Why is learning prone to fail?

Optimization issues: SGD+momentum and its convergence rate, Adagrad, Adam, diminishing/exploding gradient, oscillations

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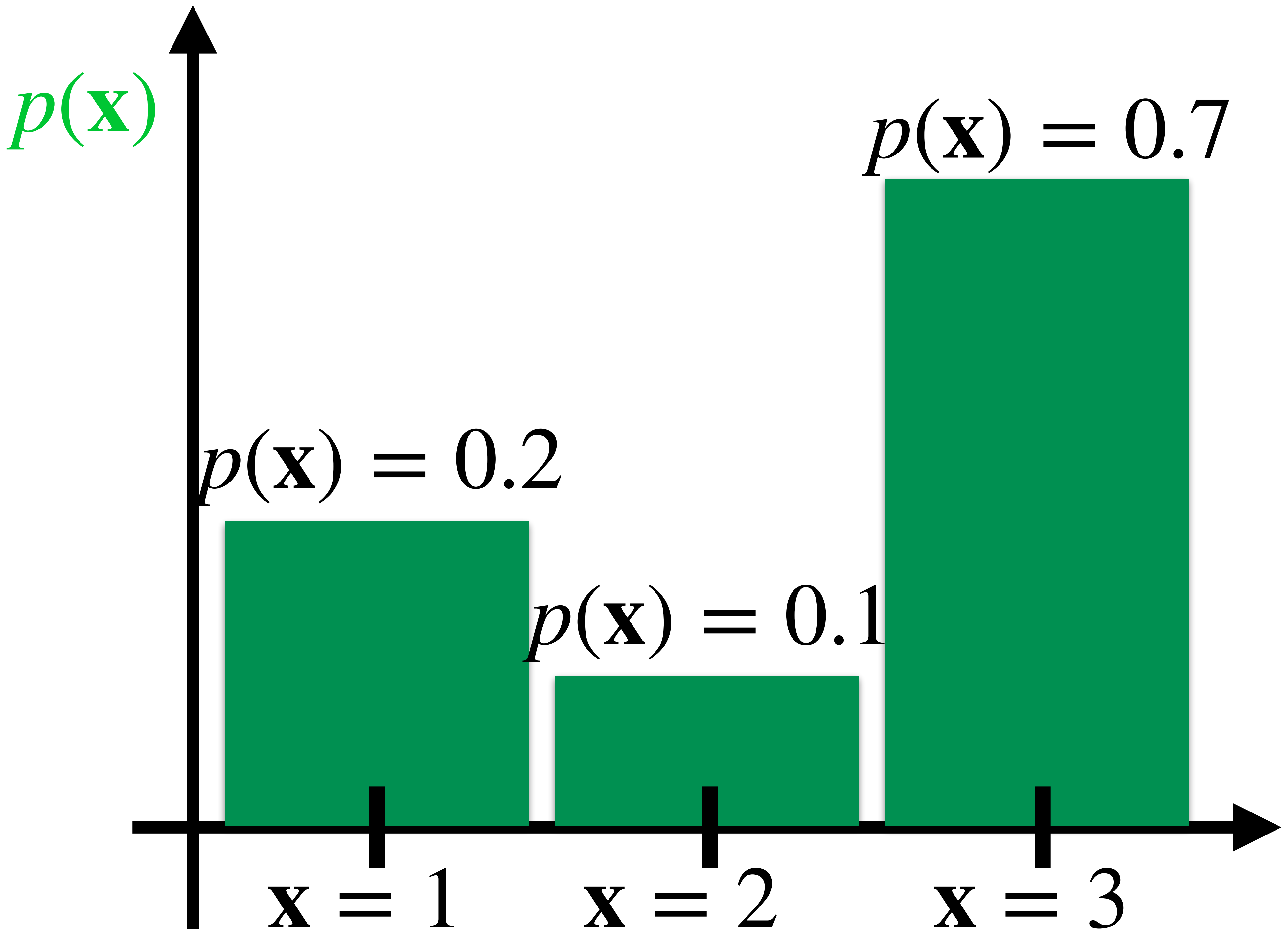
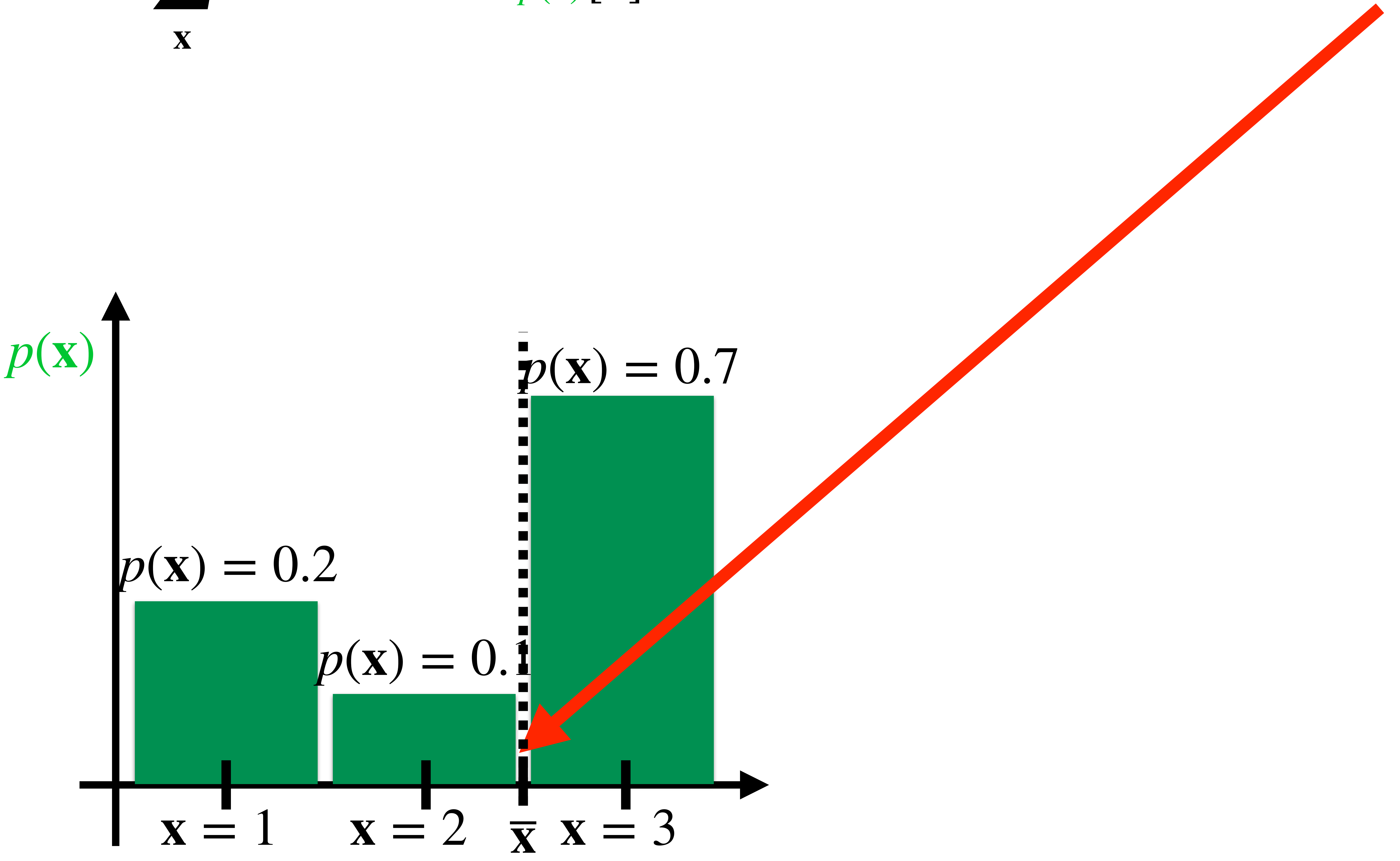
Prerequisites: Mean and average

