Neural networks

STAT 471

November 23, 2021

Where we are

- **Unit 1:** Intro to modern data mining
- **Unit 2:** Tuning predictive models
- **Unit 3:** Regression-based methods
- **Unit 4:** Tree-based methods
- **Unit 5:** Deep learning

Lecture 1: Deep learning preliminaries

Lecture 2: Neural networks

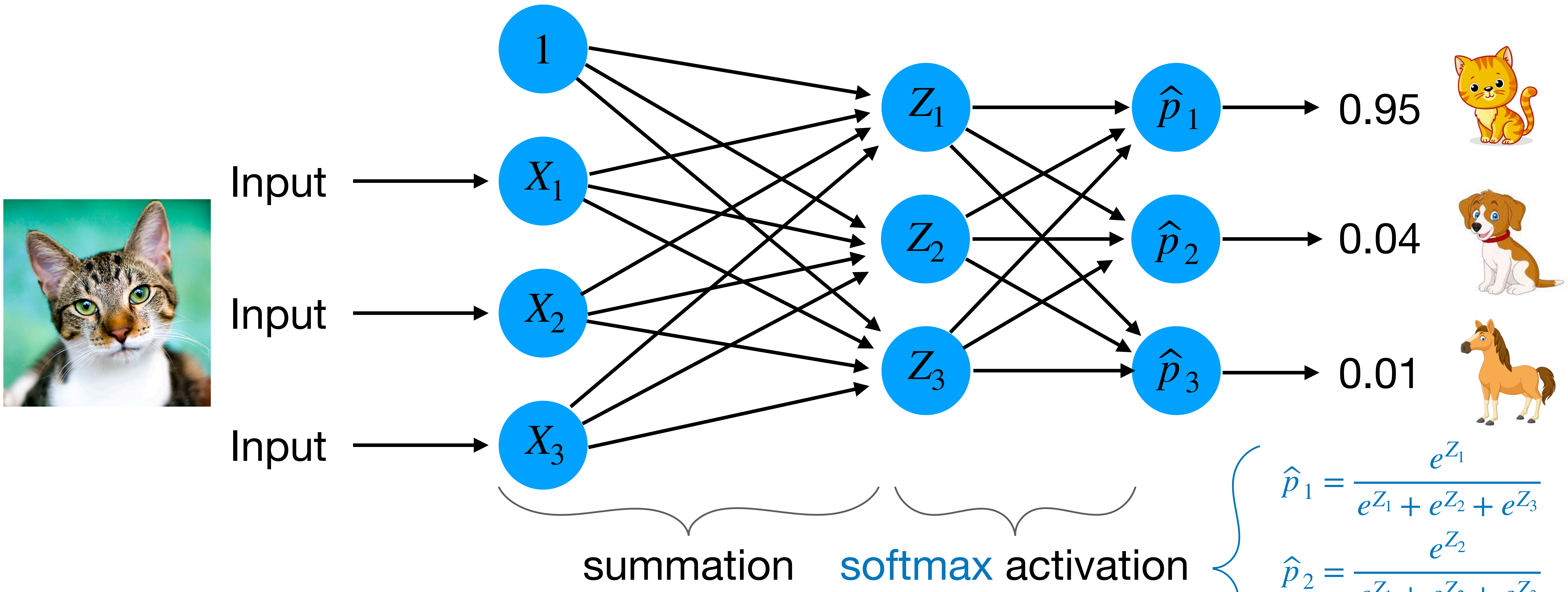
Lecture 3: Deep learning for images

Lecture 4: Deep learning for text

Lecture 5: Unit review and quiz in class

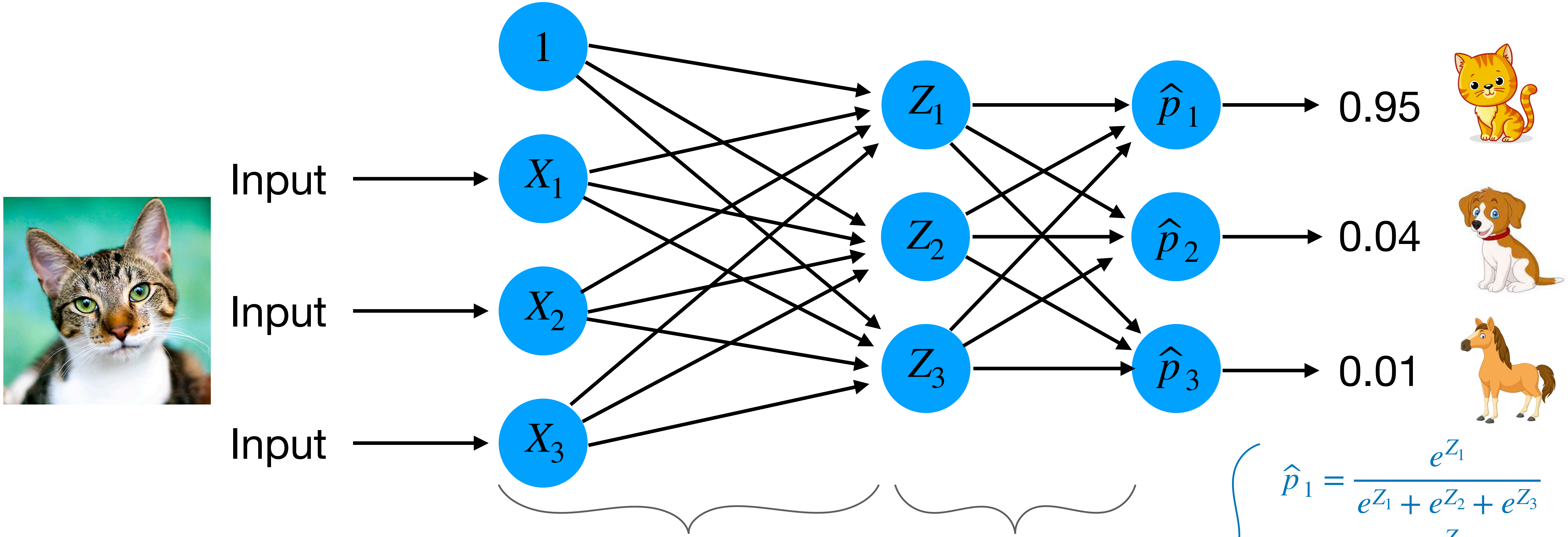
Homework 5 due the following Wednesday.

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



summation softmax activation

$$
\left\{
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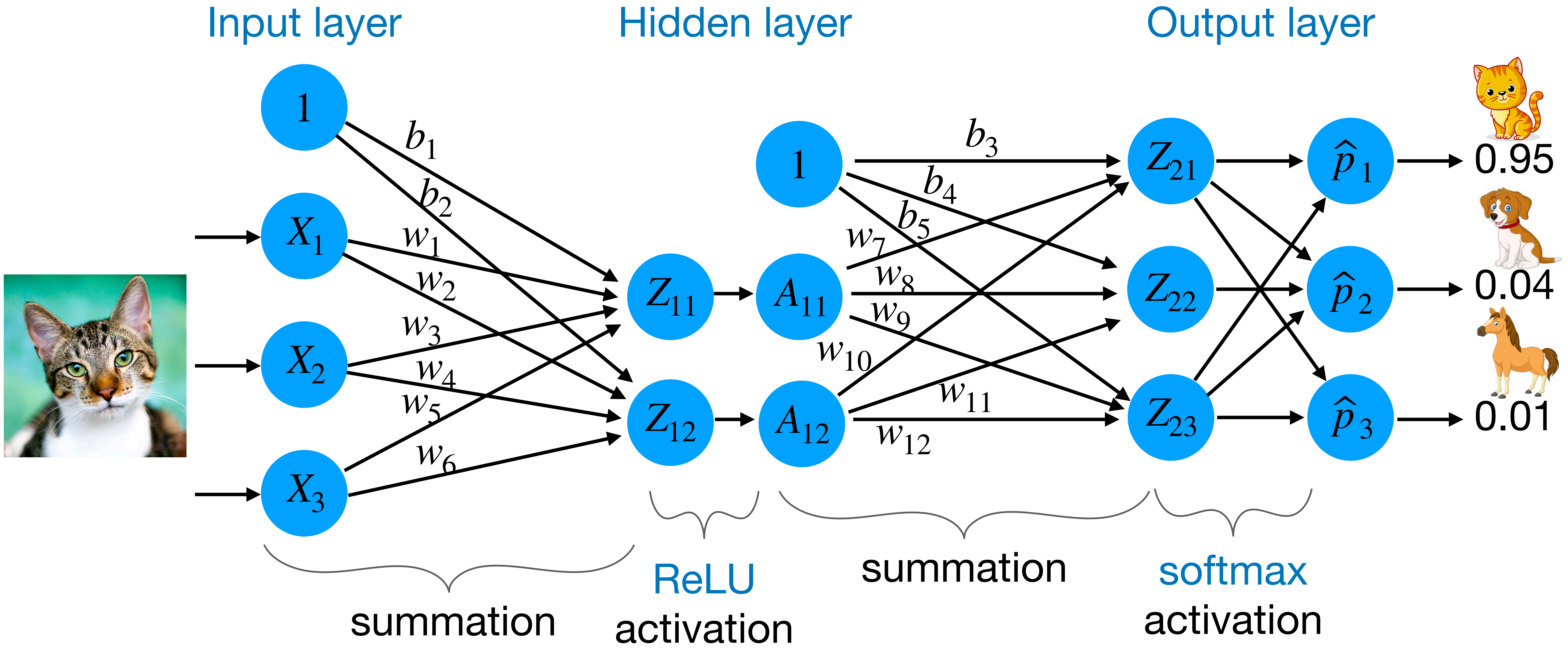
\end{aligned}
\right.
$$

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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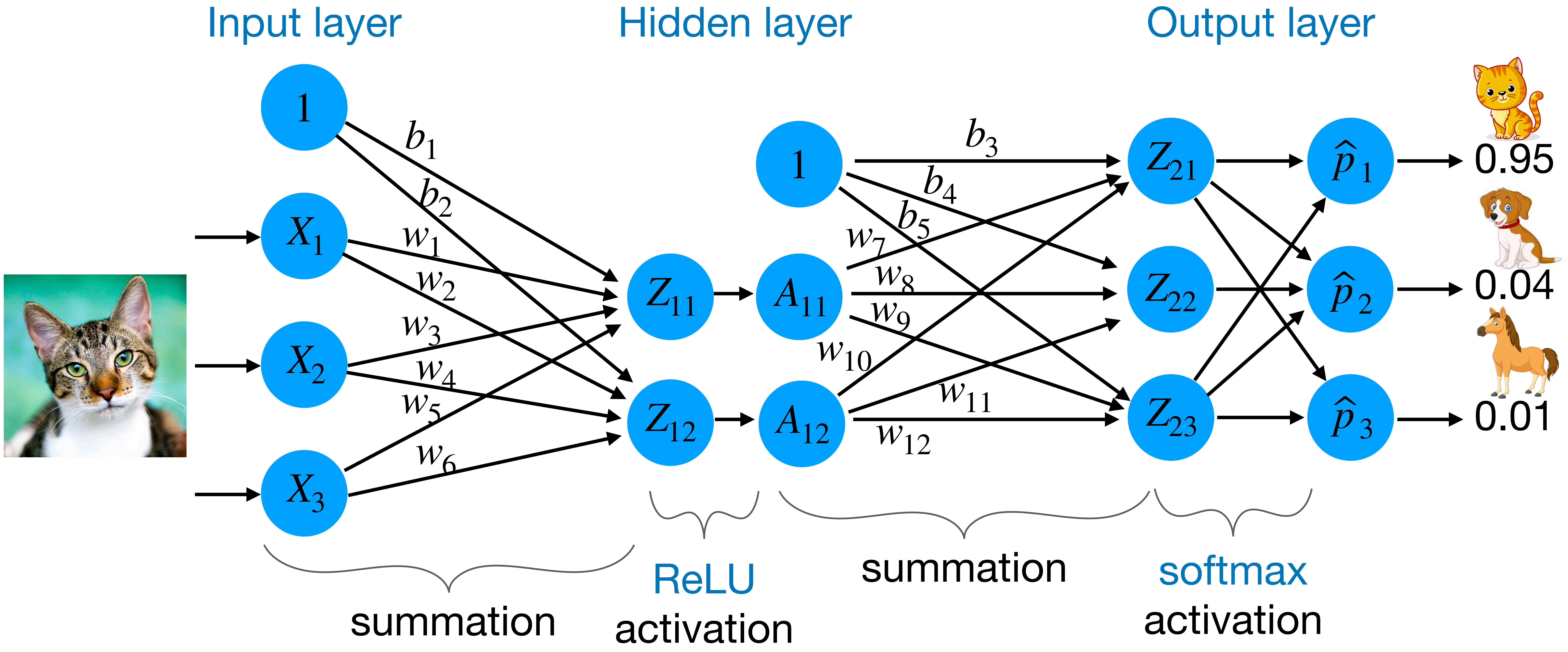

E.g., $Z_{12} = b_2 + w_2 X_1 + w_4 X_2 + w_6 X_3$

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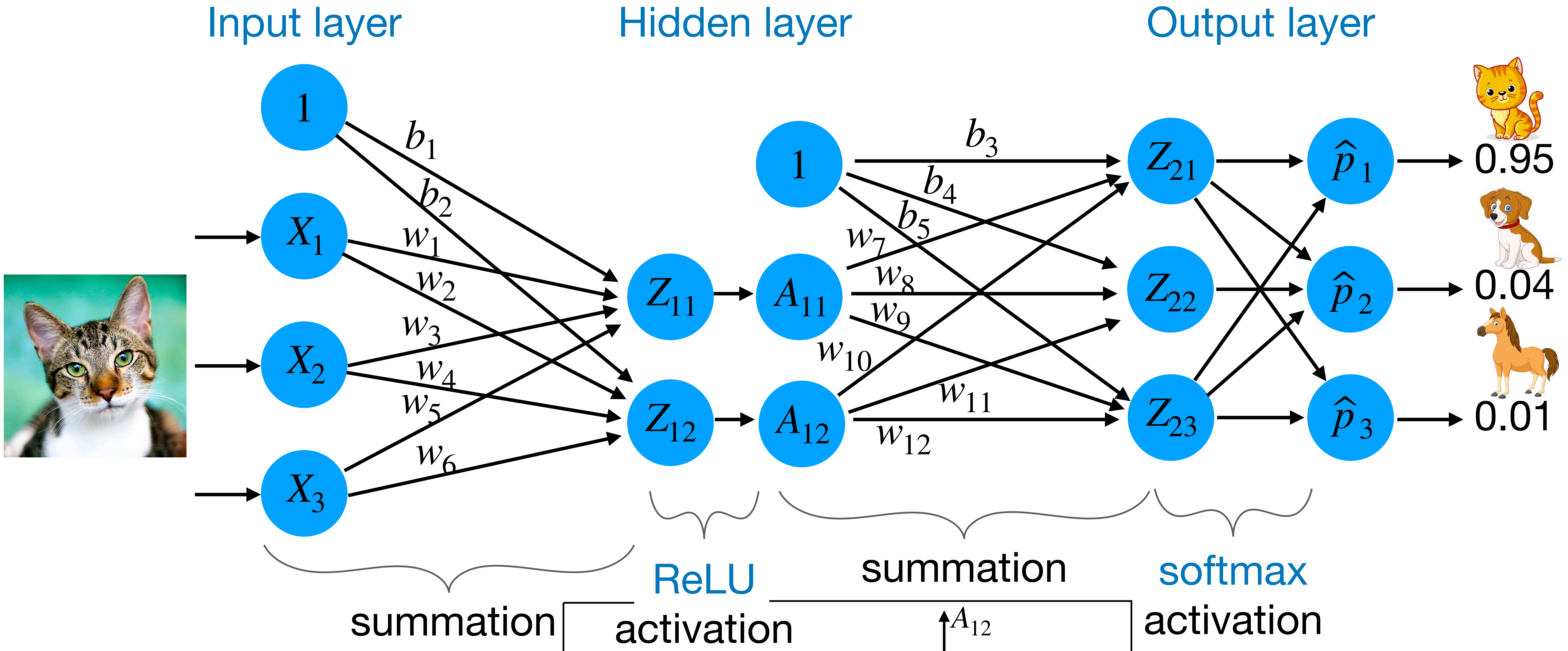

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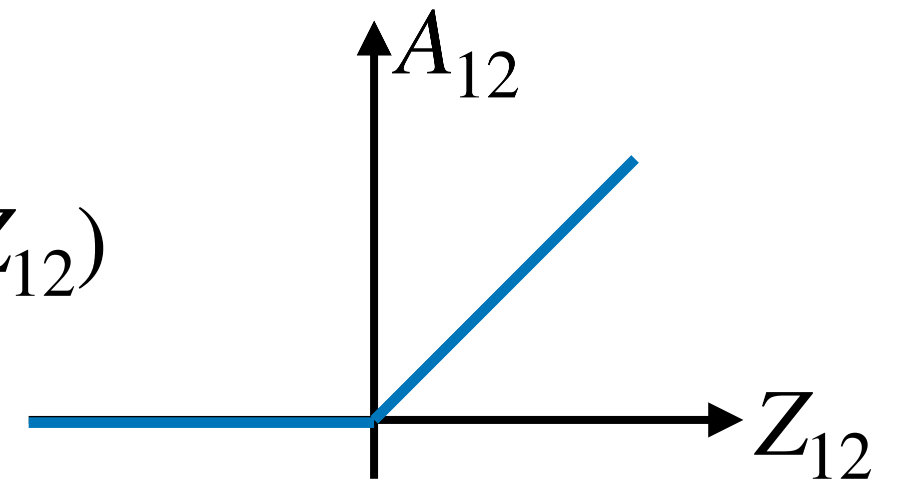
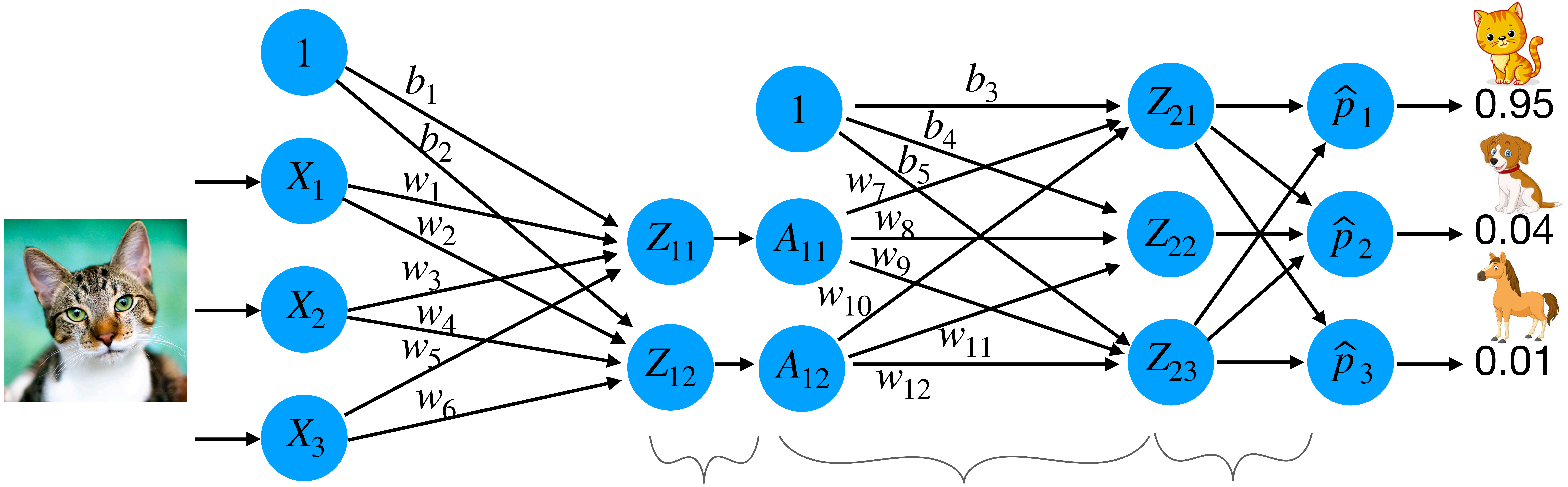
E.g., $A_{12} = \max(0, Z_{12})$



