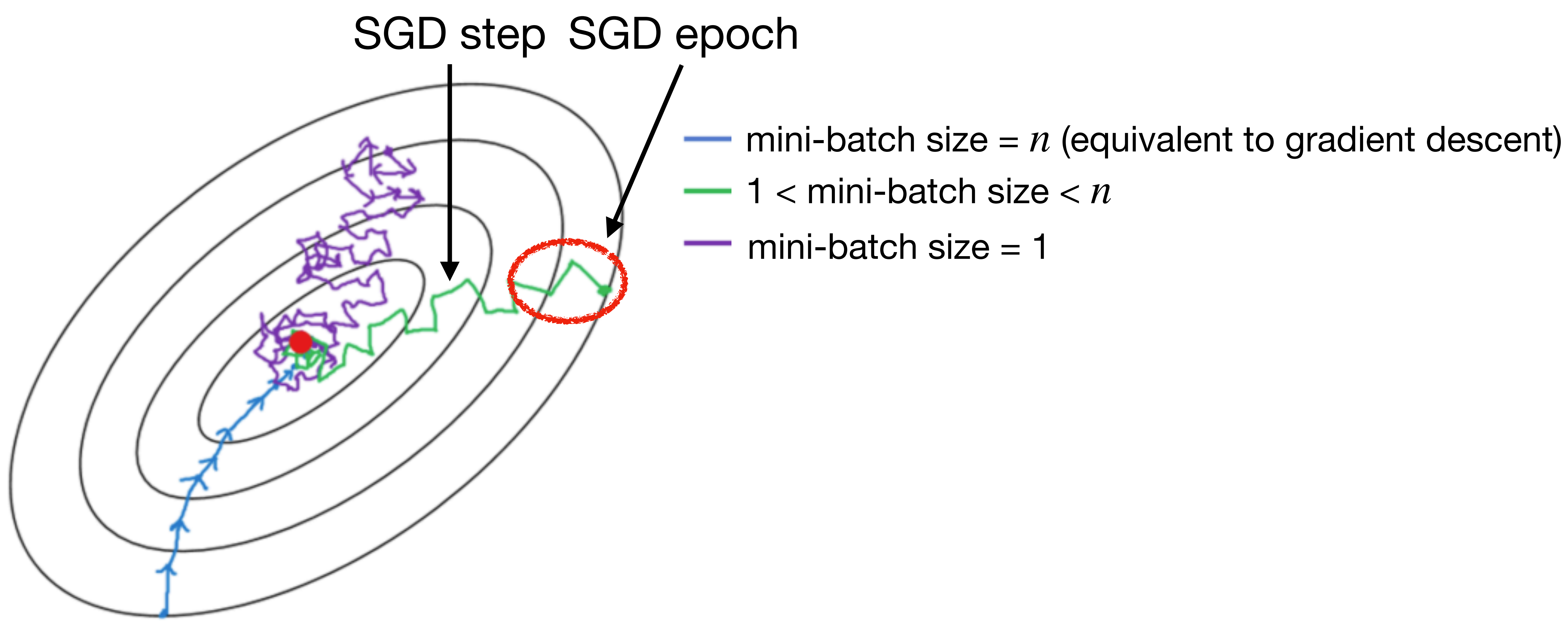

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SGD step (mini-batch size 3)	Step 1			Step 2			Step 3			Step 4			Step 5			Step 6		