$$\bar{\mathbf{x}} = \sum_{\mathbf{x}} p(\mathbf{x}) \cdot \mathbf{x} = \mathbb{E}_{\mathbf{x} \sim p(\mathbf{x})}[\mathbf{x}] = ??$$



Prerequisites: Mean and average

$$\bar{\mathbf{x}} = \sum_{\mathbf{x}} p(\mathbf{x}) \cdot \mathbf{x} = \mathbb{E}_{\mathbf{x} \sim p(\mathbf{x})}\left[\mathbf{x}\right] = 0.2 \cdot 1 \ + \ 0.1 \cdot 2 \ + \ 0.7 \cdot 3 = 2.5$$



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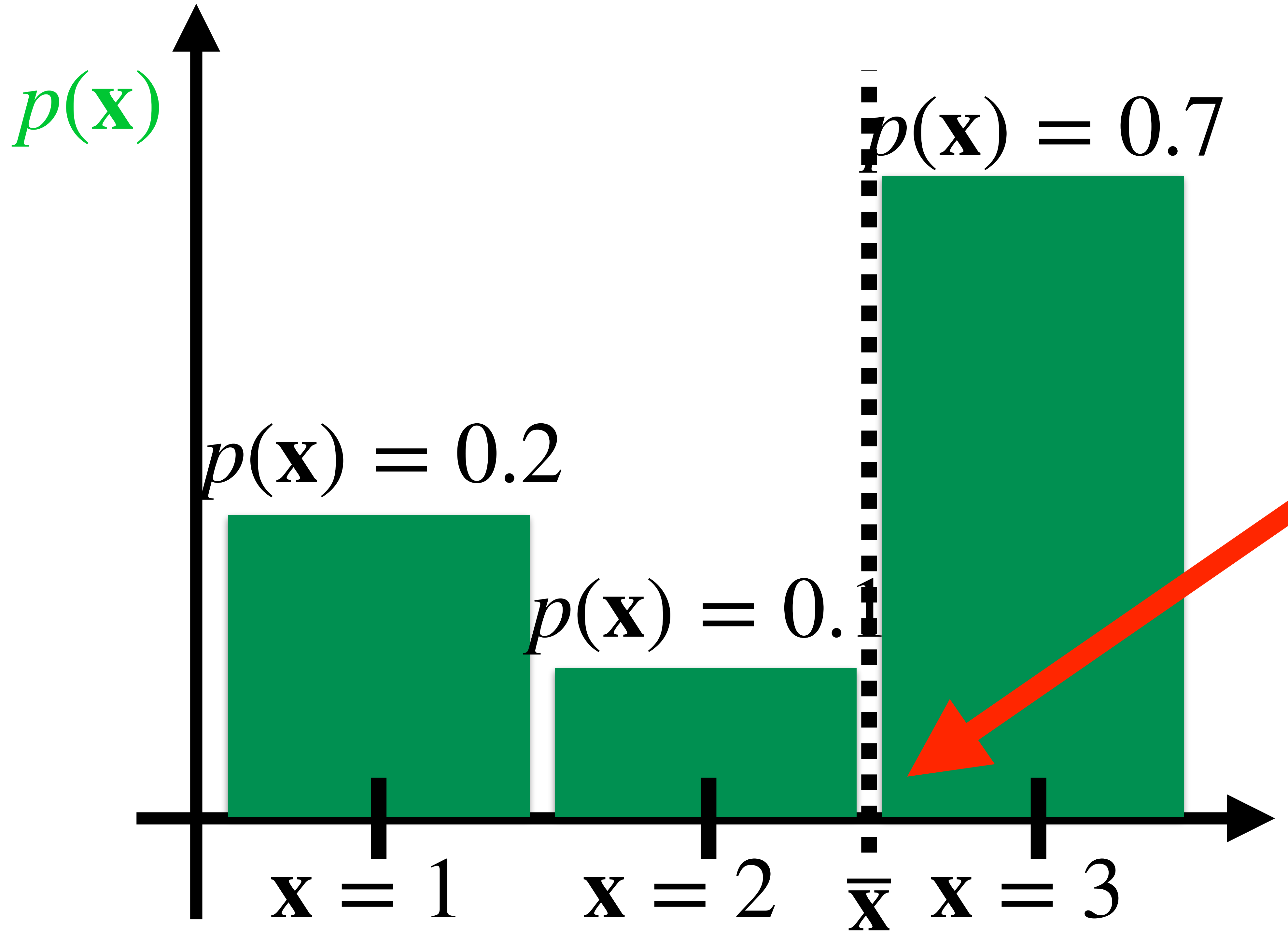
$$\approx \frac{1}{N} \sum_{i} \mathbf{x}_i \ = \frac{1}{10}(1 + 1 + 2 + 3 + 3 + 3 + 3 + 3 + 3 + 3) = 2.5$$

where $\mathbf{x}_i \sim p$



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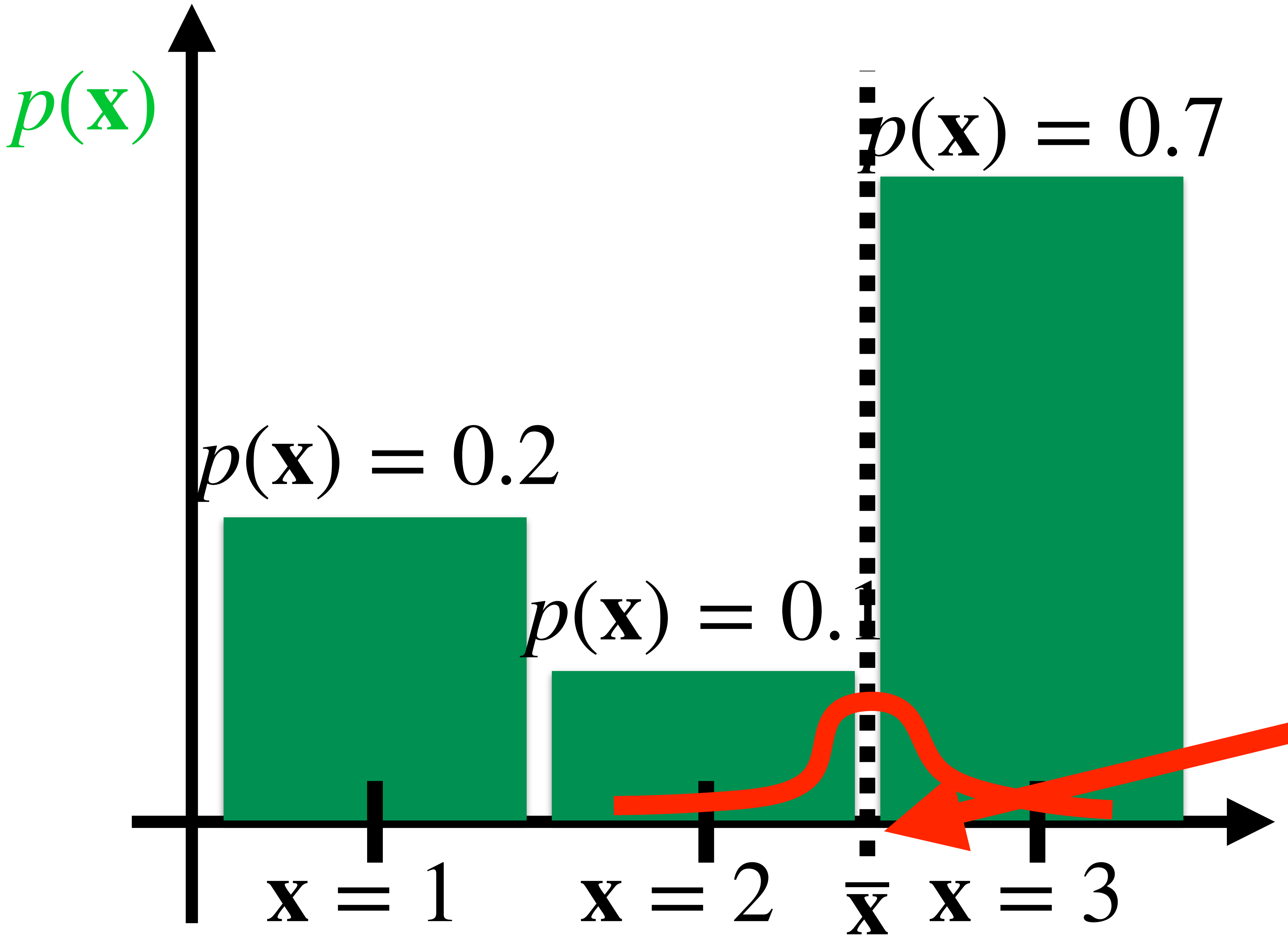
For $N \to \infty$