One-hidden-layer neural network

Input layer | Hidden layer | Output layer

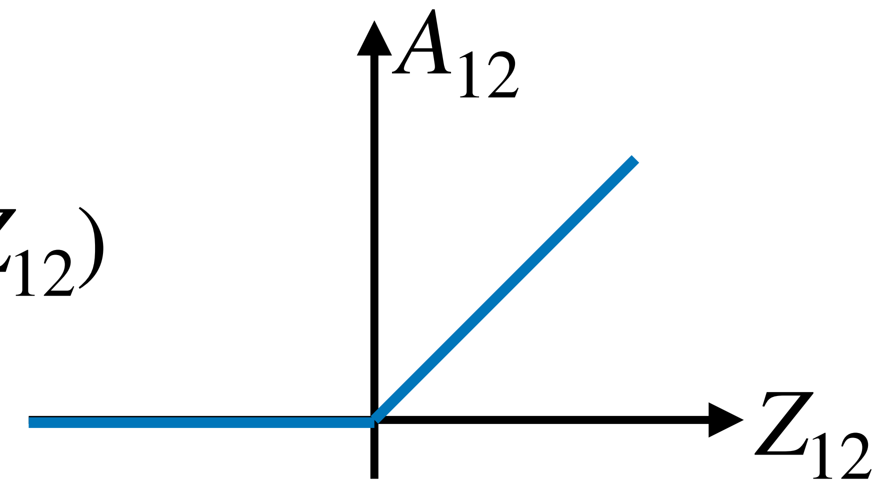


summation

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

softmax activation

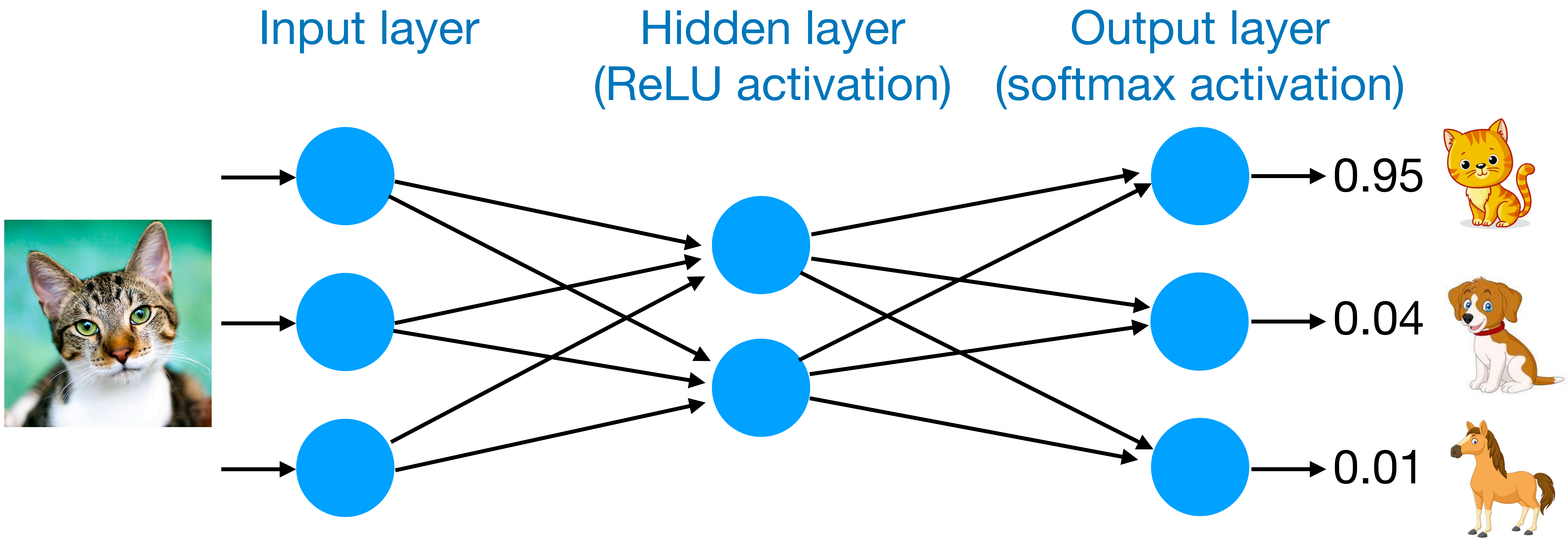
Terminology:

b_j: biases

w_j: weights

One-hidden-layer neural network

Concise representation



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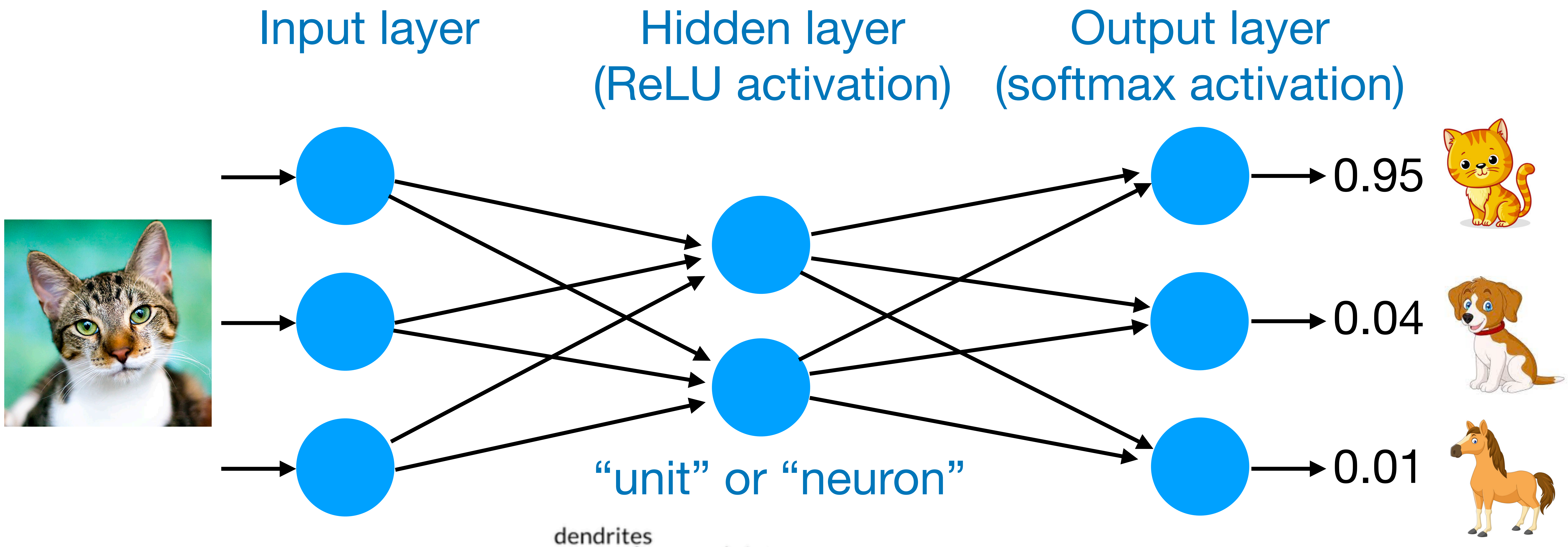

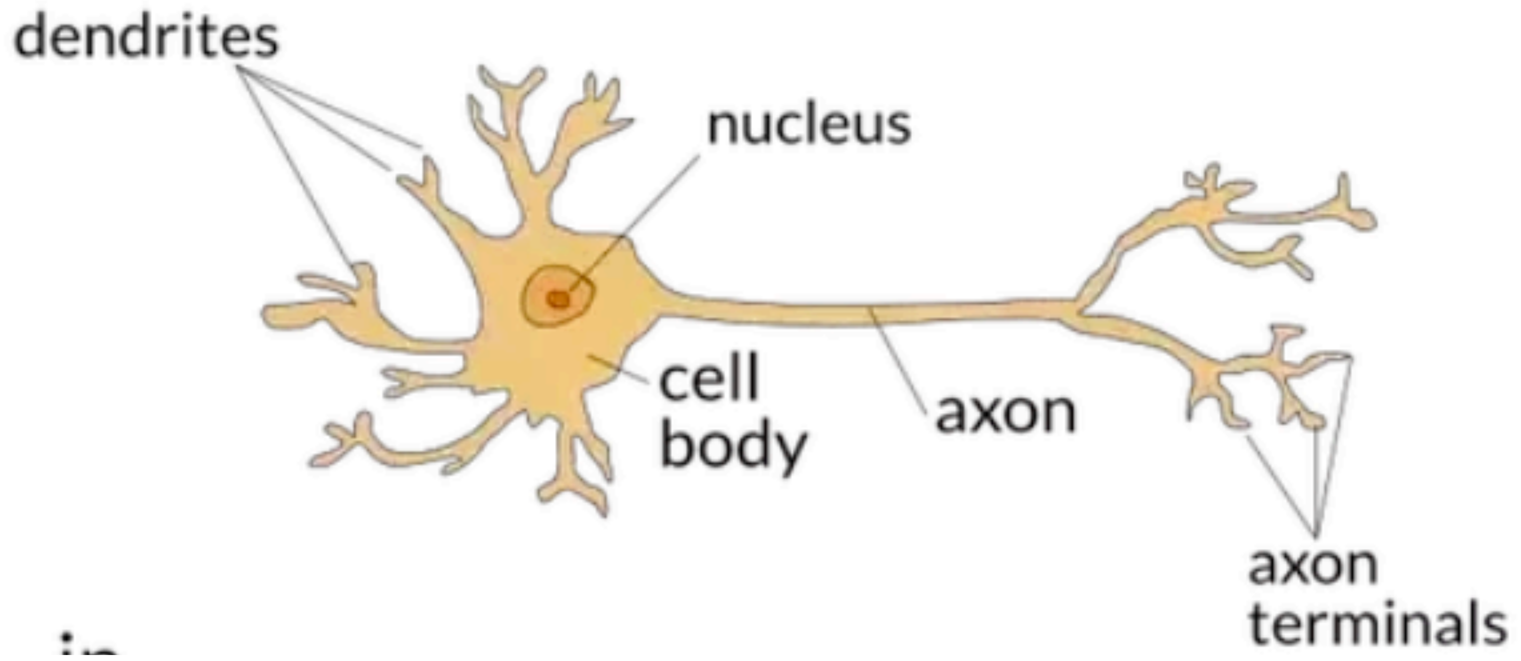

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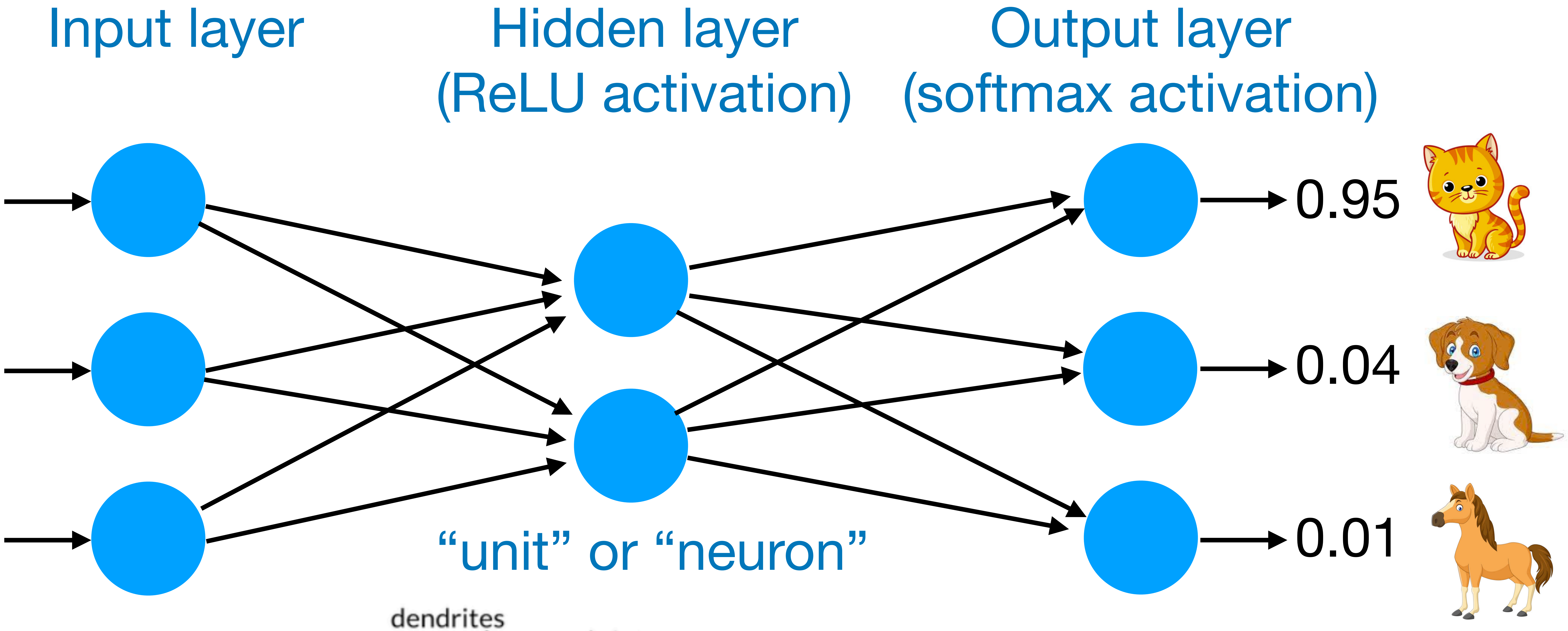
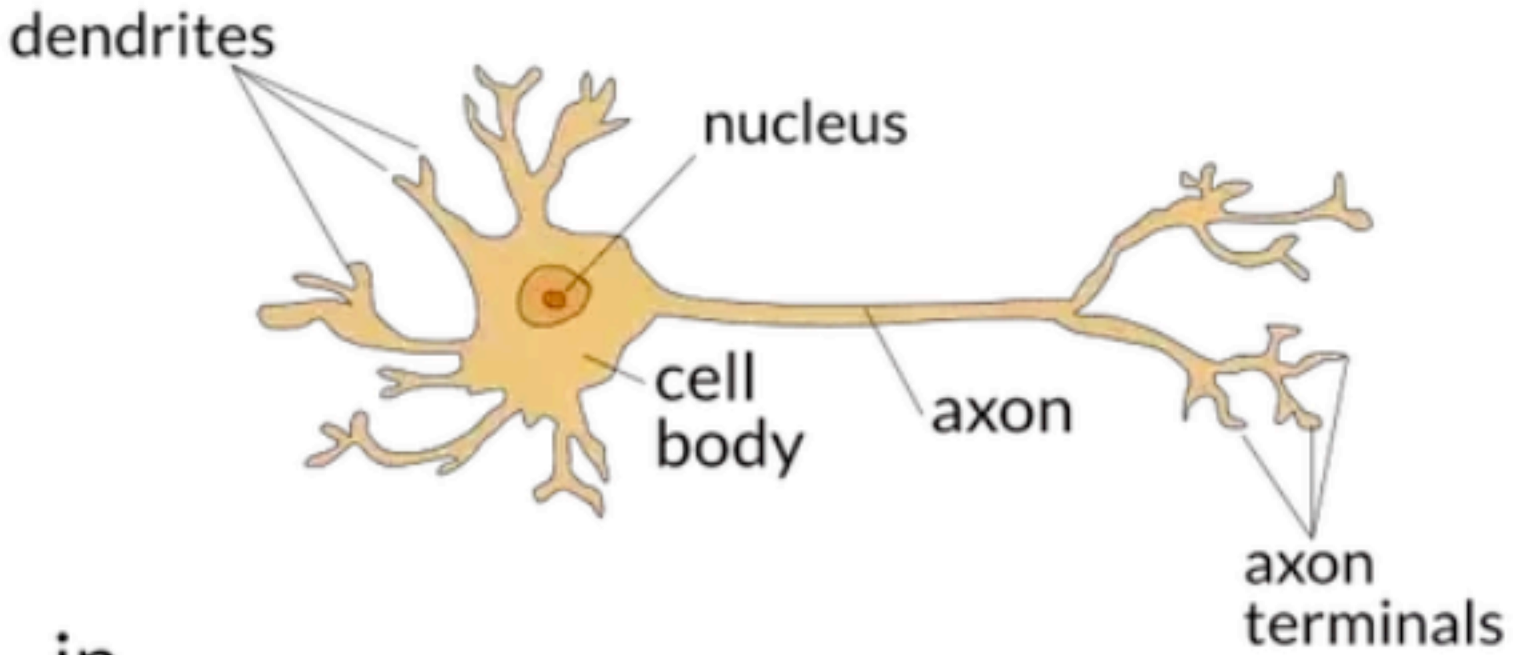


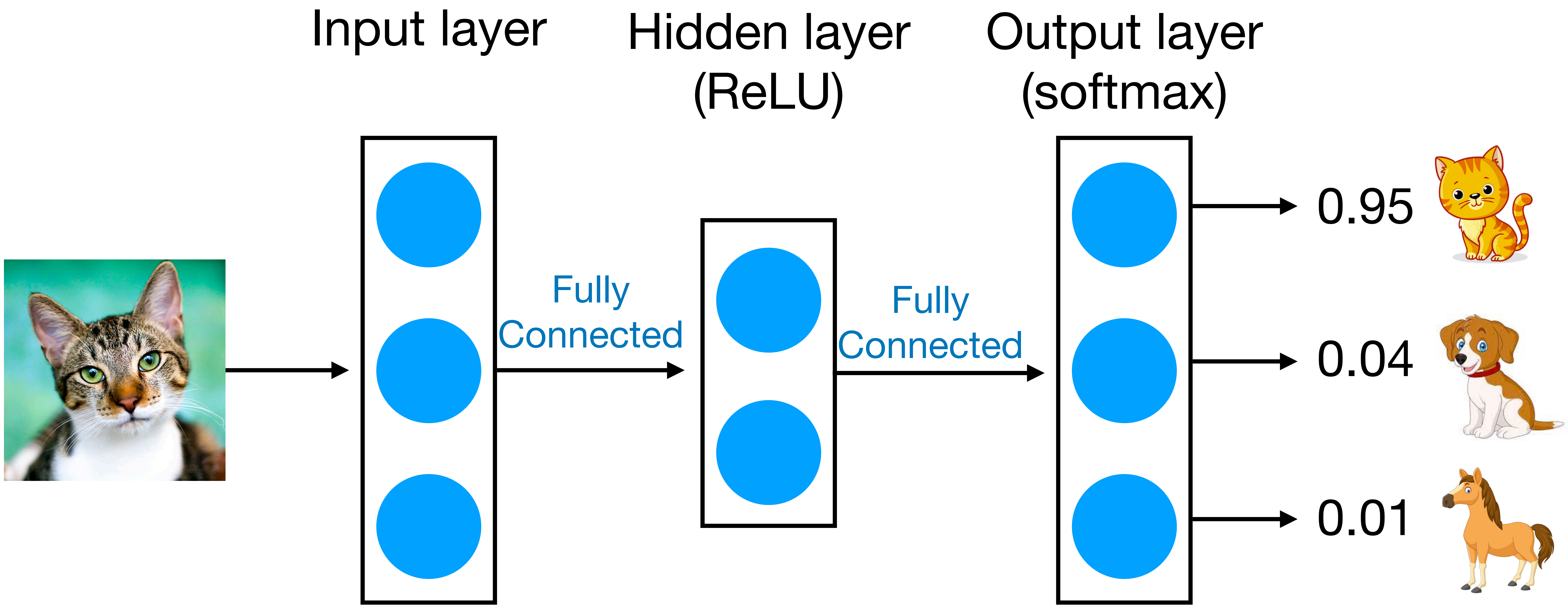


Notes:

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

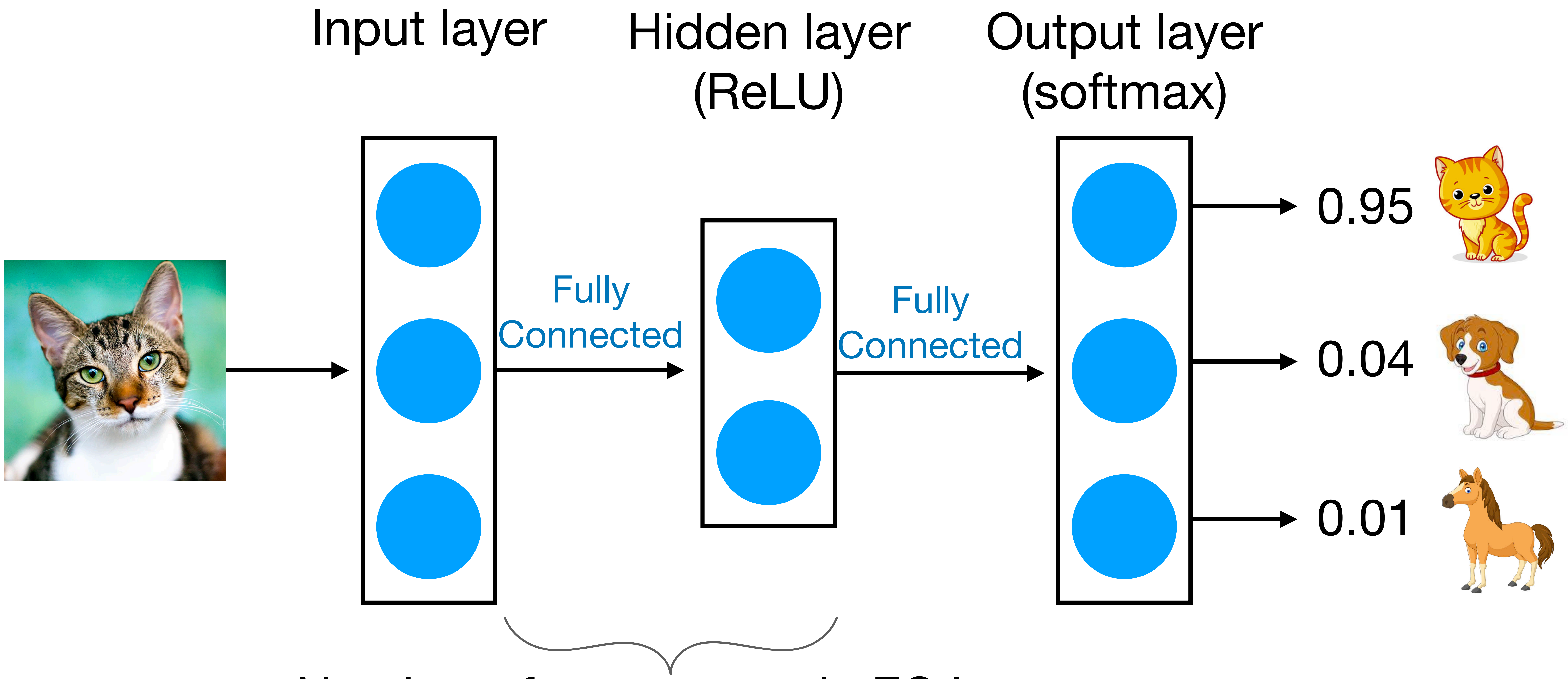
One-hidden-layer neural network

Even more concise representation



One-hidden-layer neural network

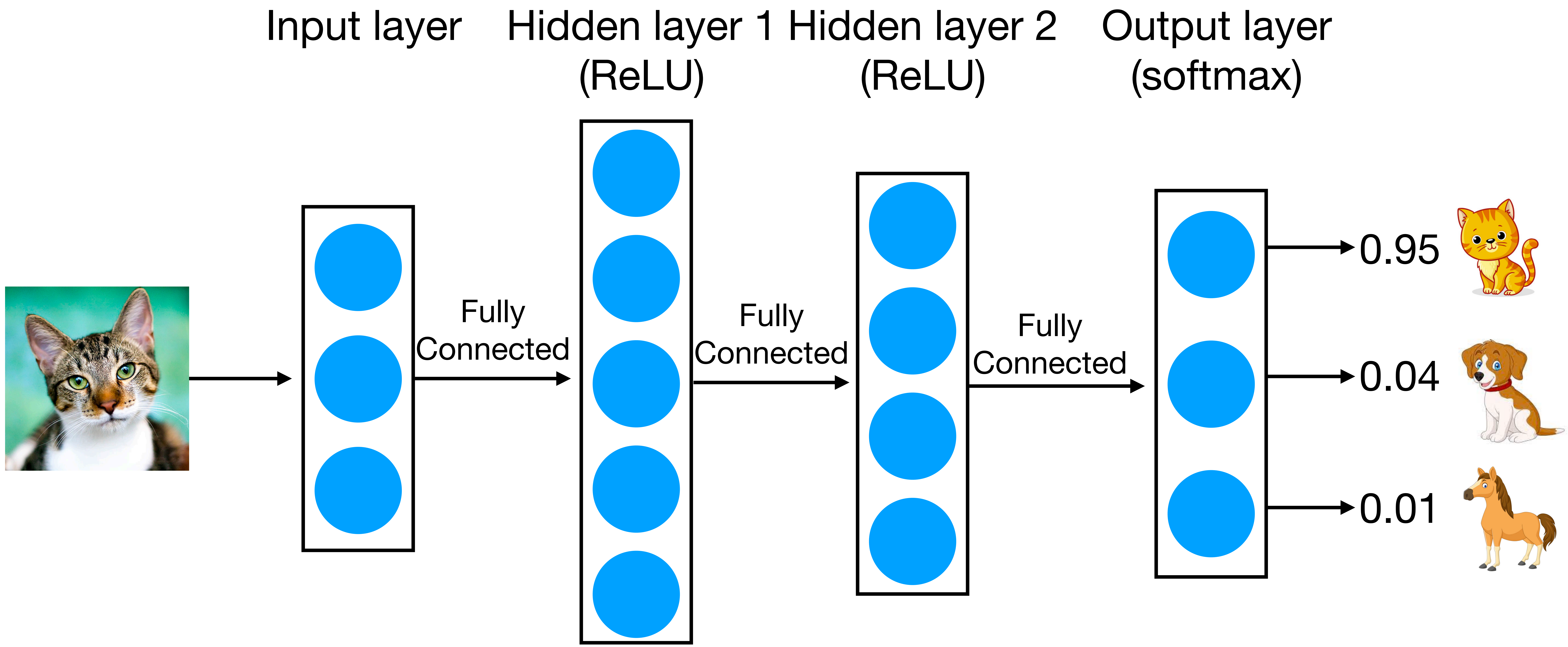
Even more concise representation



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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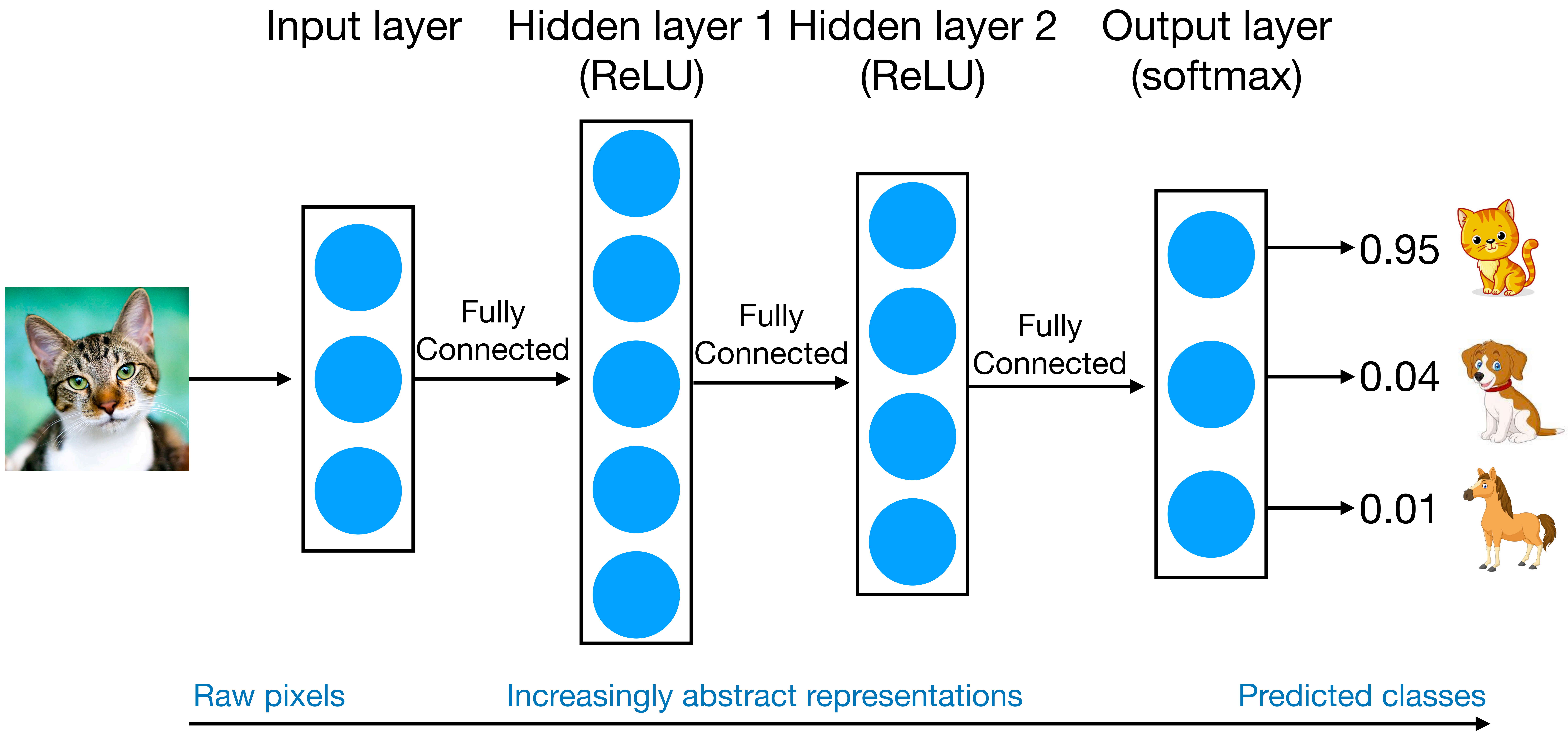

Training deep learning models

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

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

Unfortunately, neural networks have non-convex objective functions, causing issues discussed in the previous lecture.

In practice, deep learning models are trained using stochastic gradient descent, which is a variant of gradient descent.

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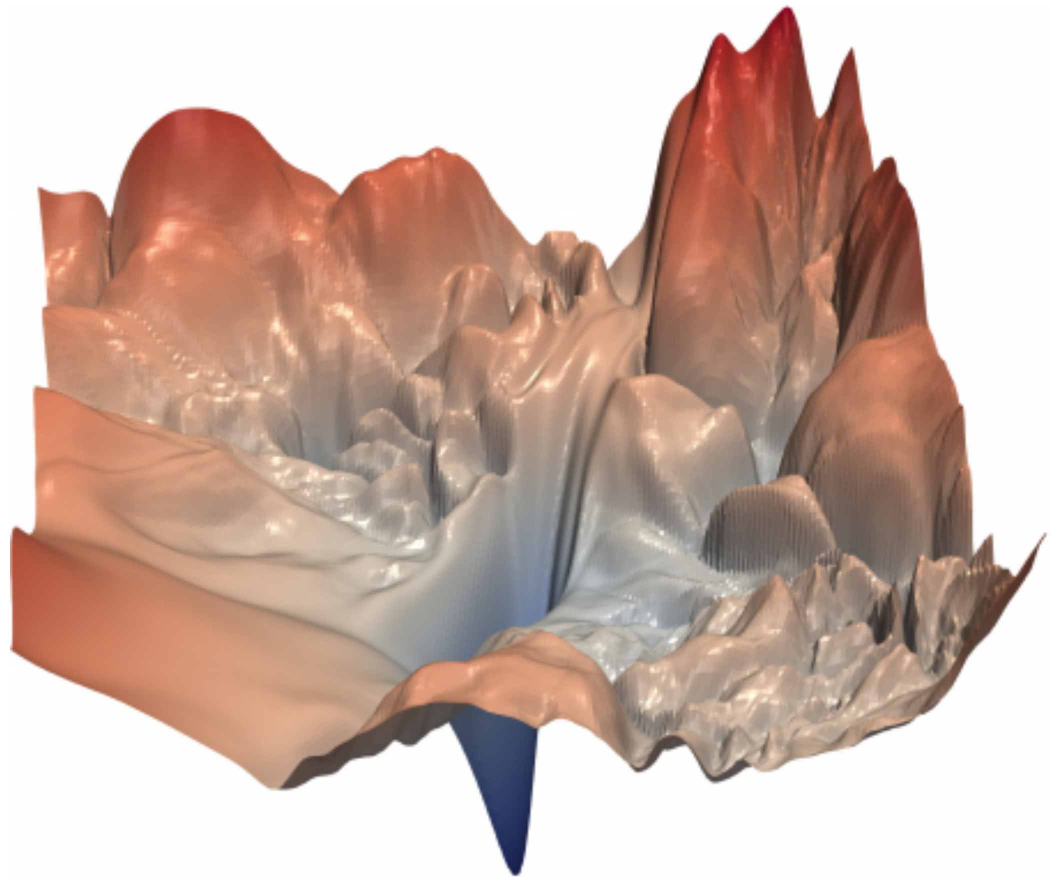

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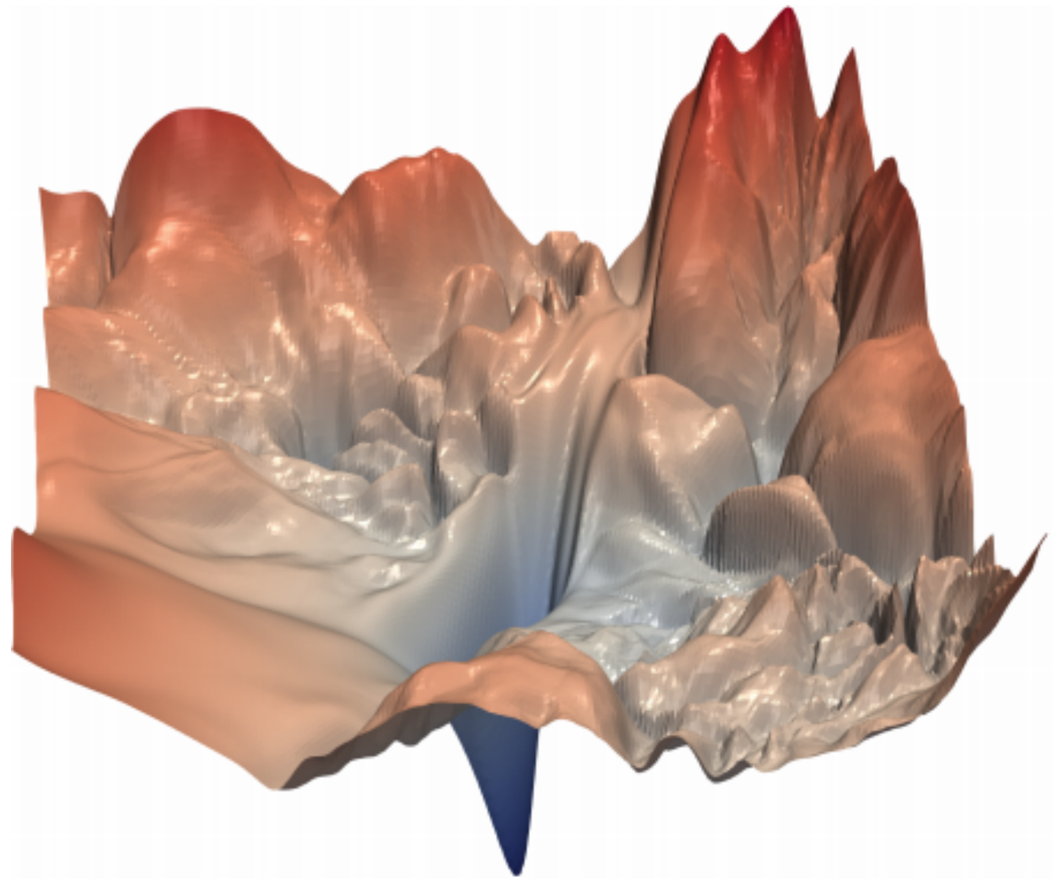

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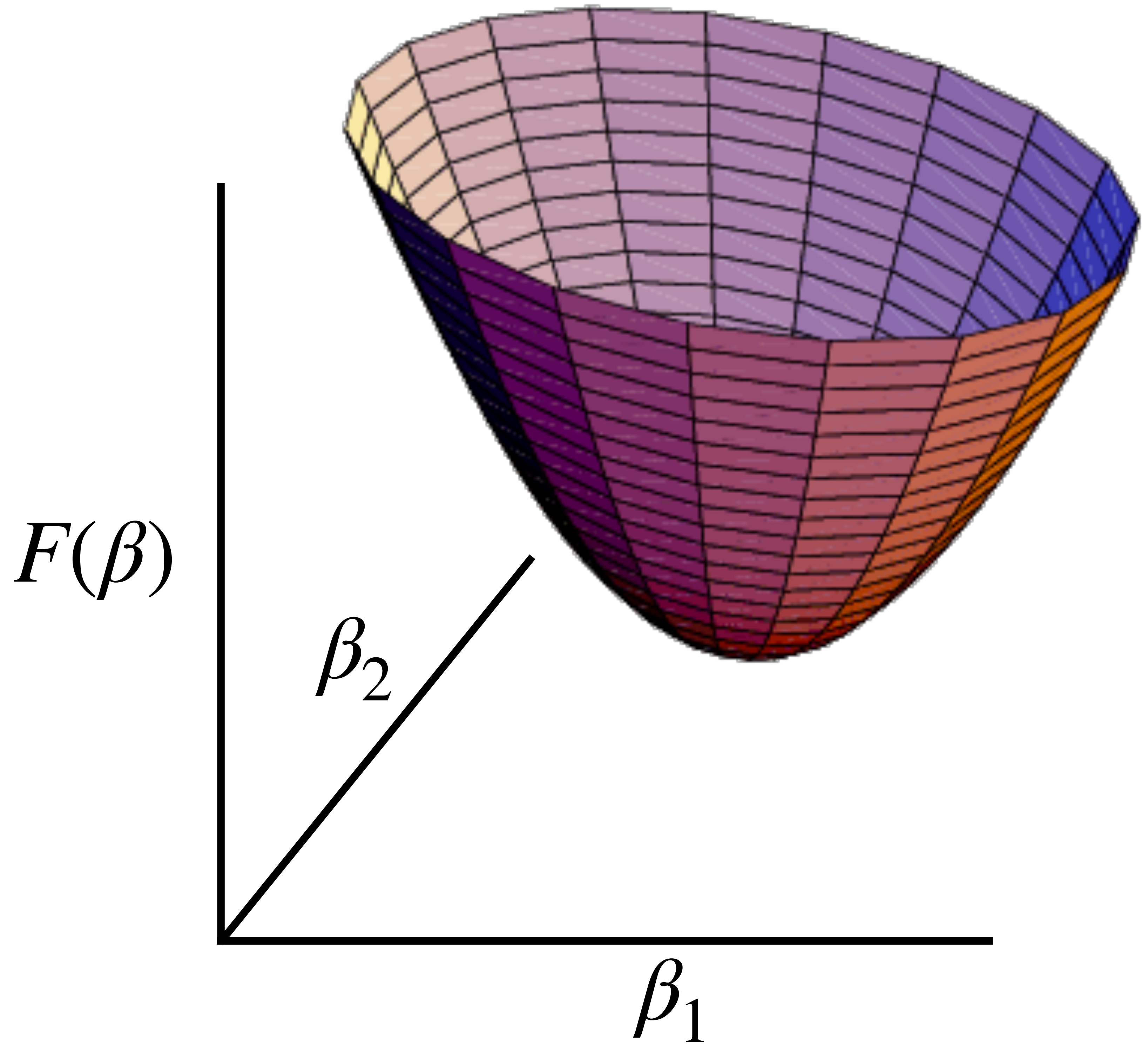