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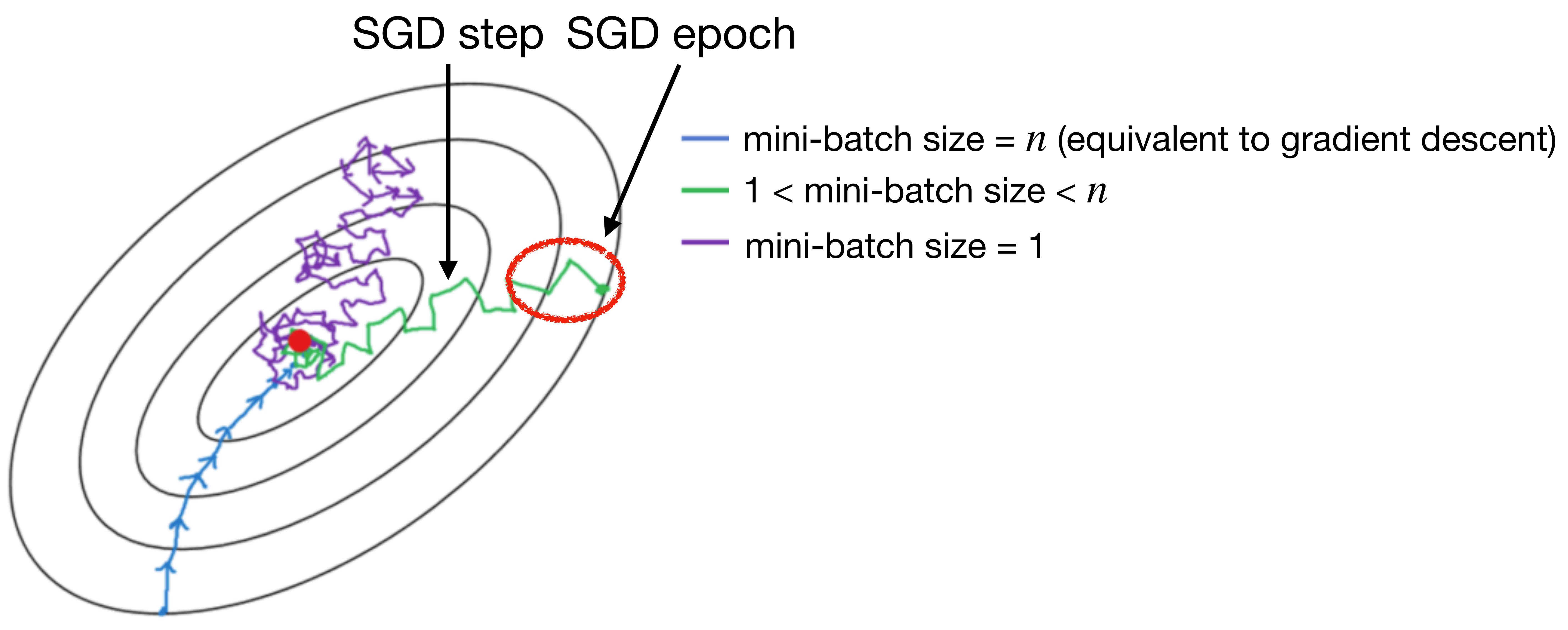

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E.g. $n = 9$, mini-batch size 3. Then each epoch consists of three SGD steps.

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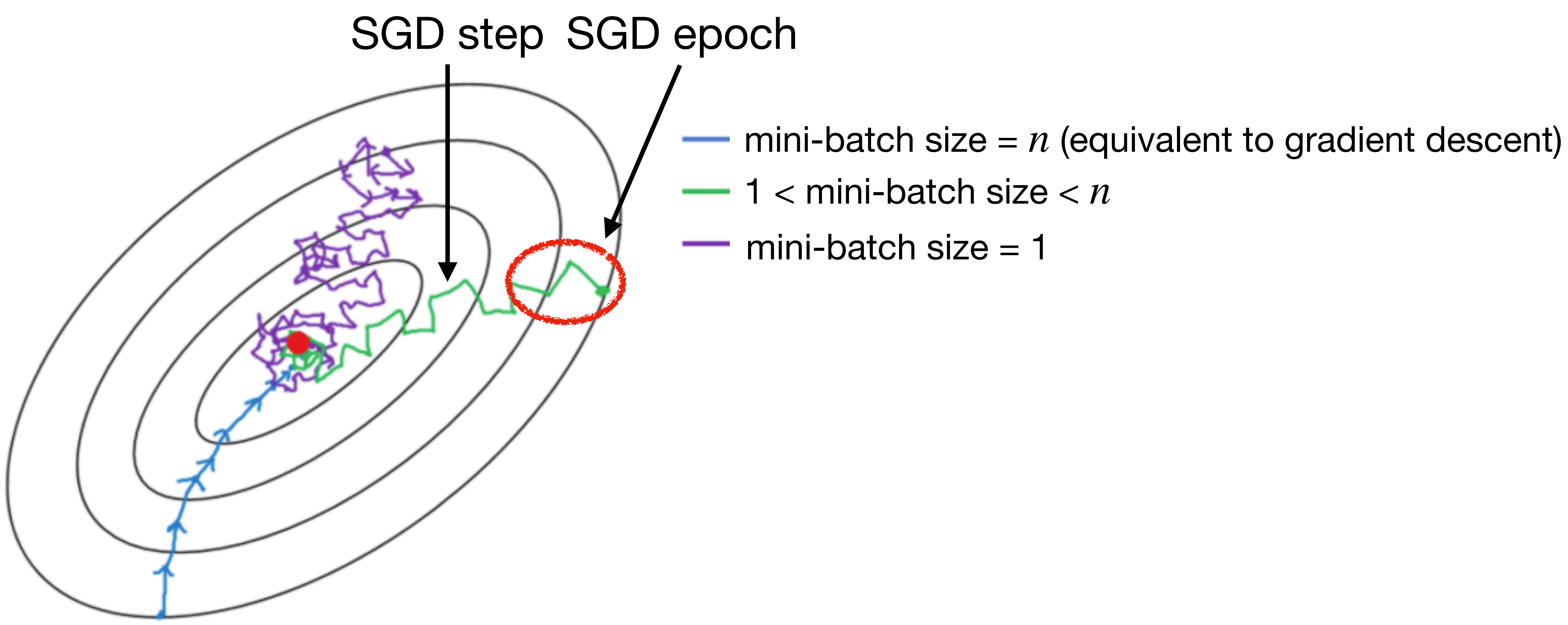