$$\mathcal{N}(\bar{\mathbf{x}}_i; \ \ \bar{\mathbf{x}}, \frac{\sigma^2_{\mathbf{x}}}{\sqrt{N}})$$



$$\bar{\mathbf{x}}_1 = \frac{1}{10}(1 + 1 + 1 + 1 + 3 + 3 + 3 + 3 + 3 + 3) = 2.2$$

$$\bar{\mathbf{x}}_2 = \frac{1}{10}(3 + 3 + 3 + 3 + 3 + 3 + 3 + 3 + 3 + 3) = 3.0$$

$$\bar{\mathbf{x}}_3 = \frac{1}{10}(2 + 2 + 2 + 2 + 3 + 3 + 3 + 3 + 3 + 3) = 2.6$$

$$\bar{\mathbf{x}}_4 = \frac{1}{10}(1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 2 + 2) = 1.2$$

$$\bar{\mathbf{x}}_5 = \frac{1}{10}(1 + 1 + 1 + 1 + 1 + 3 + 3 + 3 + 3 + 3) = 2.0$$

Prerequisites: Learning vs optimization

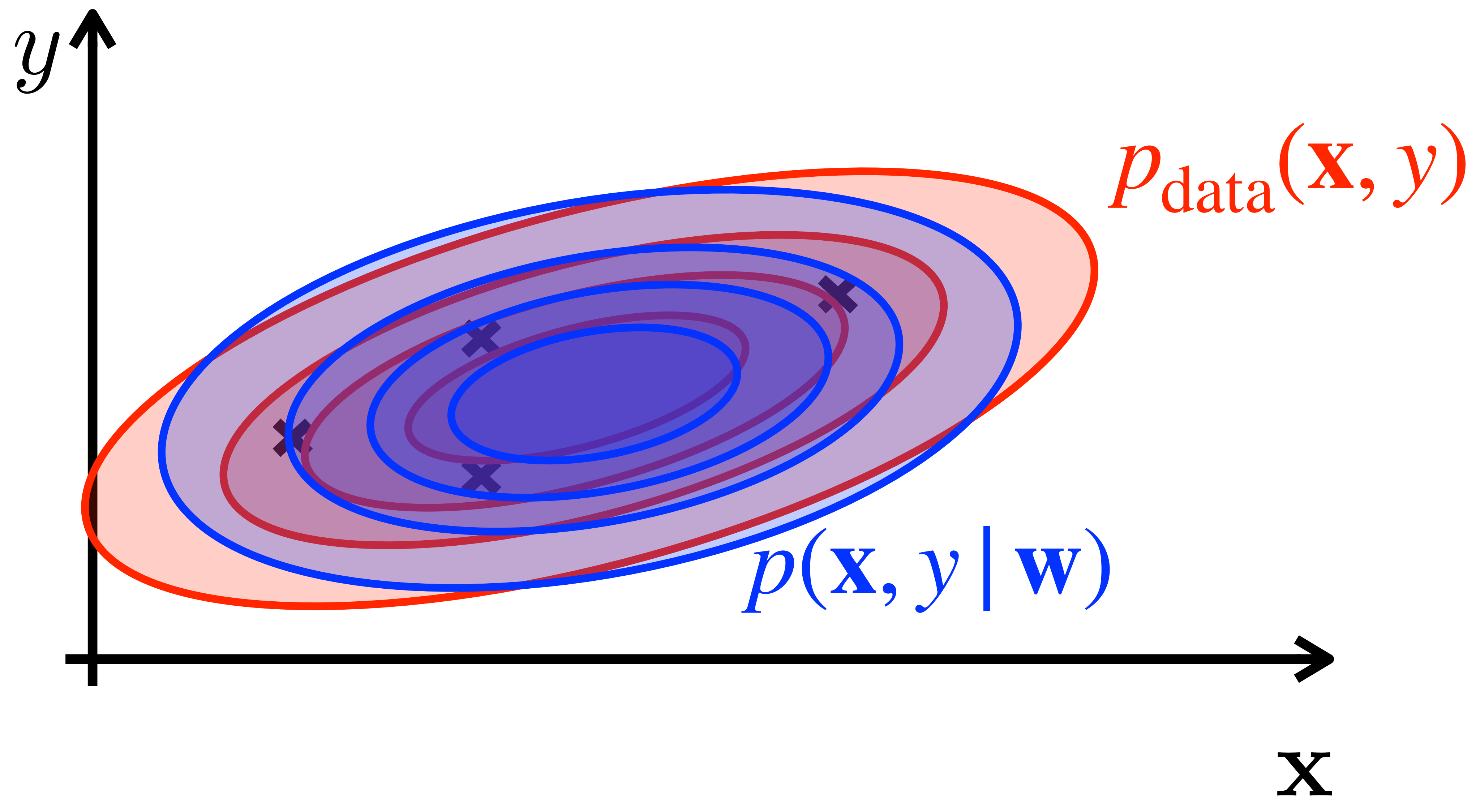
$$\mathbf{w}^\star = \arg\min_{\mathbf{w}} D_{KL}\big(p_{\text{data}}(\mathbf{x}, y) \,\|\, p(\mathbf{x}, y \,|\, \mathbf{w})\big) = \int_{(\mathbf{x},y)} p_{\text{data}}(\mathbf{x}, y) \cdot \log \frac{p_{\text{data}}(\mathbf{x}, y)}{p(\mathbf{x}, y \,|\, \mathbf{w})}$$