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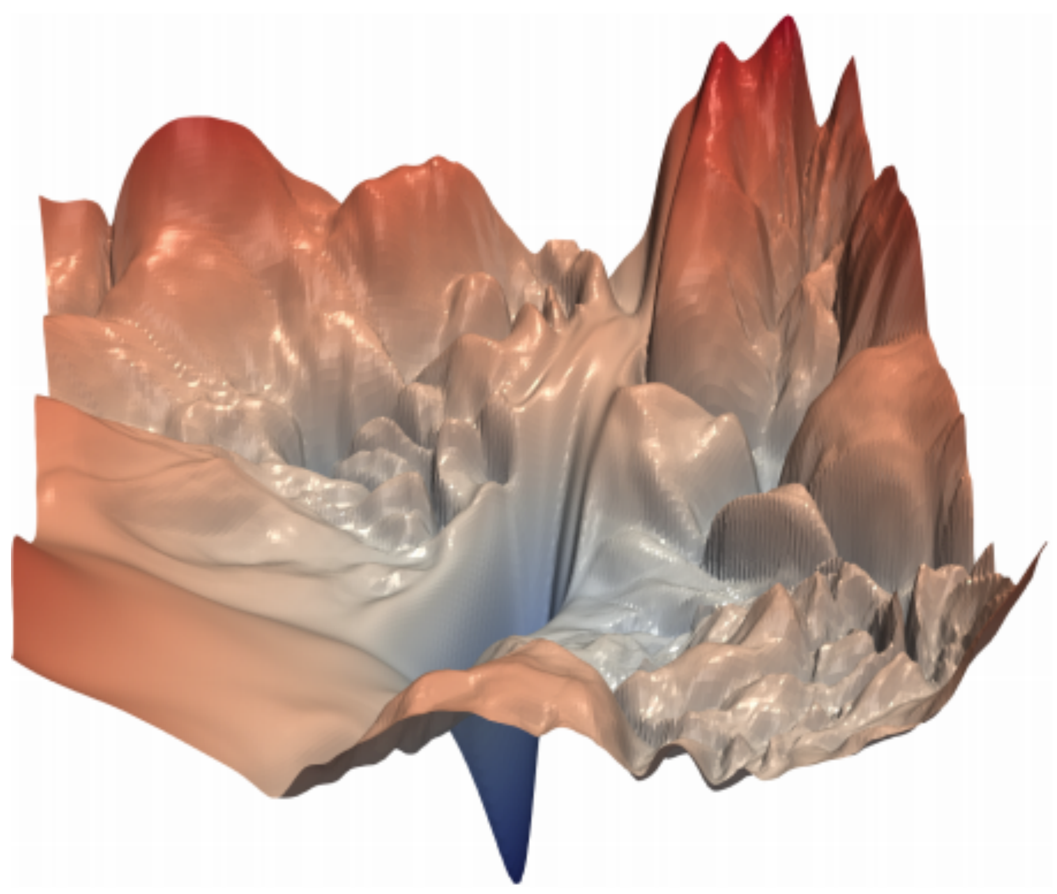

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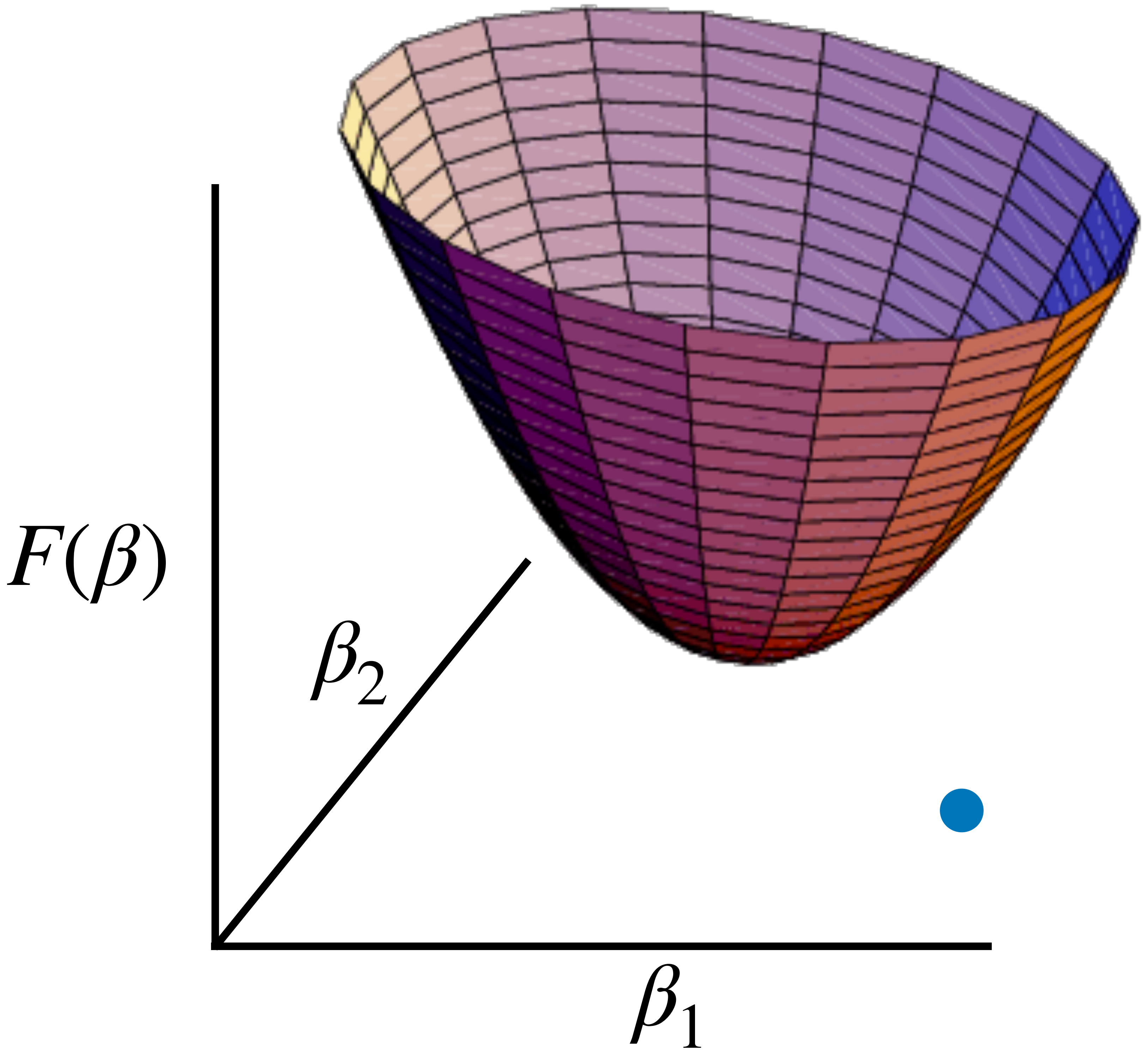

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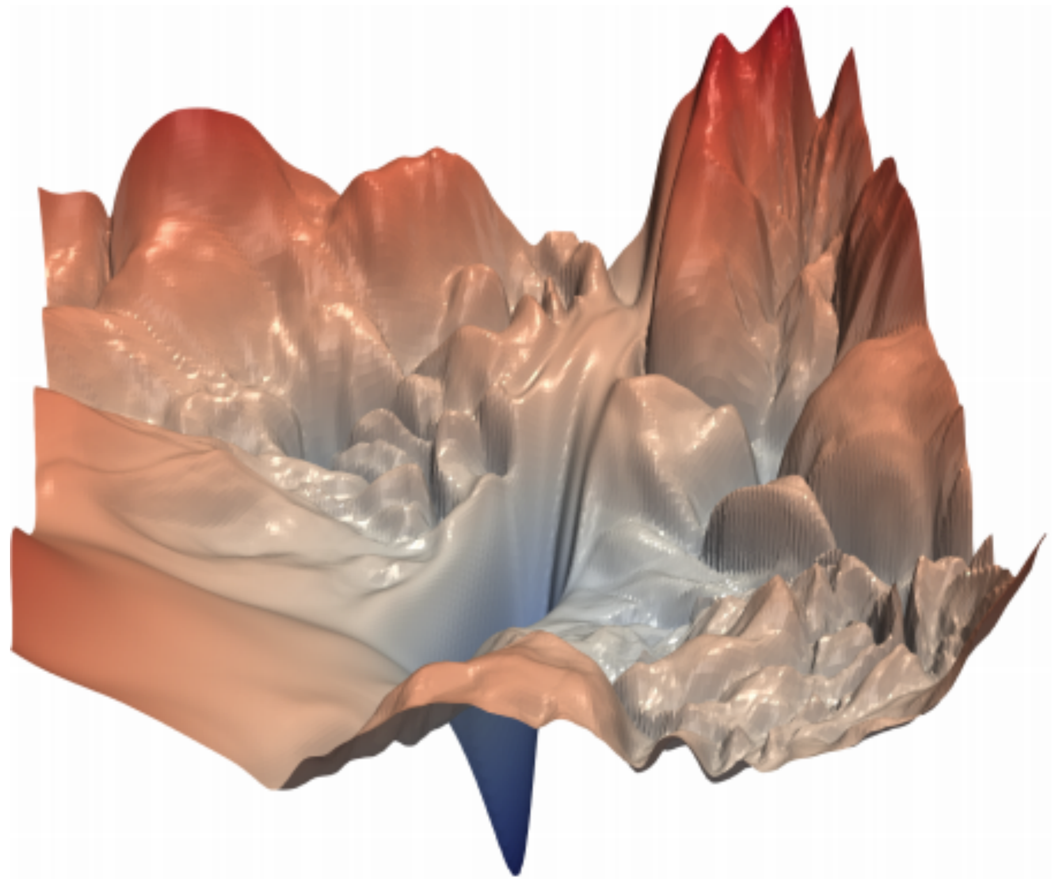

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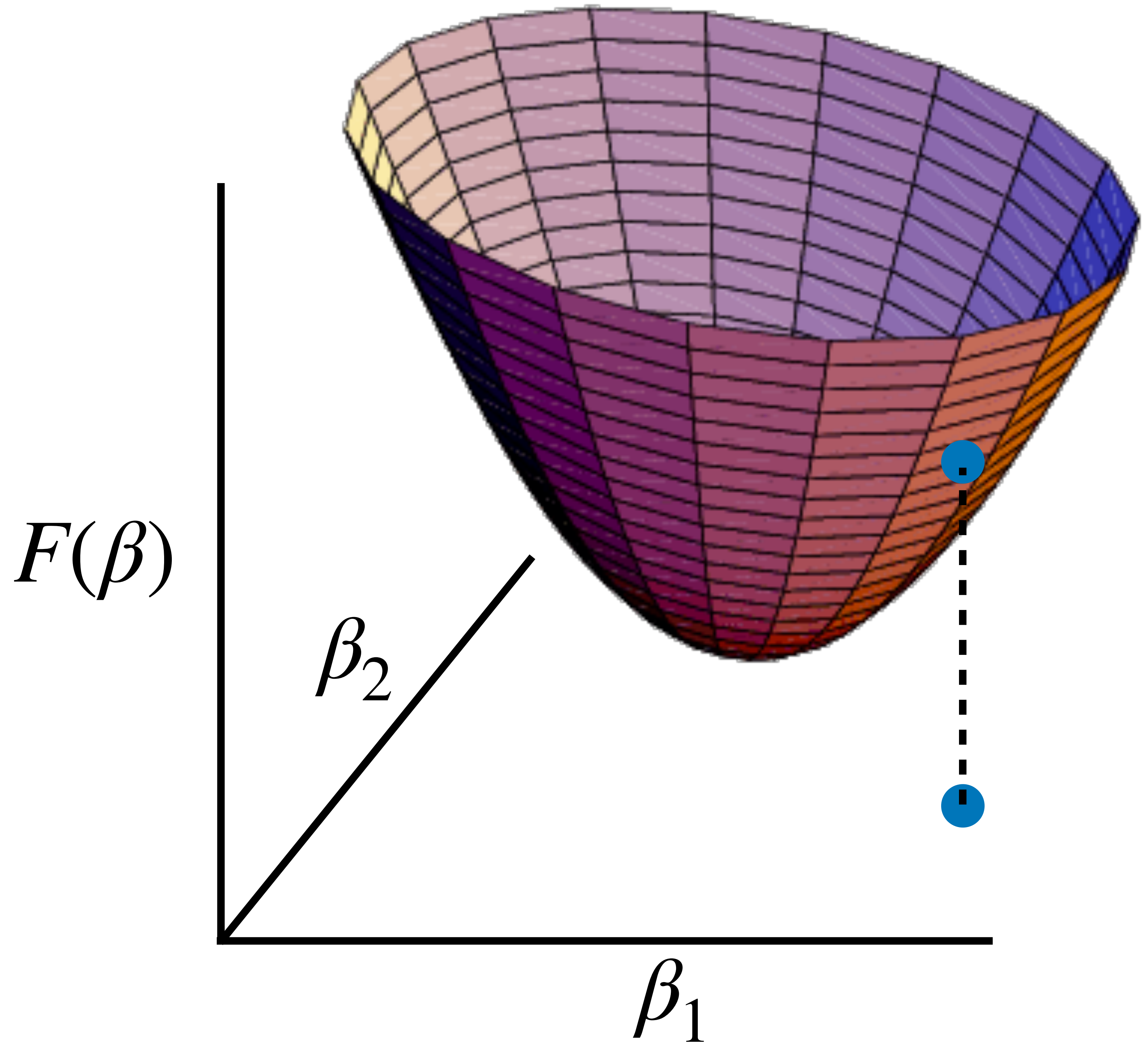

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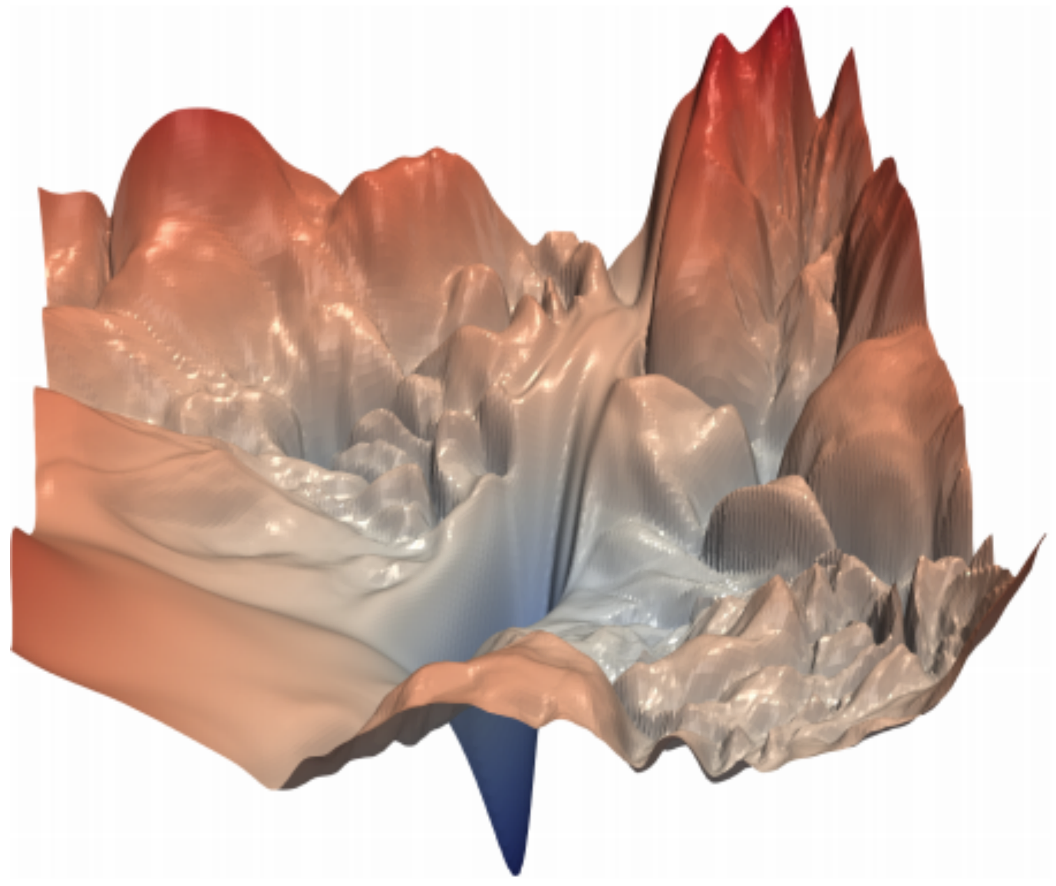