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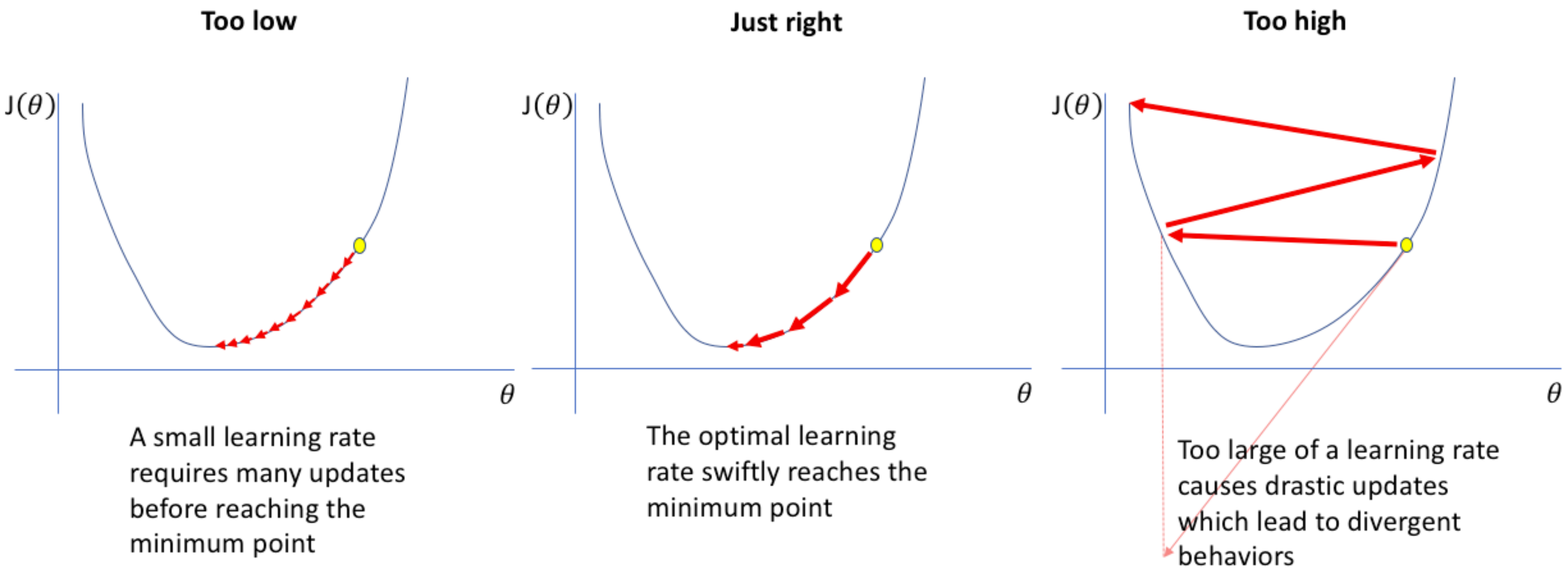
Gradient step	Step 1									Step 2								