$$= \arg\min_{\mathbf{w}} \mathbb{E}_{(\mathbf{x},y)\sim p_{\text{data}}}\left[\log \frac{p_{data}(\mathbf{x}, y)}{p(\mathbf{x}, y \,|\, \mathbf{w})}\right] = \arg\min_{\mathbf{w}} \mathbb{E}_{(\mathbf{x},y)\sim p_{\text{data}}}\left[-\log p(\mathbf{x}, y \,|\, \mathbf{w})\right]$$

$$= \arg\min_{\mathbf{w}} \mathbb{E}_{(\mathbf{x},y)\sim p_{\text{data}}}\left[-\log p(y \,|\, \mathbf{x}, \mathbf{w})\right] \approx \arg\min_{\mathbf{w}} \frac{1}{N} \sum_{(\mathbf{x}_i, y_i) \sim p_{\text{data}}(\mathbf{x}, y)} \left[-\log p(y_i \,|\, \mathbf{x}_i, \mathbf{w})\right]$$

True criterium we want to maximize:

$$J(\mathbf{w}) = \mathbb{E}_{(\mathbf{x},y)\sim p_{\text{data}}}\left[-\log p(y \,|\, \mathbf{x}, \mathbf{w})\right]$$



True gradient:

$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \mathbb{E}_{(\mathbf{x},y)\sim p_{\text{data}}}\left[-\nabla_{\mathbf{w}} \log\big(p(y \,|\, \mathbf{x}, \mathbf{w})\big)\right]$$

$$\approx \frac{1}{N} \sum_i -\nabla_{\mathbf{w}} \log\big(p(y_i \,|\, \mathbf{x}_i, \mathbf{w})\big)$$

$|\mathcal{T}| < \infty$: Learning from a finite dataset

- Is the minibatch gradient unbiased estimate of the true gradient if $|\mathcal{T}| < \infty$?
- I want to maximize $J(\mathbf{w})$
- I recycle samples from $\mathcal{T}$ => Criterion $\hat{J}(\mathbf{w})$ is biased by the training set
- This causes overfitting, requires strong priors and data augmentation !!!!