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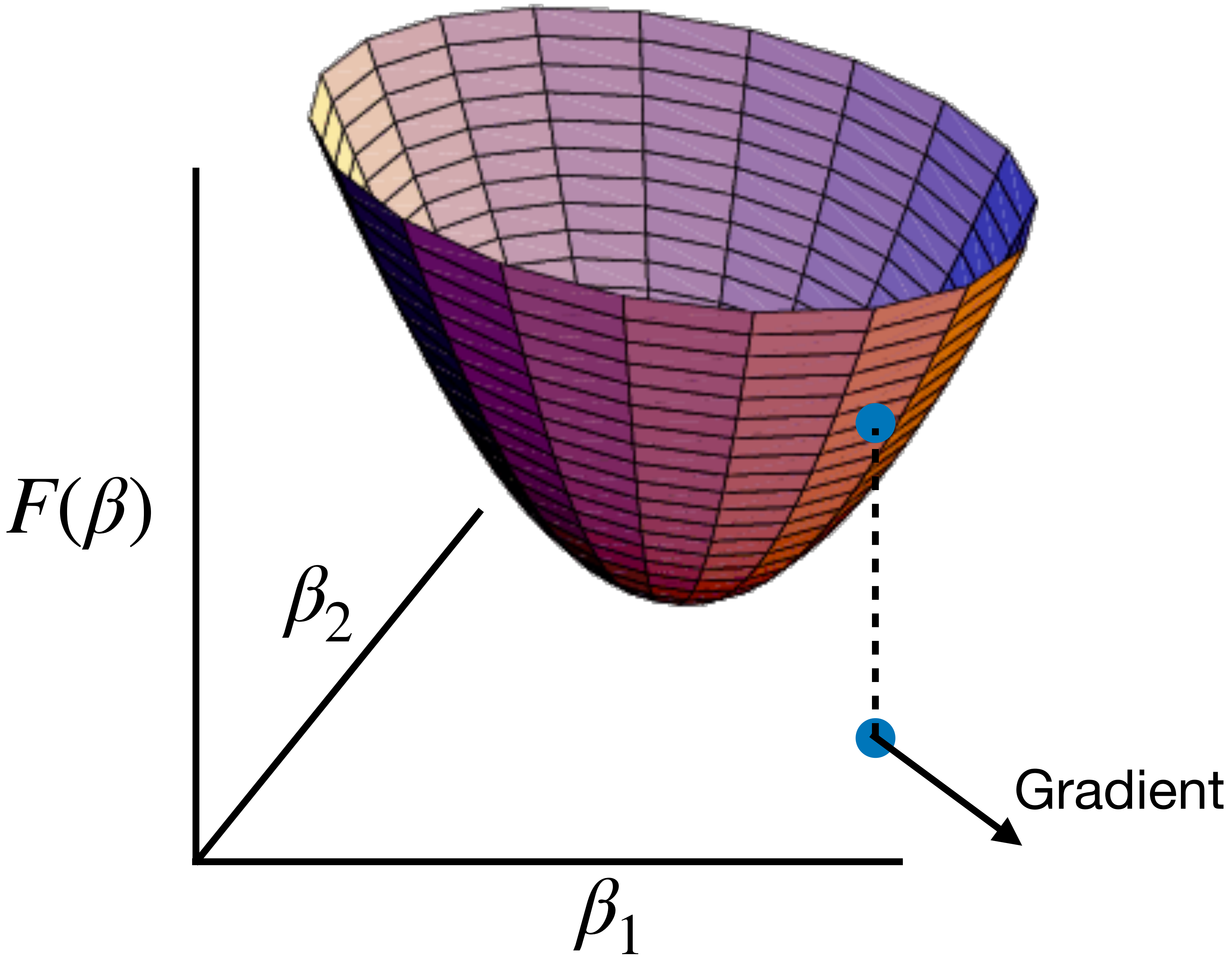

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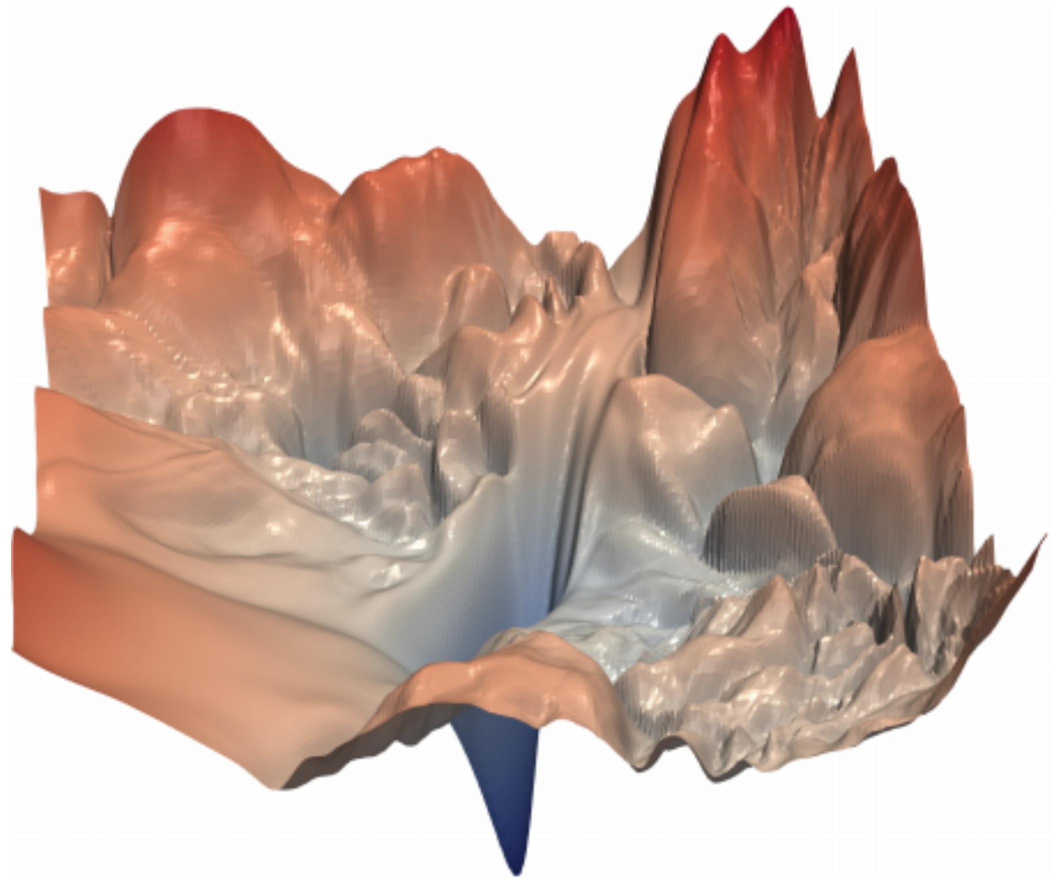

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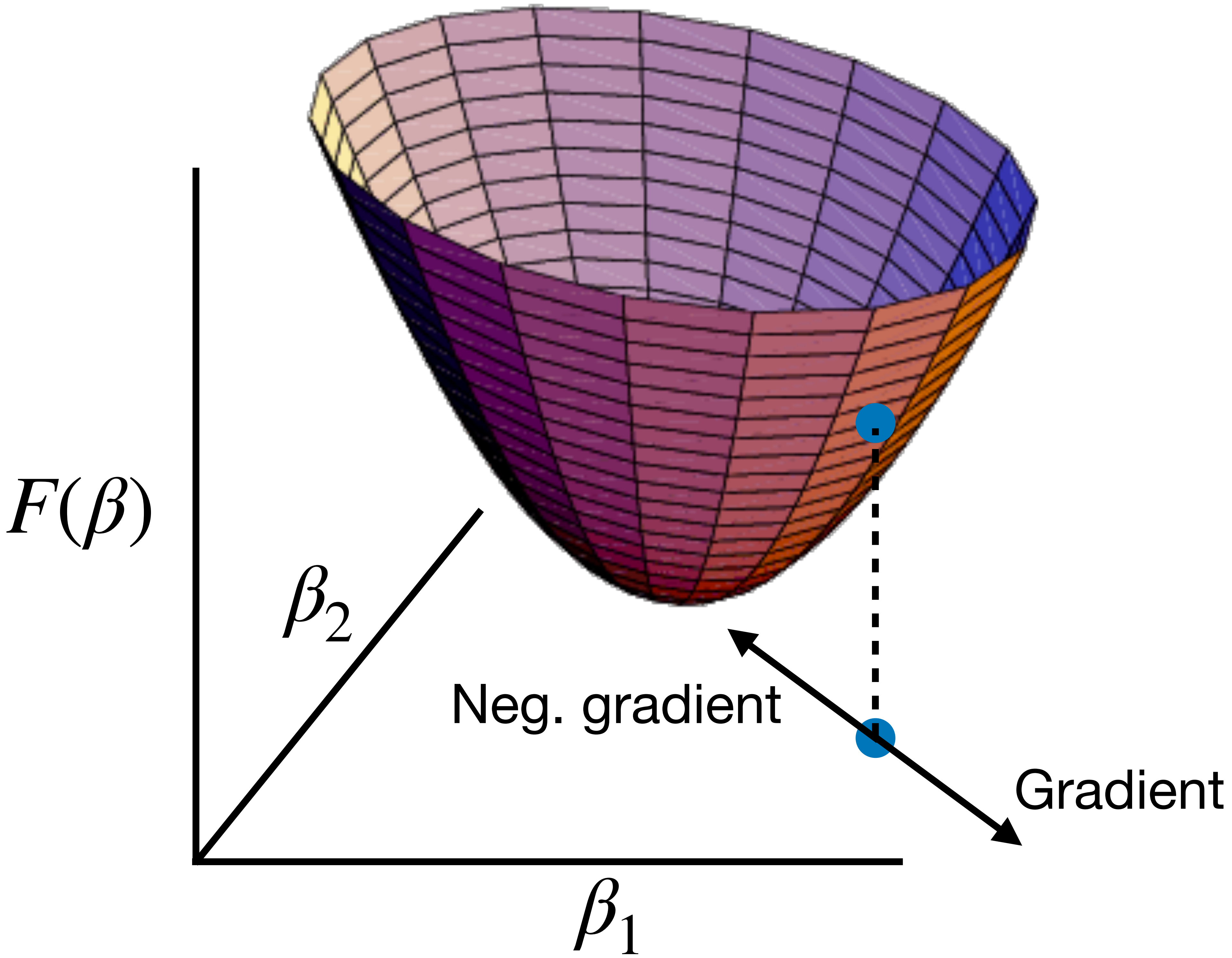

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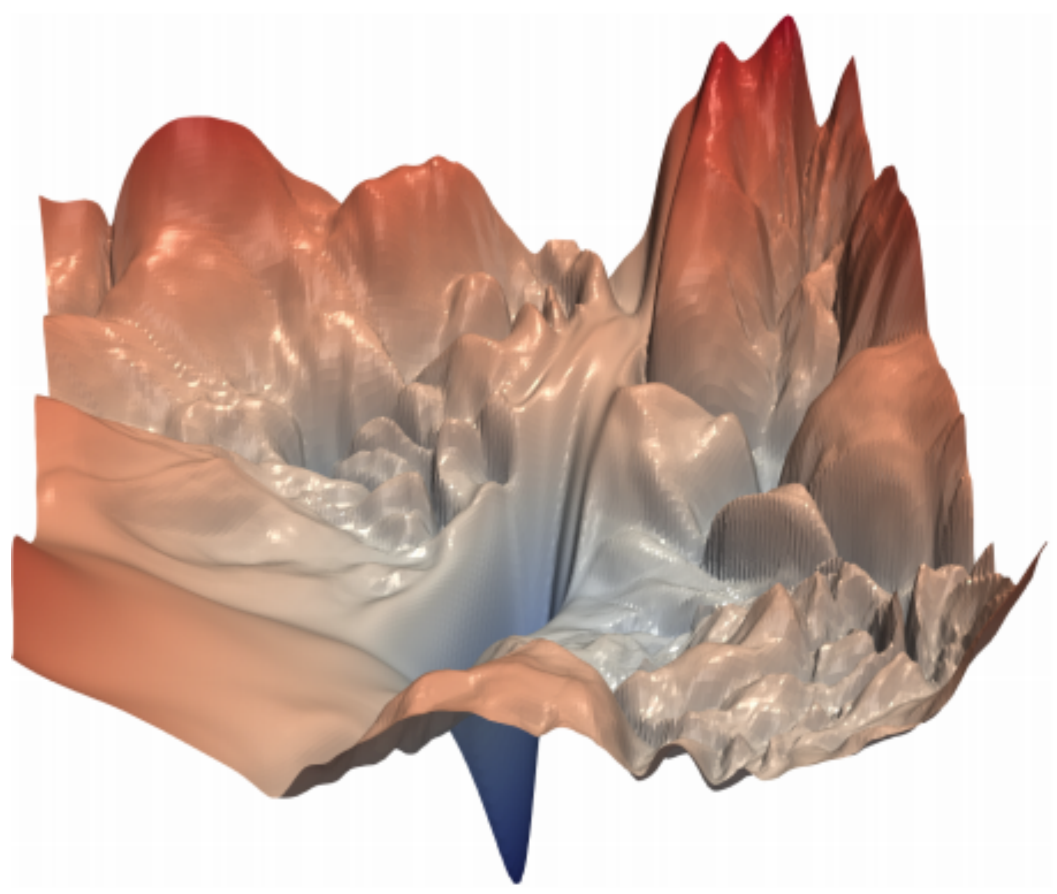

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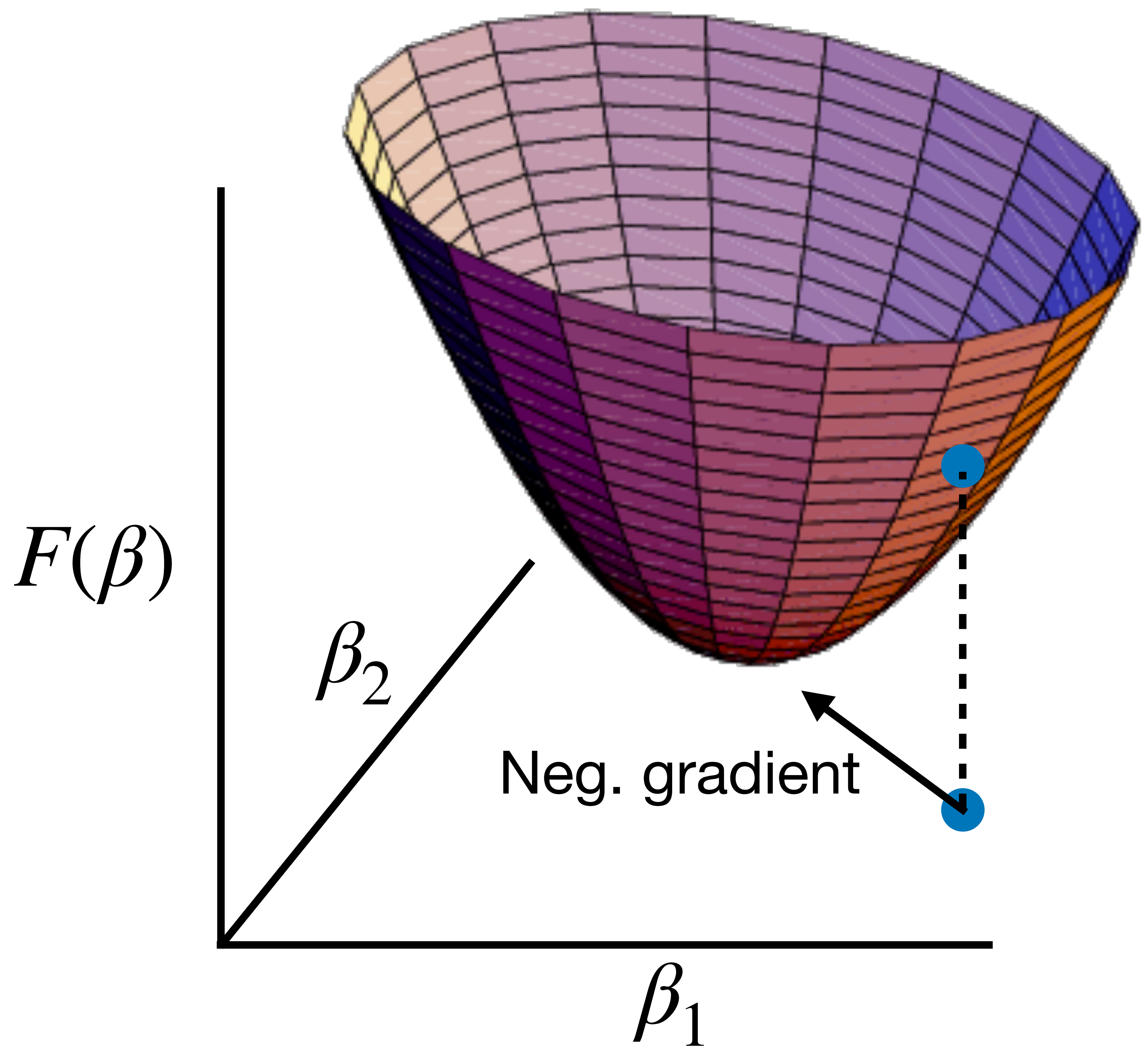

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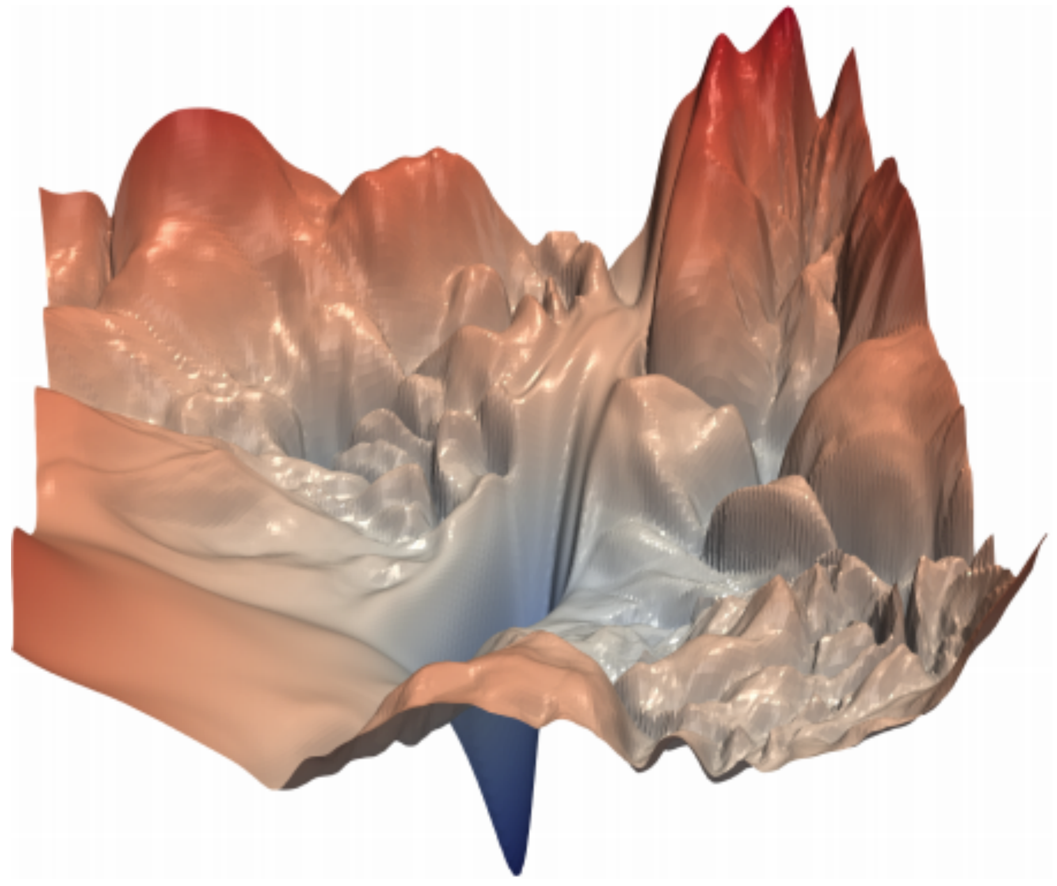