The learning rate for (stochastic) gradient descent



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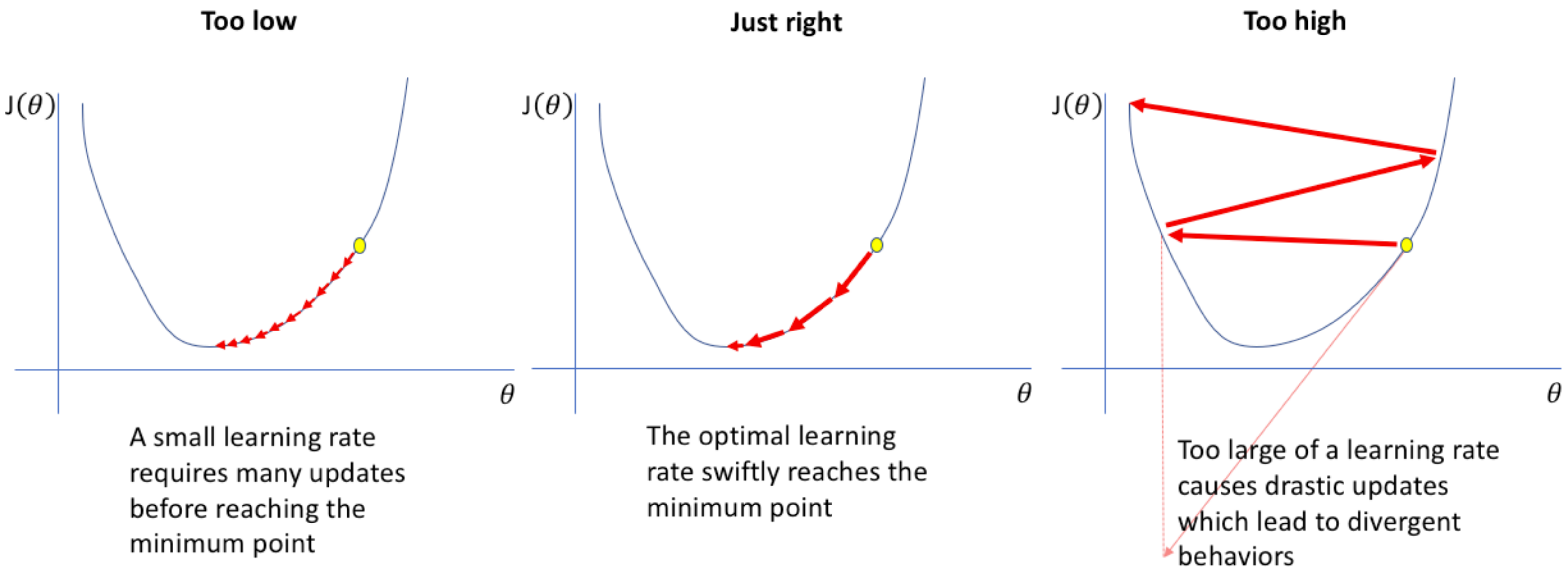