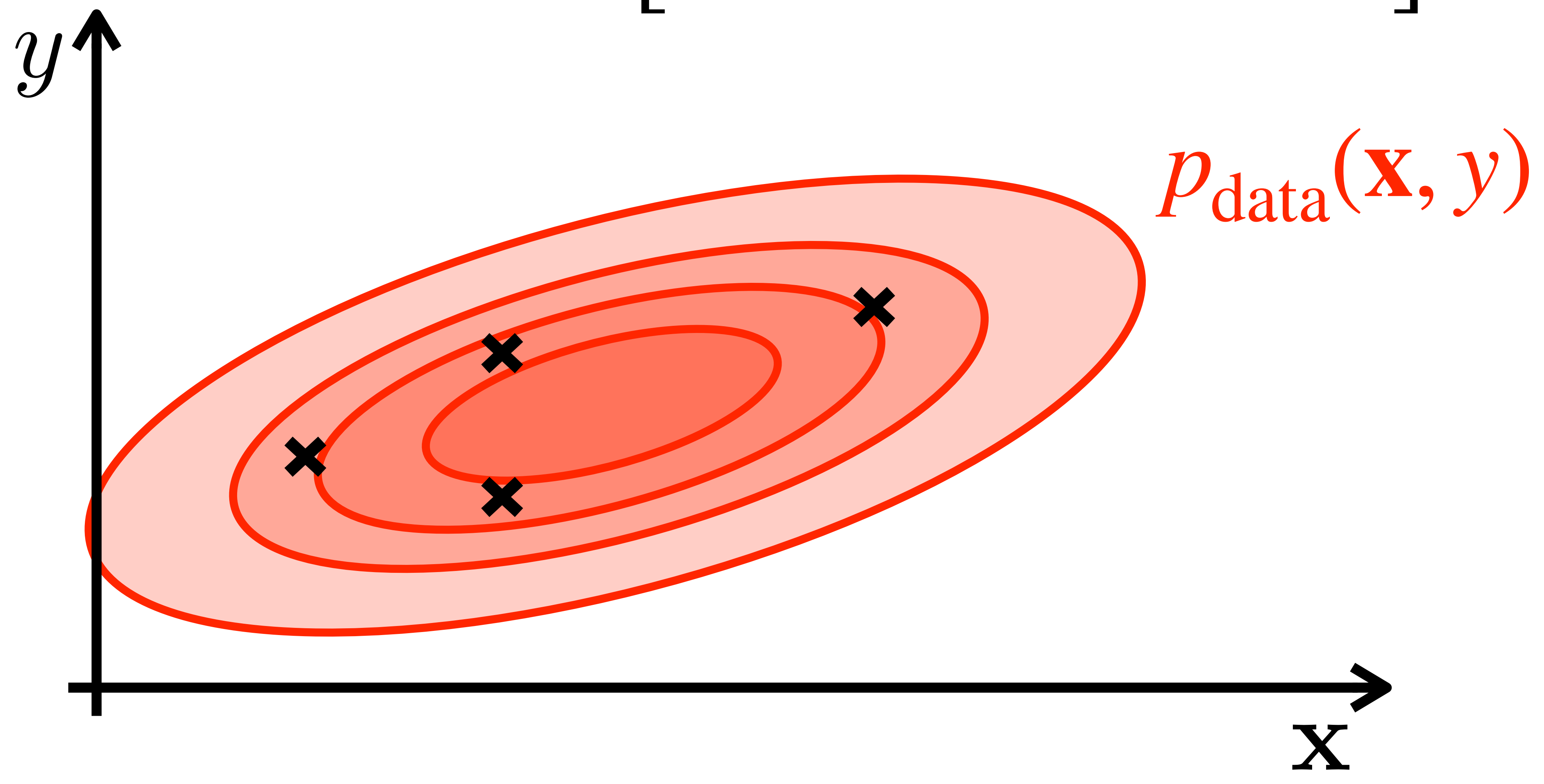
$$J(\mathbf{w}) = \mathbb{E}_{(\mathbf{x},y)\sim p_{\text{data}}}\left[\log p(\mathbf{x}, y \,|\, \mathbf{w})\right]$$

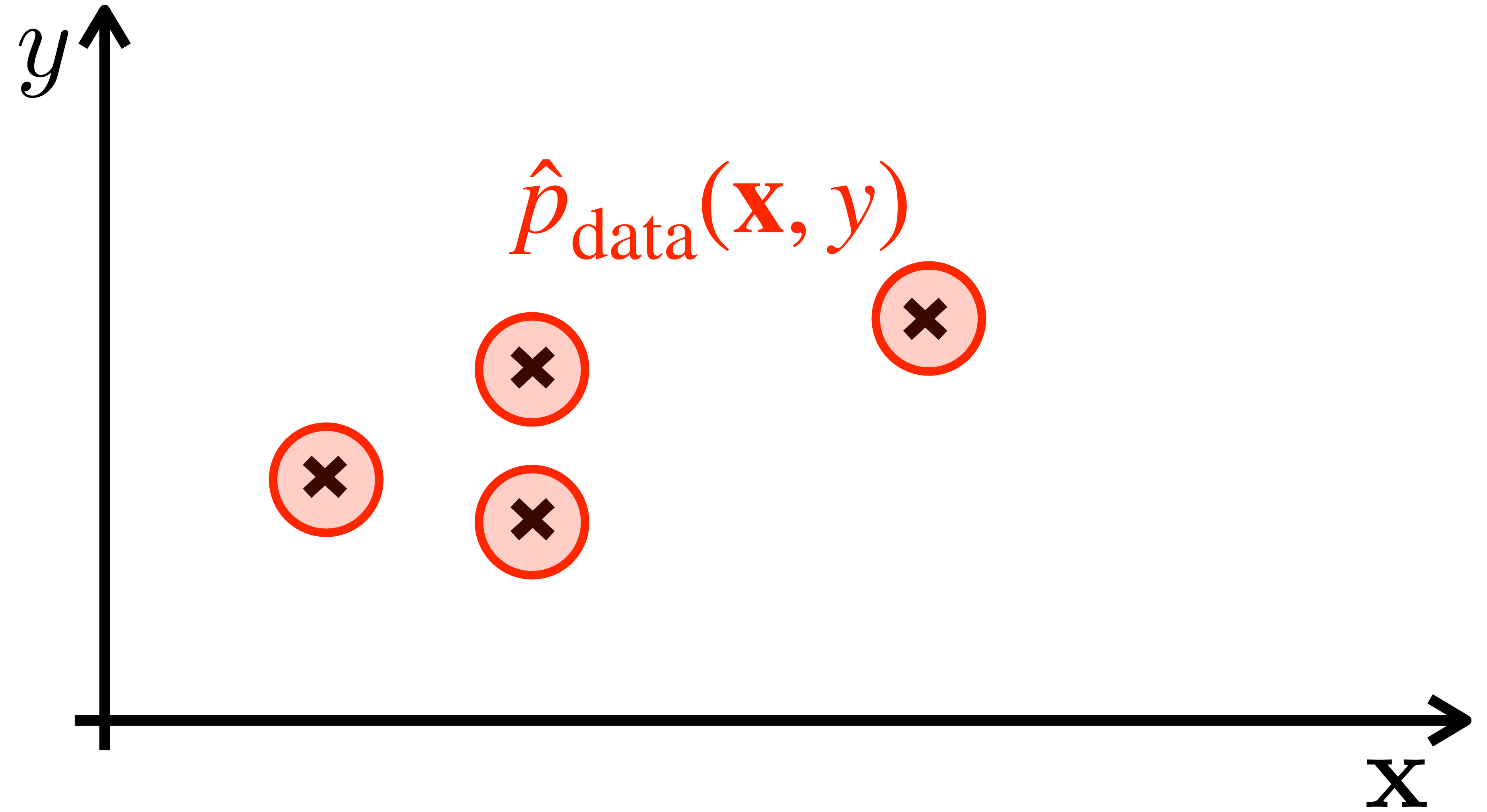
$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \mathbb{E}_{(\mathbf{x},y)\sim p_{\text{data}}}\left[\nabla_{\mathbf{w}} \log\left(p(\mathbf{x}, y \,|\, \mathbf{w})\right)\right]$$