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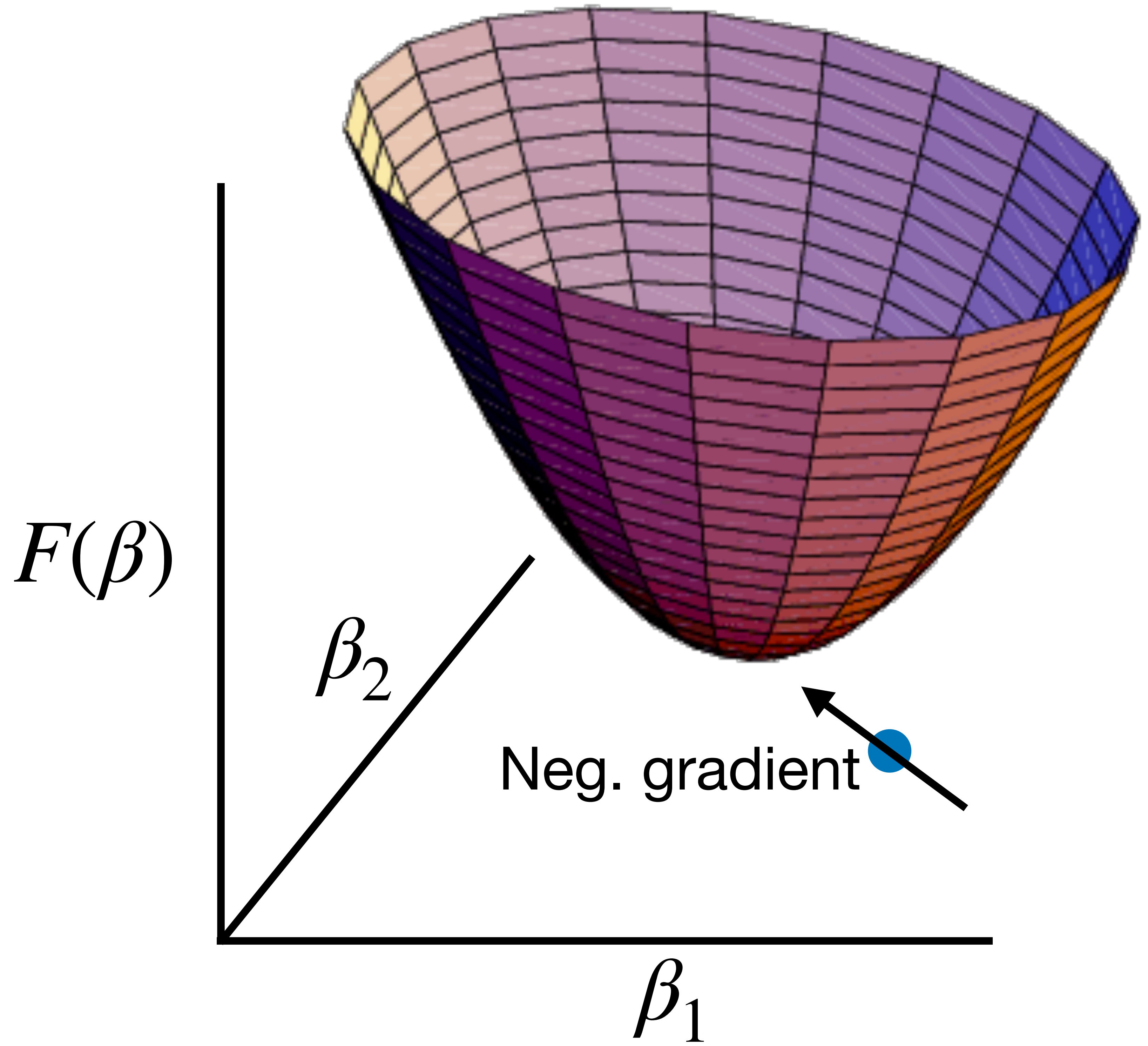

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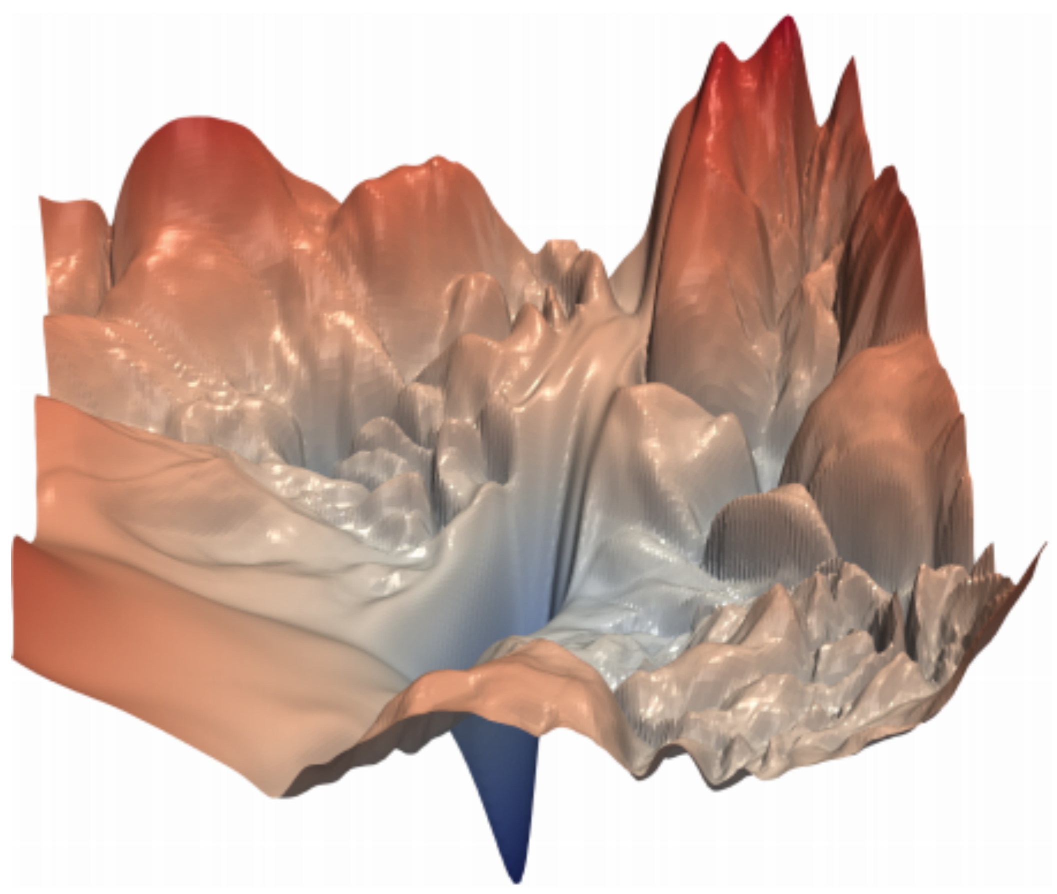

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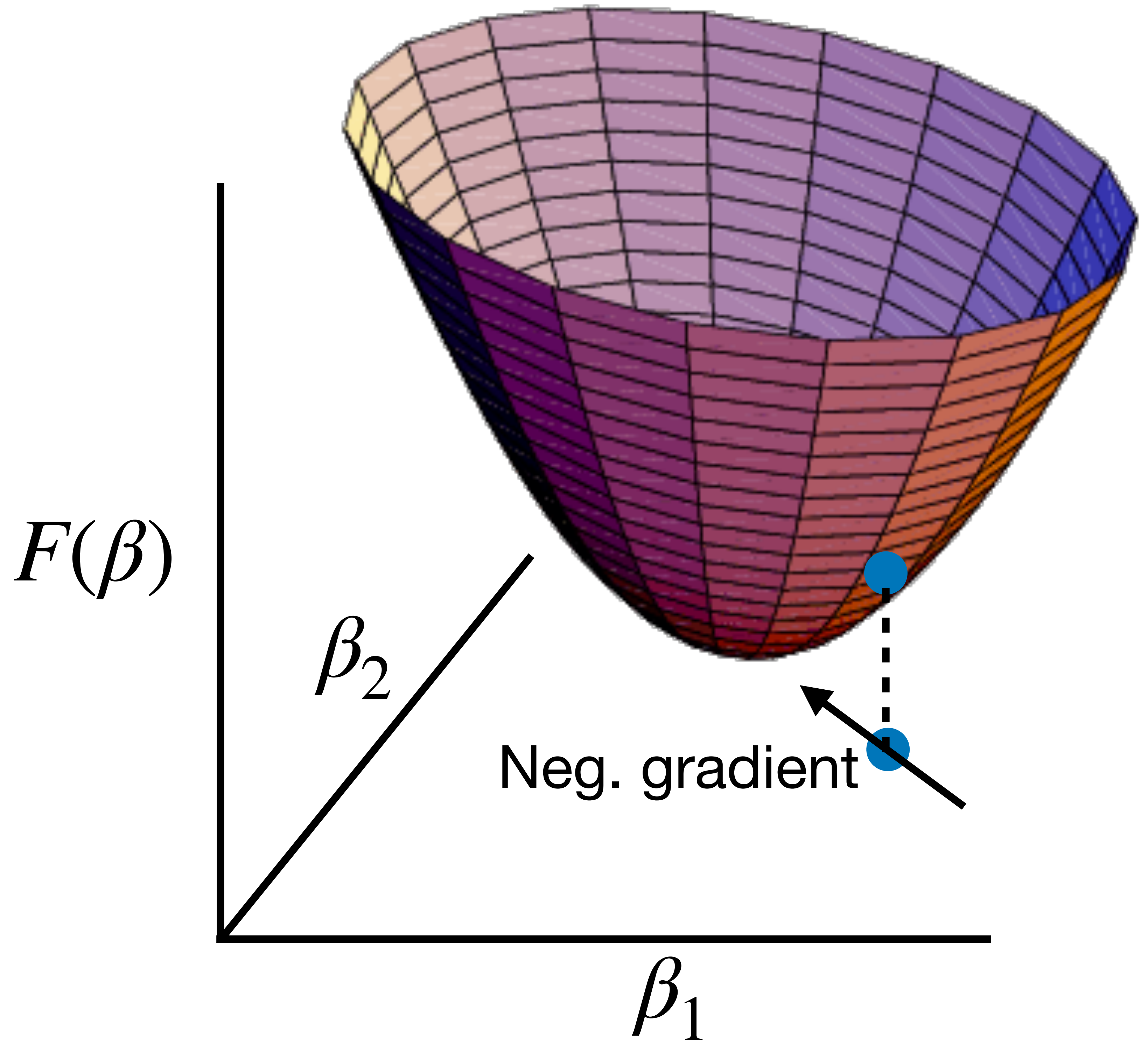

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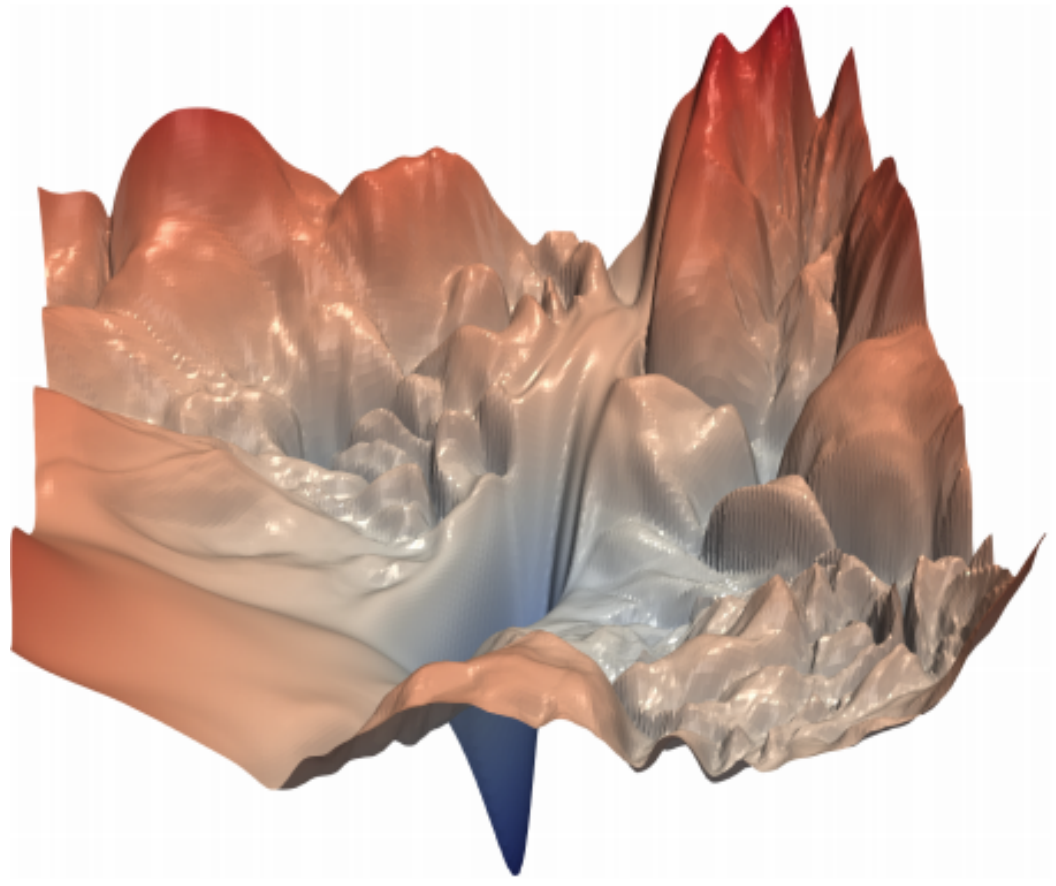

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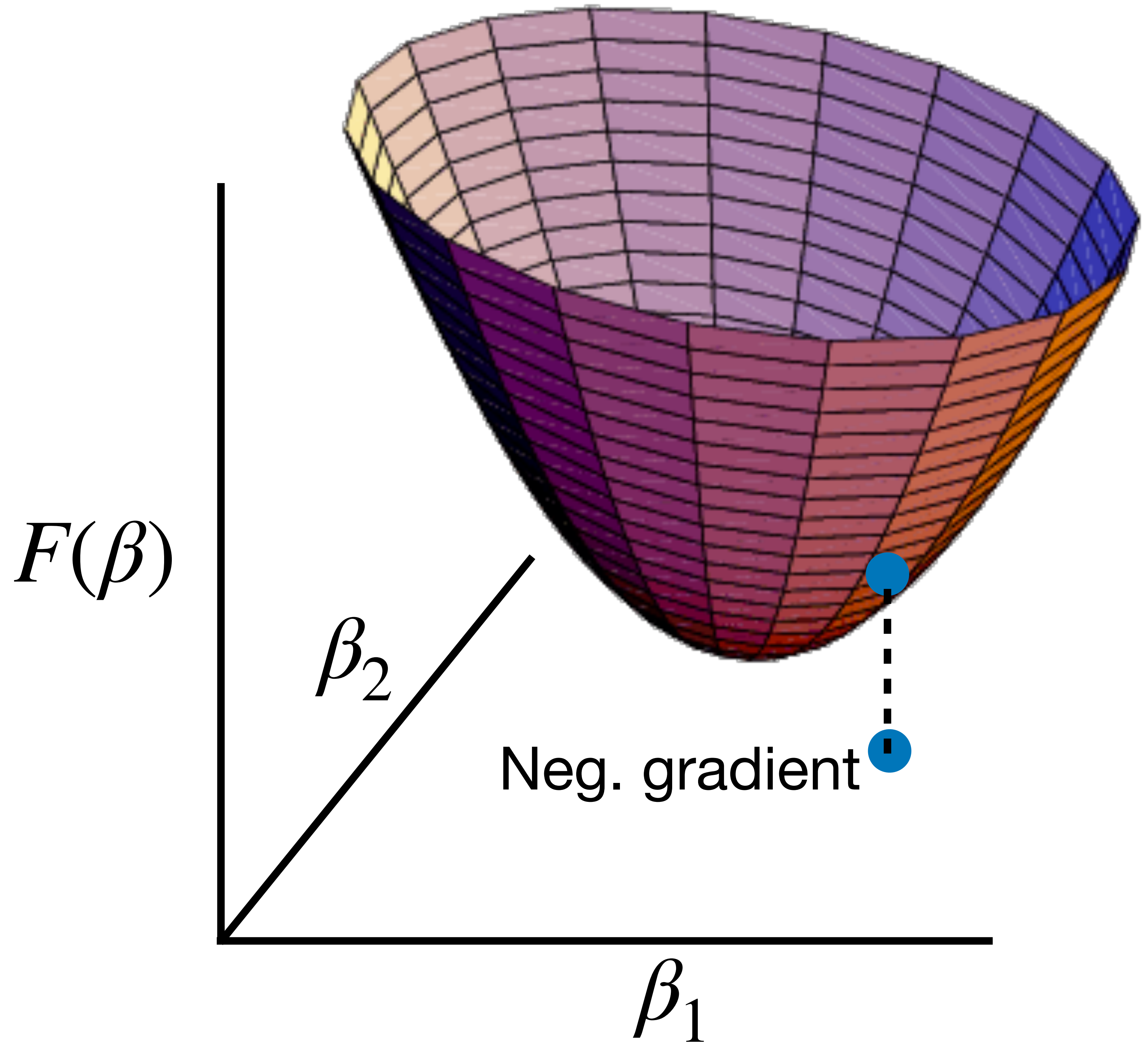

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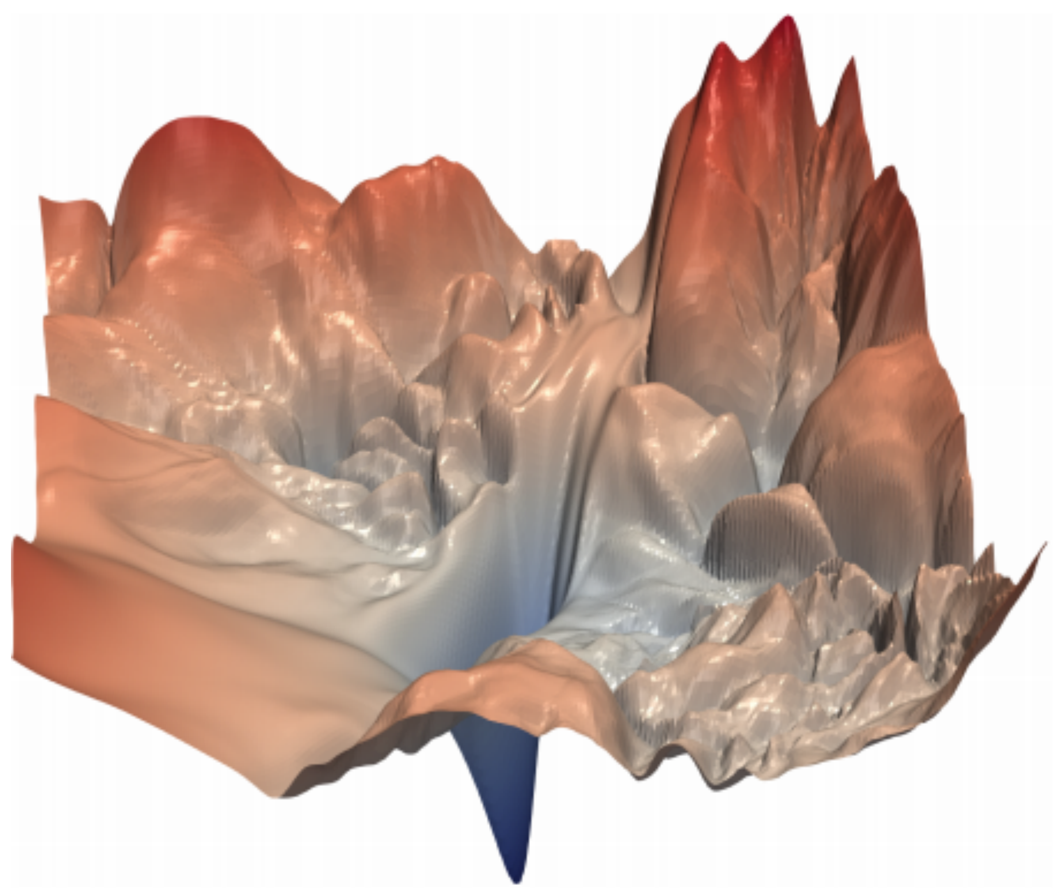