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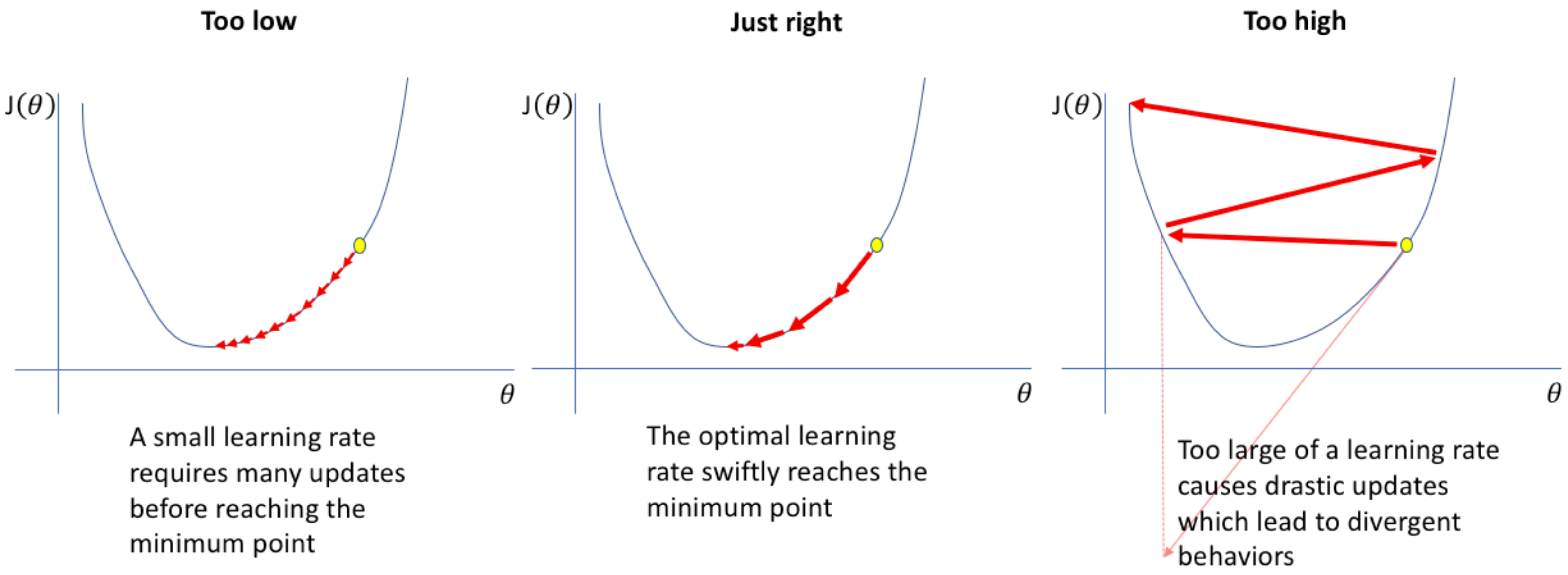

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- Setting the learning rate is more of an art than a science; might need to try a few values to get a good one.
- Especially for non-convex optimization, people come up with clever strategies like shrinking learning rates, cycling learning rates, adaptive learning rates, etc. (RMSprop, Adam, AdaGrad, AdaDelta, …)

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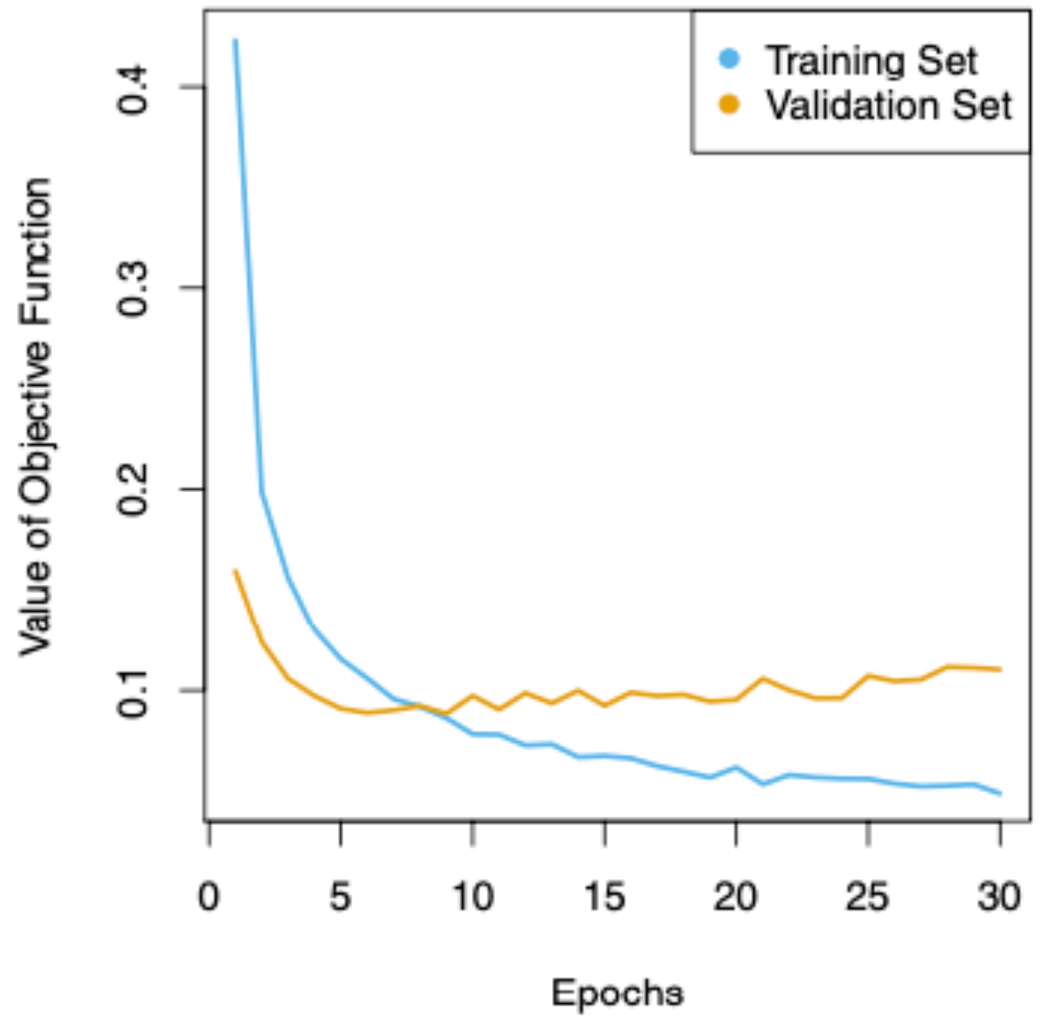