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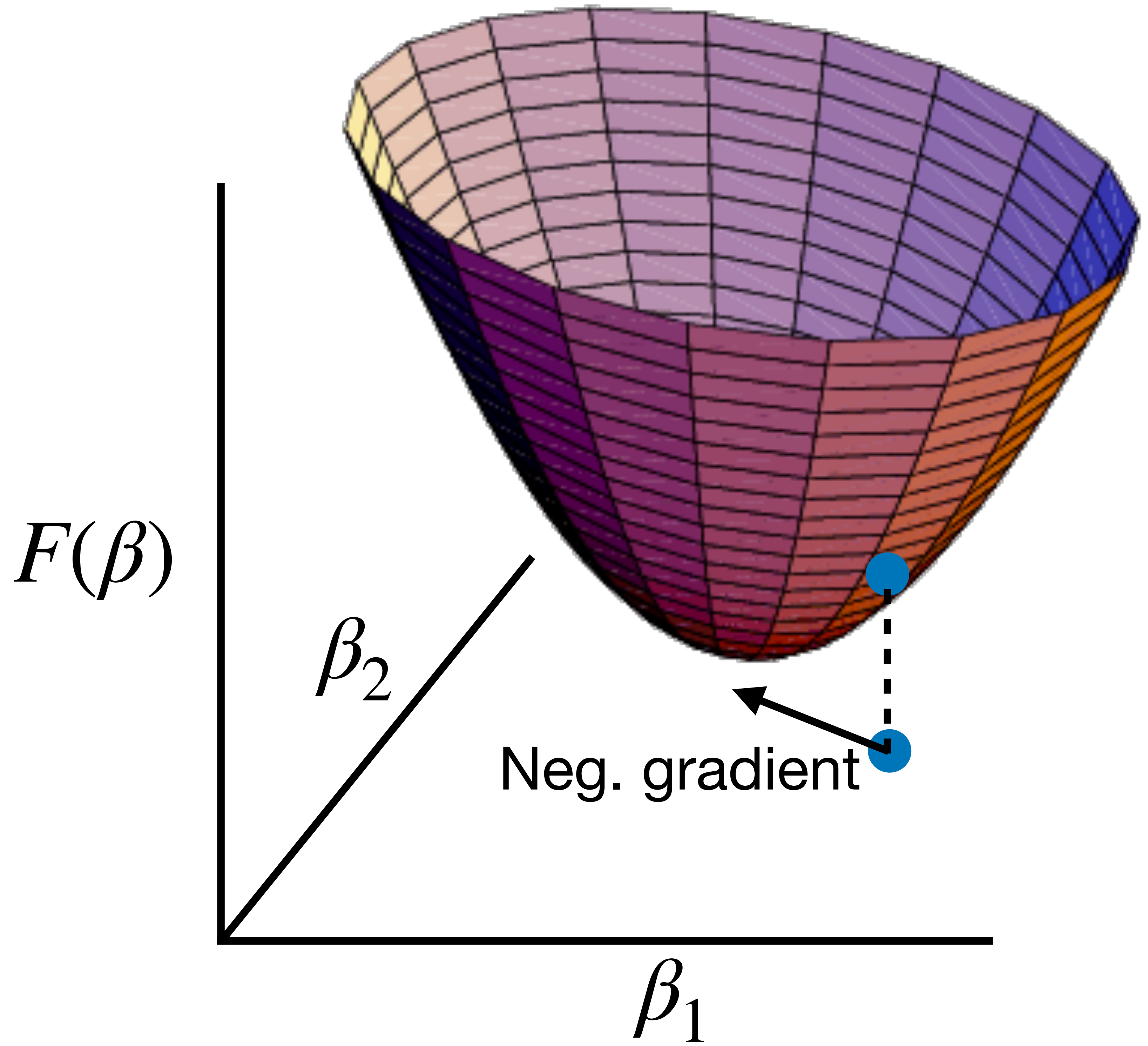

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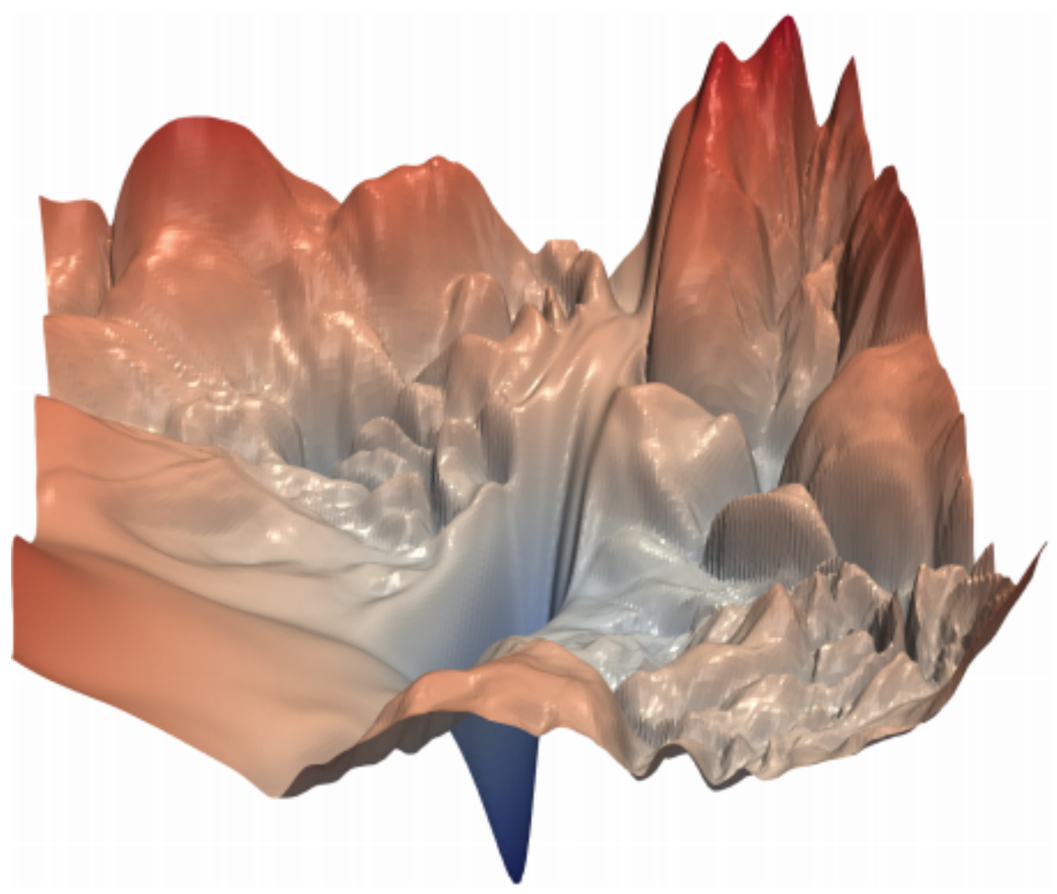

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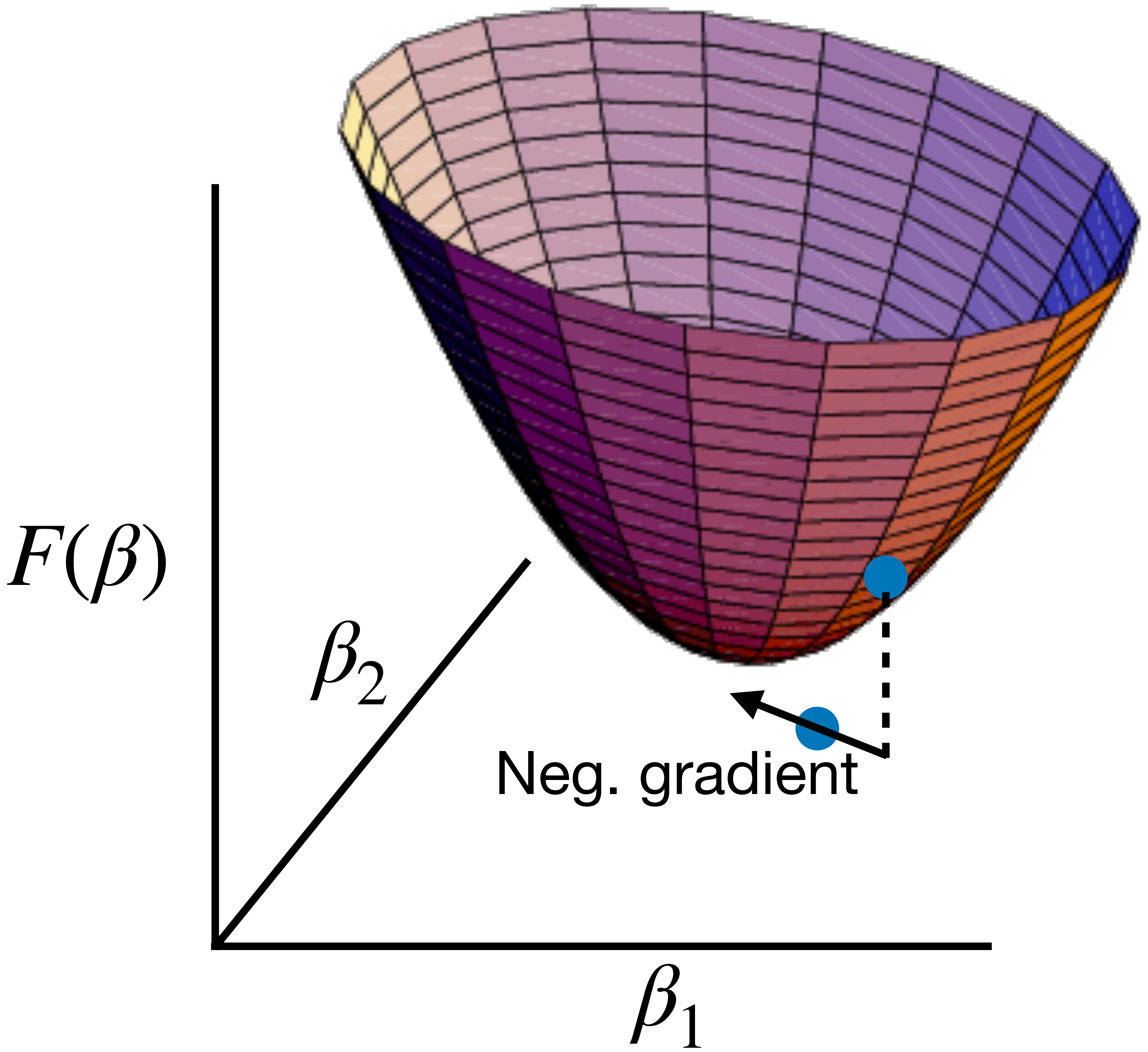

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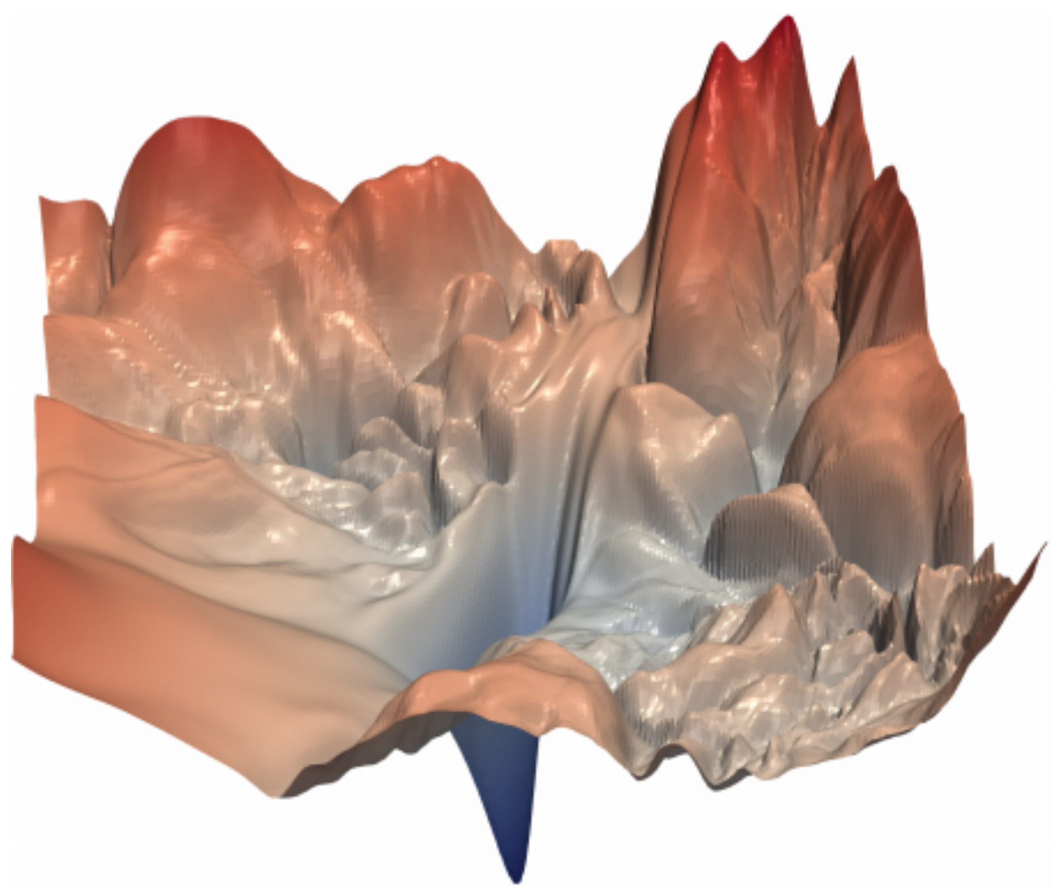

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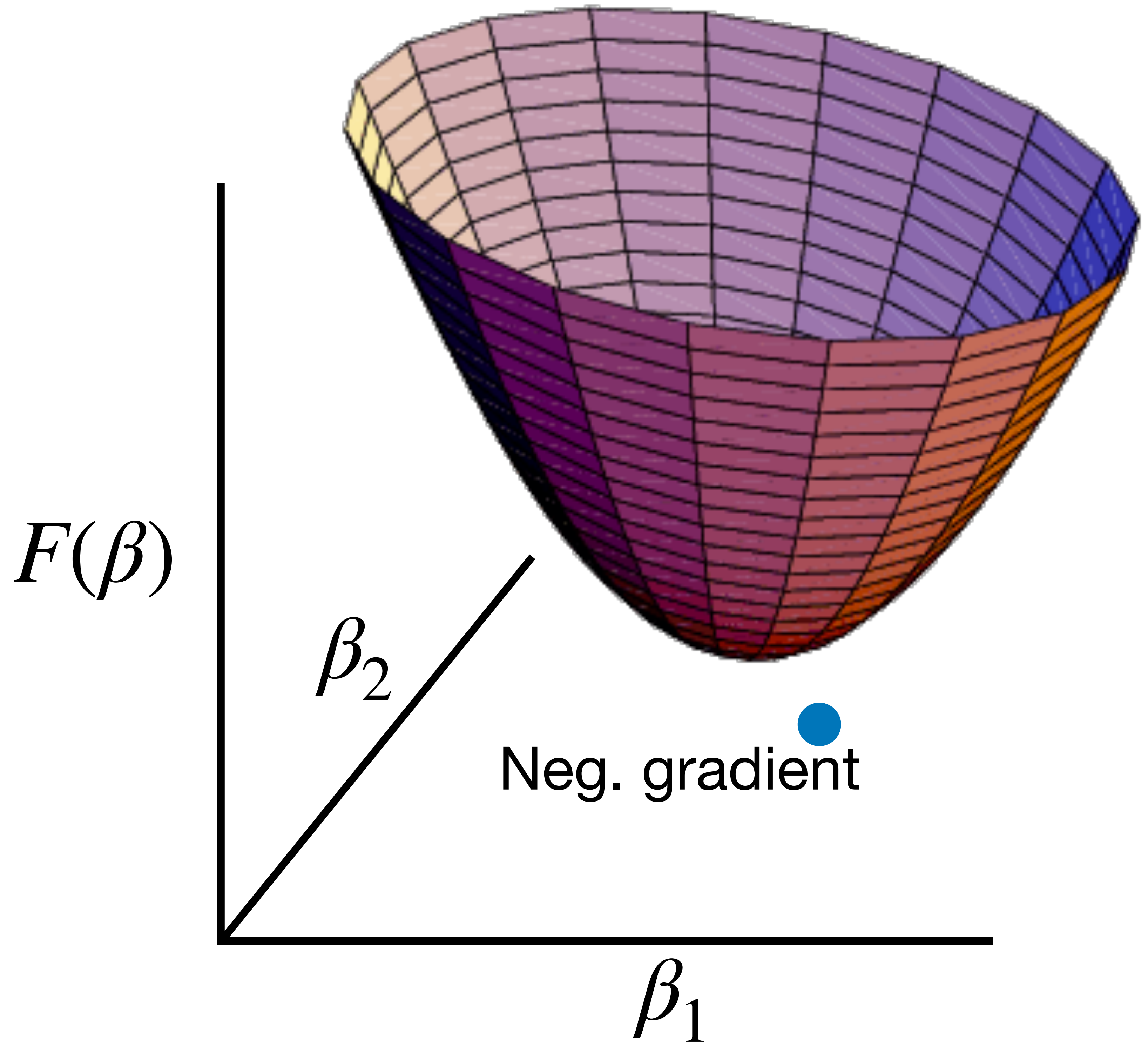

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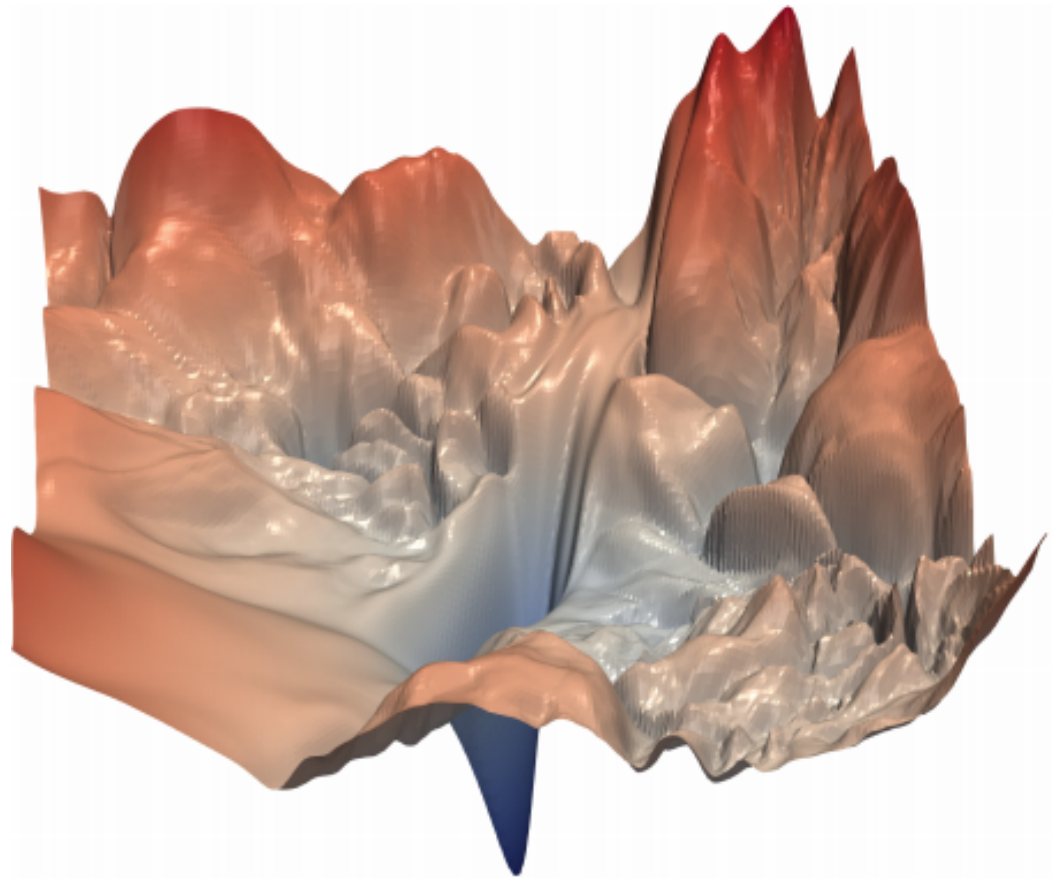