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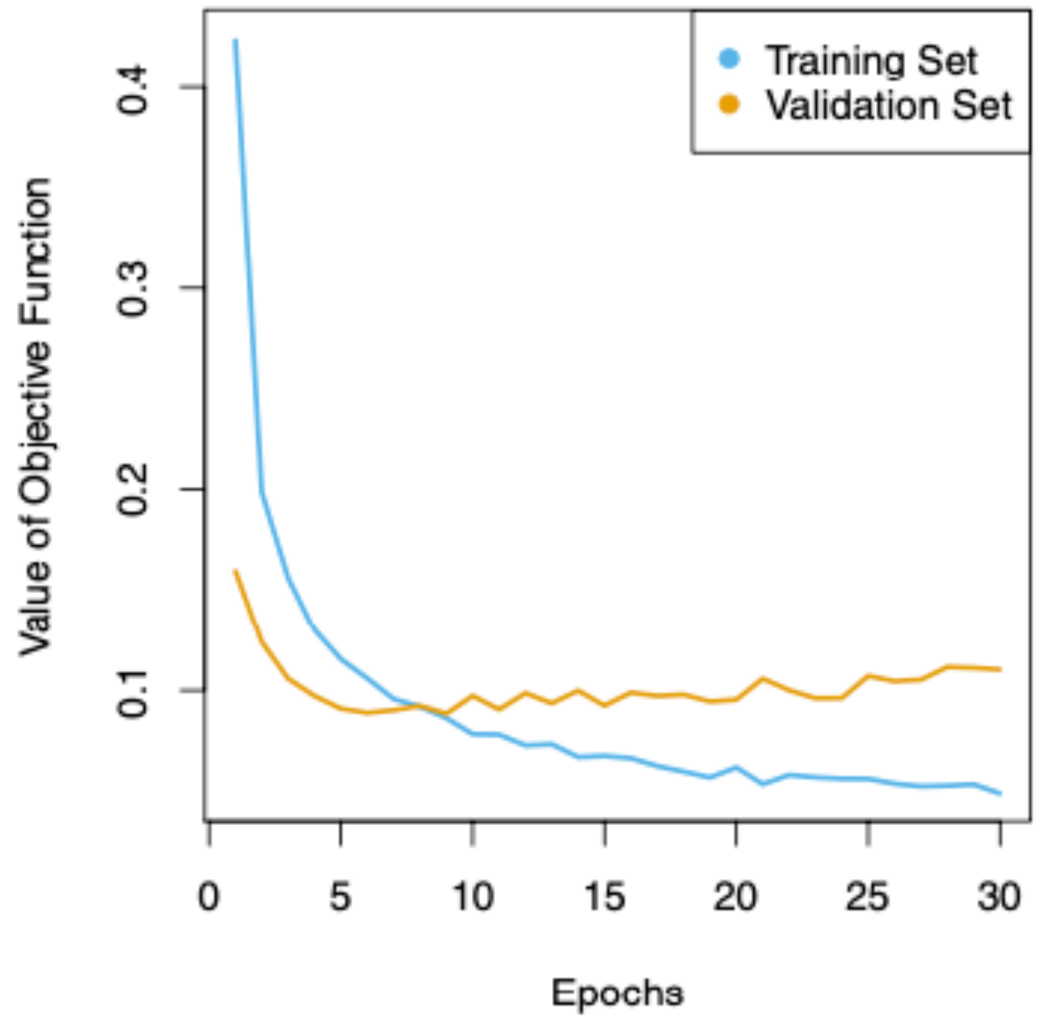
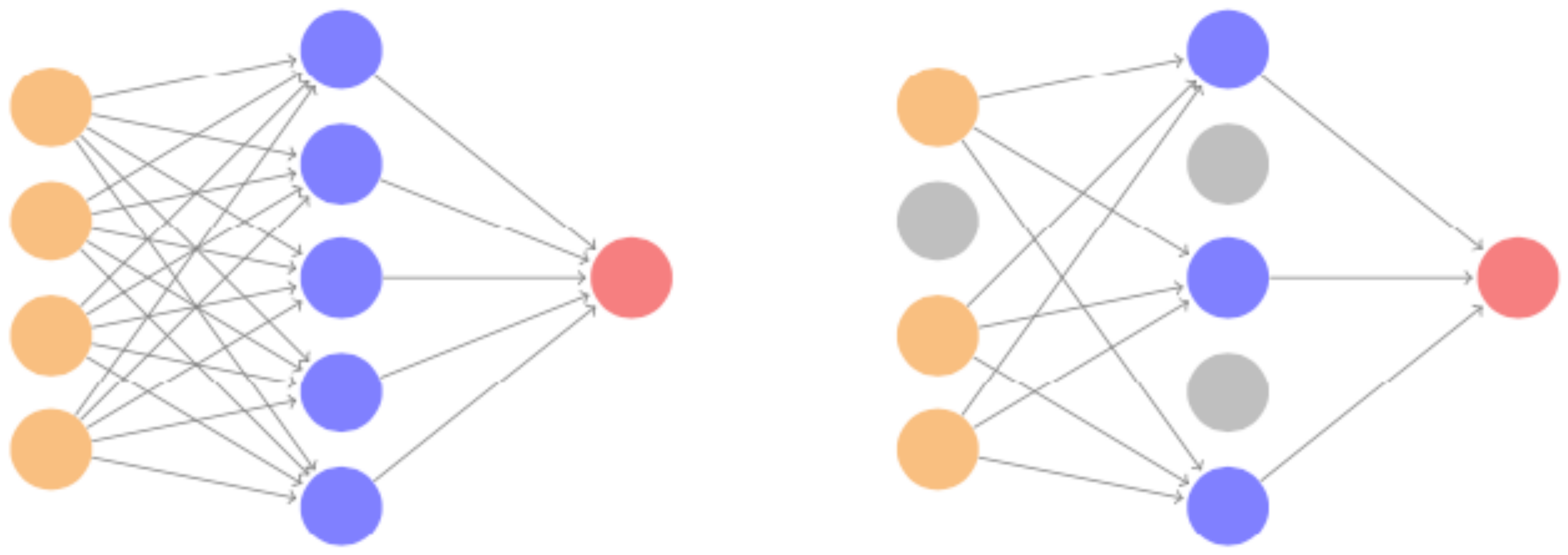


- Dropout: At each SGD iteration, remove a randomly selected set of nodes from the network (analogous to sub-sampling features for random forests).



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For computational savings, validation sets are typically employed instead of cross-validation to tune neural networks.

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- Adding hidden layers to logistic regression gives multilayer neural networks.
- Multilayer neural networks build increasingly complex representations of the input data (feature learning).
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Quiz Practice