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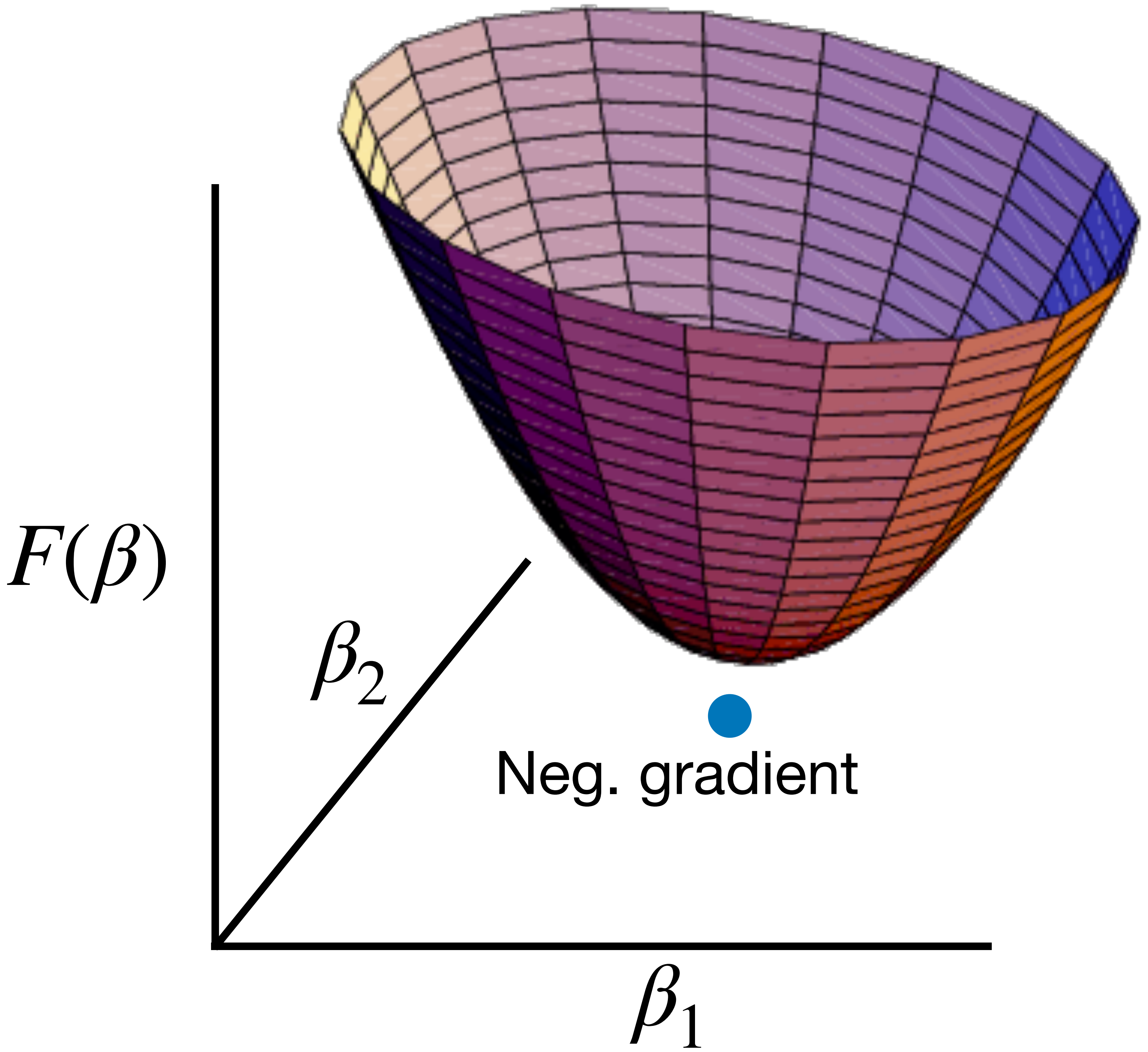

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The computational cost of gradient descent

computational cost $=$ (cost of computing the gradient) $\times$ (number of iterations)

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

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

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

Each evaluation of the gradient requires a pass through the entire training data, and modern data sets can have millions of training observations.

This can make gradient descent prohibitively expensive.

Stochastic gradient descent

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

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

1. Choose some initial value of β.
2. Randomly assign observations to mini-batches $S_1, \ldots, S_M$ of a certain size
3. Repeat until convergence:

- $\underbrace{\text{For } m = 1,\ldots,M}_{\text{One “epoch”}}$, update $\beta \leftarrow \beta - \gamma \cdot \frac{1}{|S_m|}\sum_{i\in S_m} \nabla L(Y_i, f_\beta(X_i))$.

Stochastic gradient descent

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

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

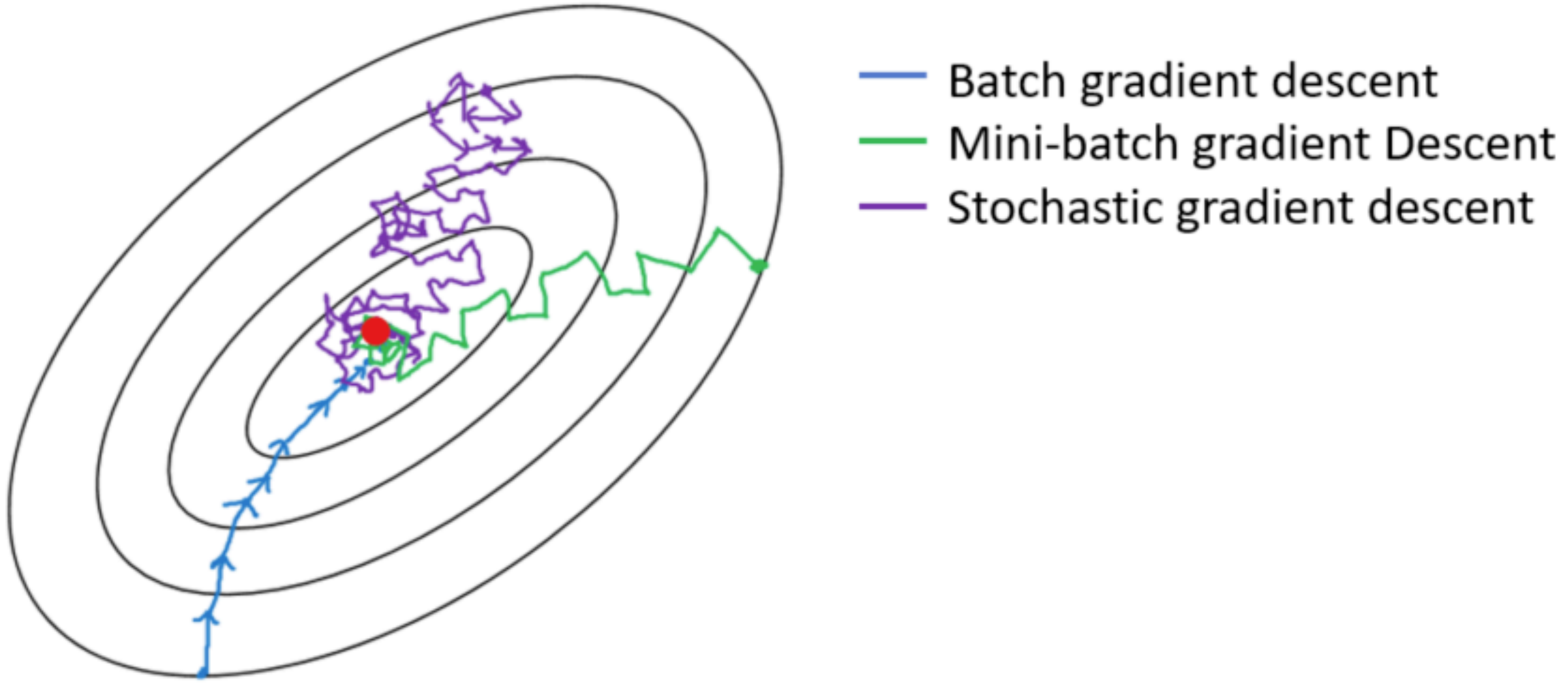
1. Choose some initial value of β.
2. Randomly assign observations to mini-batches $S_1, \ldots, S_M$ of a certain size
3. Repeat until convergence:

- $\underbrace{\text{For } m = 1,\ldots,M}_{\text{One “epoch”}}$, update $\beta \leftarrow \beta - \gamma \cdot \frac{1}{|S_m|}\sum_{i\in S_m} \nabla L(Y_i, f_\beta(X_i))$.

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:



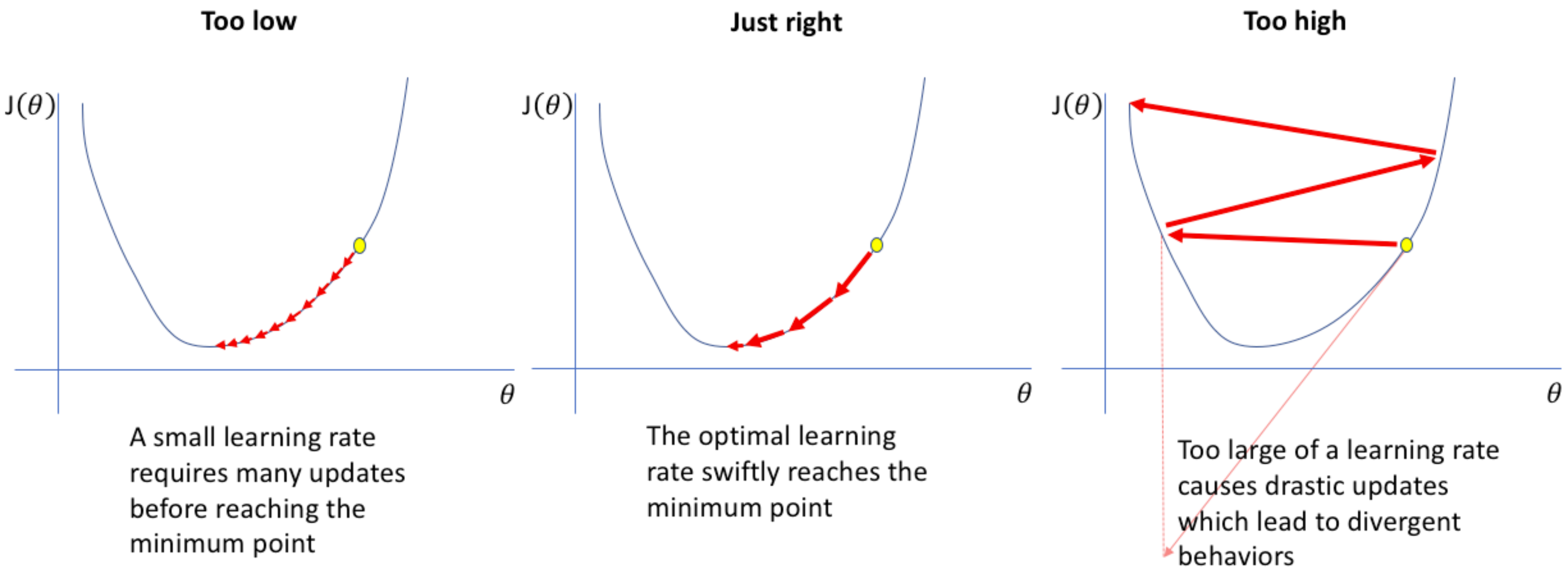
(Mini-batch size = n)
($1 <$ mini-batch size $< n$)
(Mini-batch size = 1)

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.

The learning rate for (stochastic) gradient descent



Source: https://www.jeremyjordan.me/nn-learning-rate/

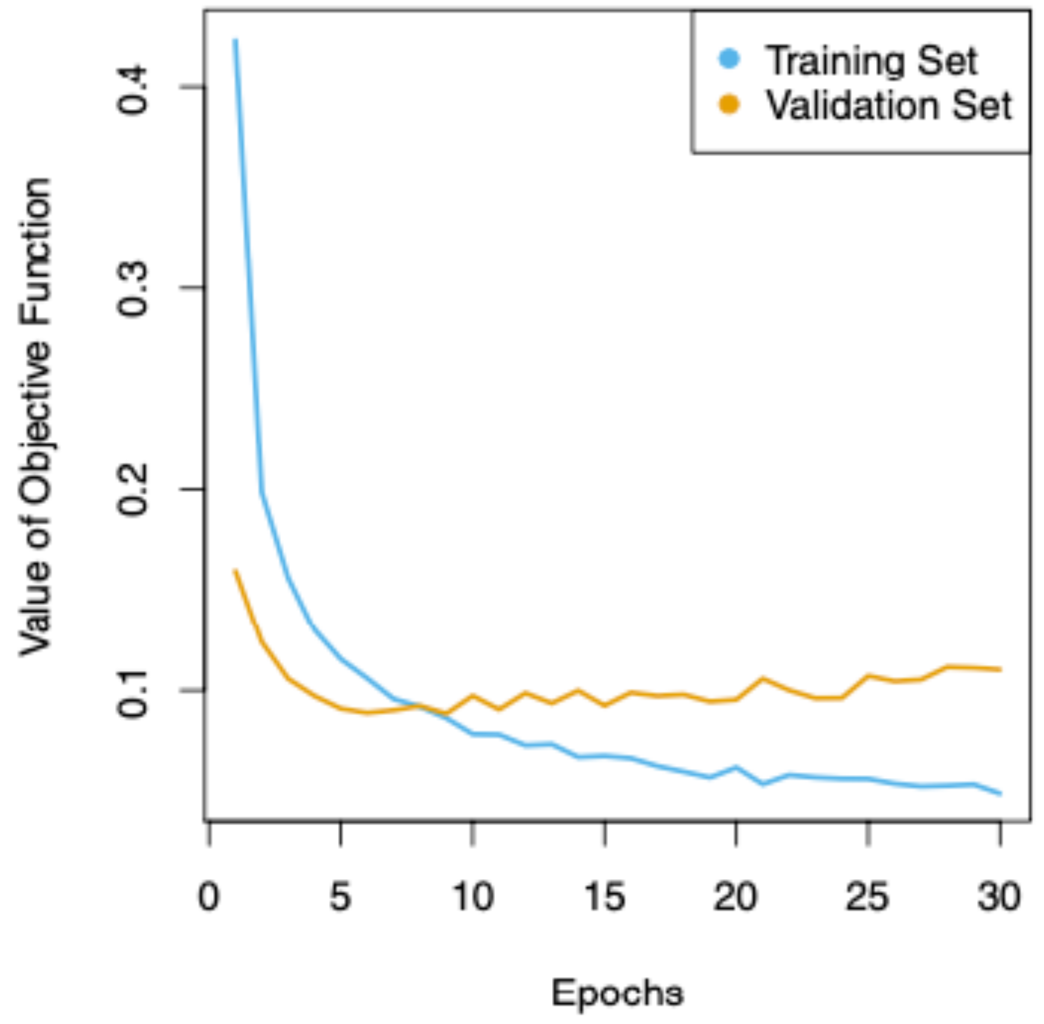
- Setting the learning rate is more of an art than a science; might need to try a few values to get a good one.
- Especially for non-convex optimization, people come up with clever strategies like shrinking learning rates, cycling learning rates, adaptive learning rates, etc. (RMSprop, Adam, AdaGrad,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

Regularization in deep learning models

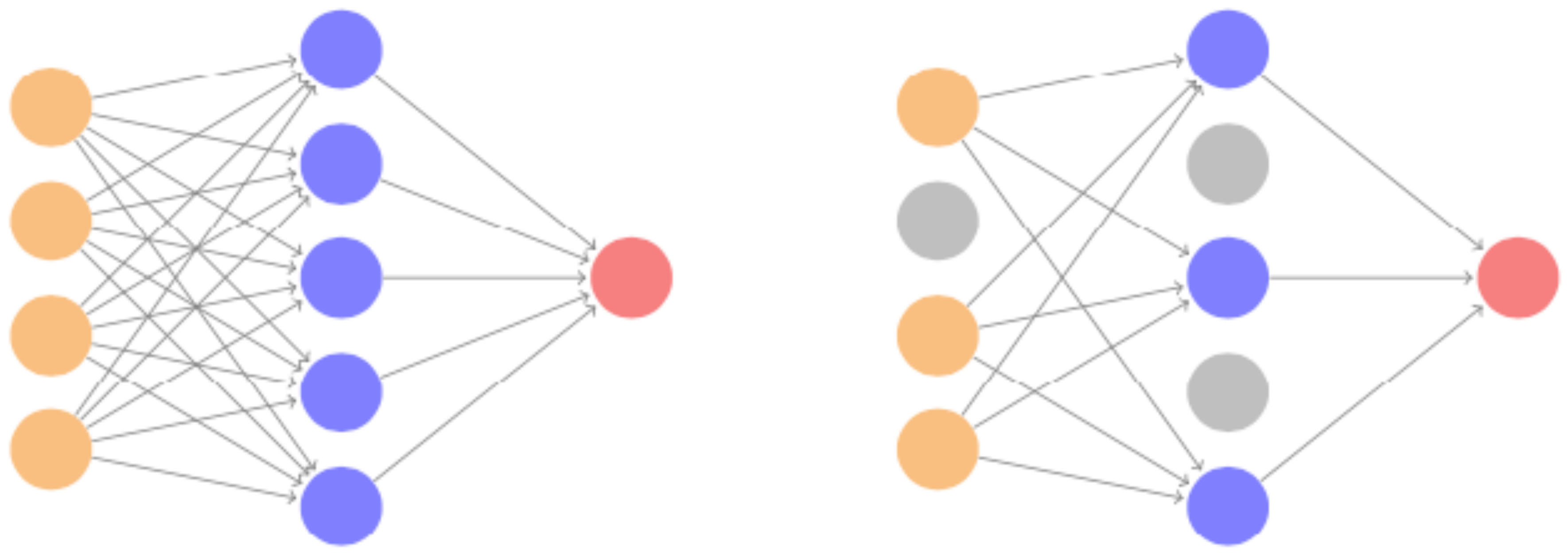
Explicit regularization via penalization. Ridge regression penalty is the most common; this kind of penalization is known as weight decay.

Implicit regularization: Other techniques to control complexity of the model.

- Early stopping: Do not run SGD until convergence; rather, stop SGD when validation error starts to increase.



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



Model complexity and model tuning in deep learning

Deep learning has many tuning parameters:

- Network architecture (number of layers, units per layer)
- Optimization algorithm used (RMSprop, Adam, etc.)
- Weight decay parameter, dropout rate, number of SGD iterations

More complex models arise from bigger networks, less weight decay, less dropout, more SGD iterations.

Deep learning performance can be sensitive to these parameters; there is no standard way to tune neural networks; tuning is computationally expensive.

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