vs.

$$\hat{J}(\mathbf{w}) = \mathbb{E}_{(\mathbf{x},y)\sim \hat{p}_{\text{data}}}\left[\log p(\mathbf{x}, y \,|\, \mathbf{w})\right]$$

$$\nabla_{\mathbf{w}} \hat{J}(\mathbf{w}) = \mathbb{E}_{(\mathbf{x},y)\sim p_{\text{data}}}\left[\nabla_{\mathbf{w}} \log\left(p(\mathbf{x}, y \,|\, \mathbf{w})\right)\right]$$





$|\mathcal{T}| = \infty$: Learning from an finite dataset

- Some datasets grows faster than we can learn from them:
  - Colorizing images (1074 imgs/sec uploaded to Instagram)
  - Autonomous cars (predicting vertical acceleration from images)
  - Youtube videos (predicting keywords in comments from video)
- The learning bottleneck stems from computational limitations (not from trn size).
- We always learn from a new “not-yet-seen” mini batch. => Gradient is unbiased estimate => Perform SGD on the true generalization error.

$$J(\mathbf{w}) = \mathbb{E}_{(\mathbf{x},y)\sim p_{\text{data}}}\left[\log p(\mathbf{x}, y \,|\, \mathbf{w})\right]$$

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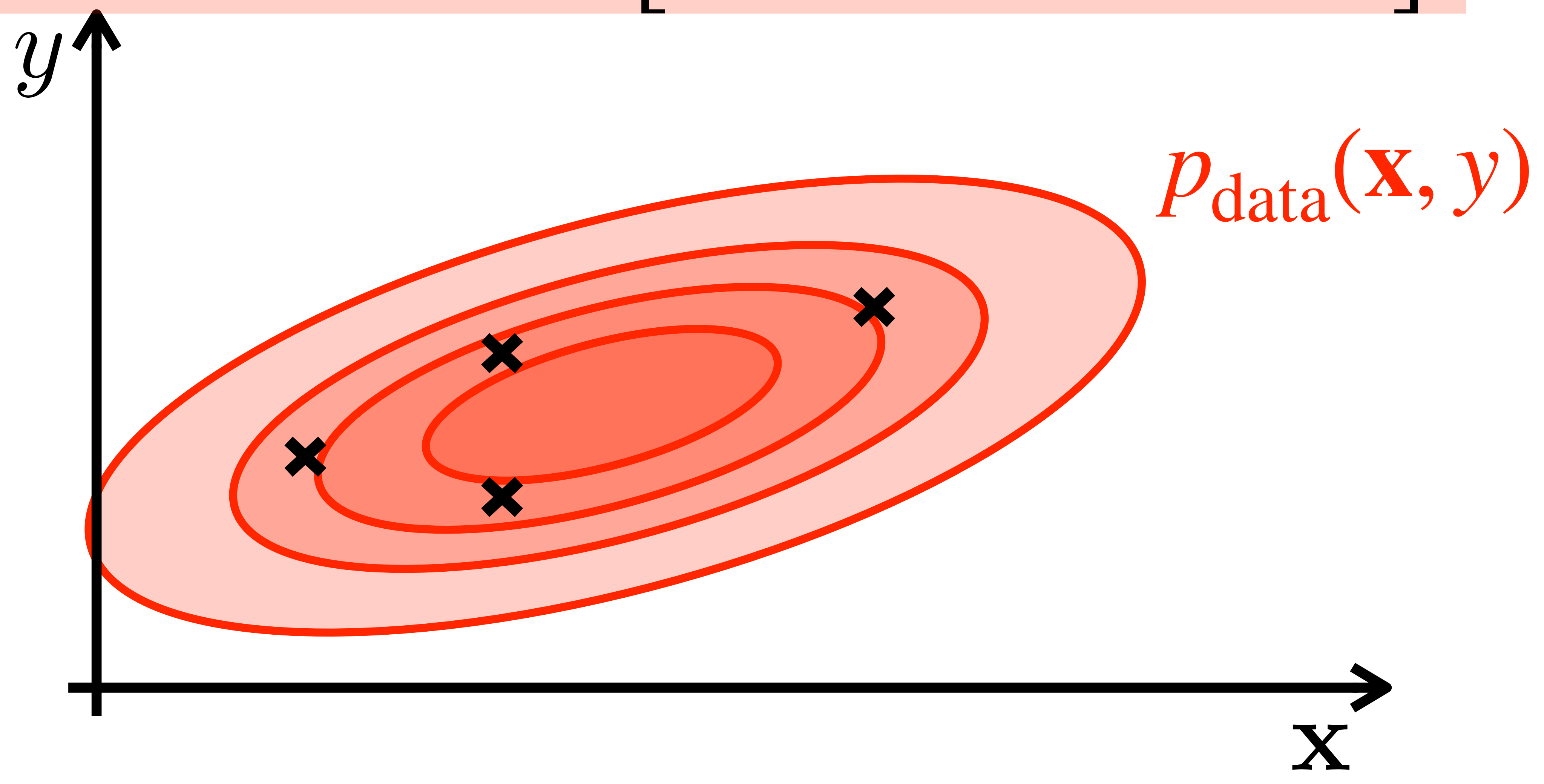
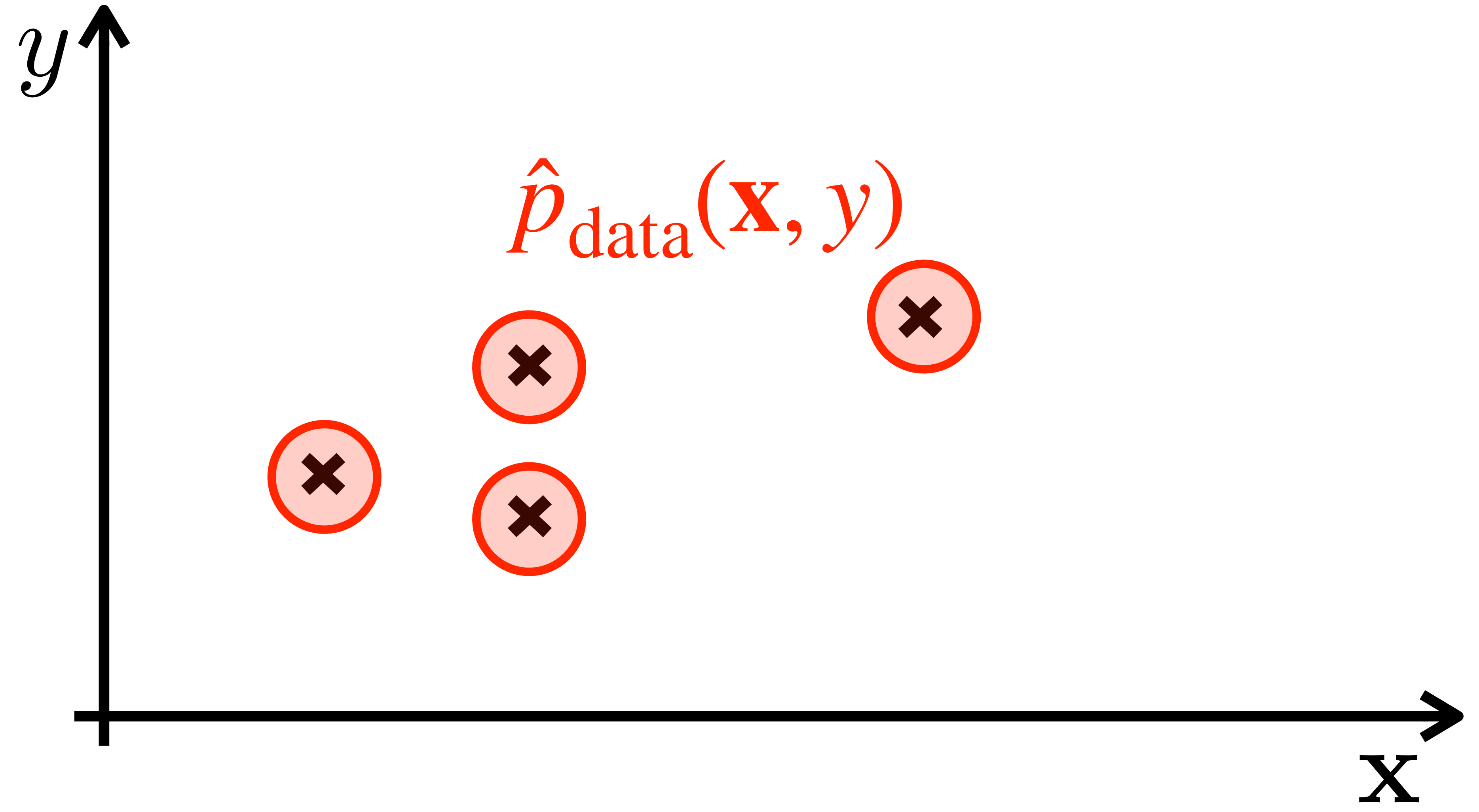




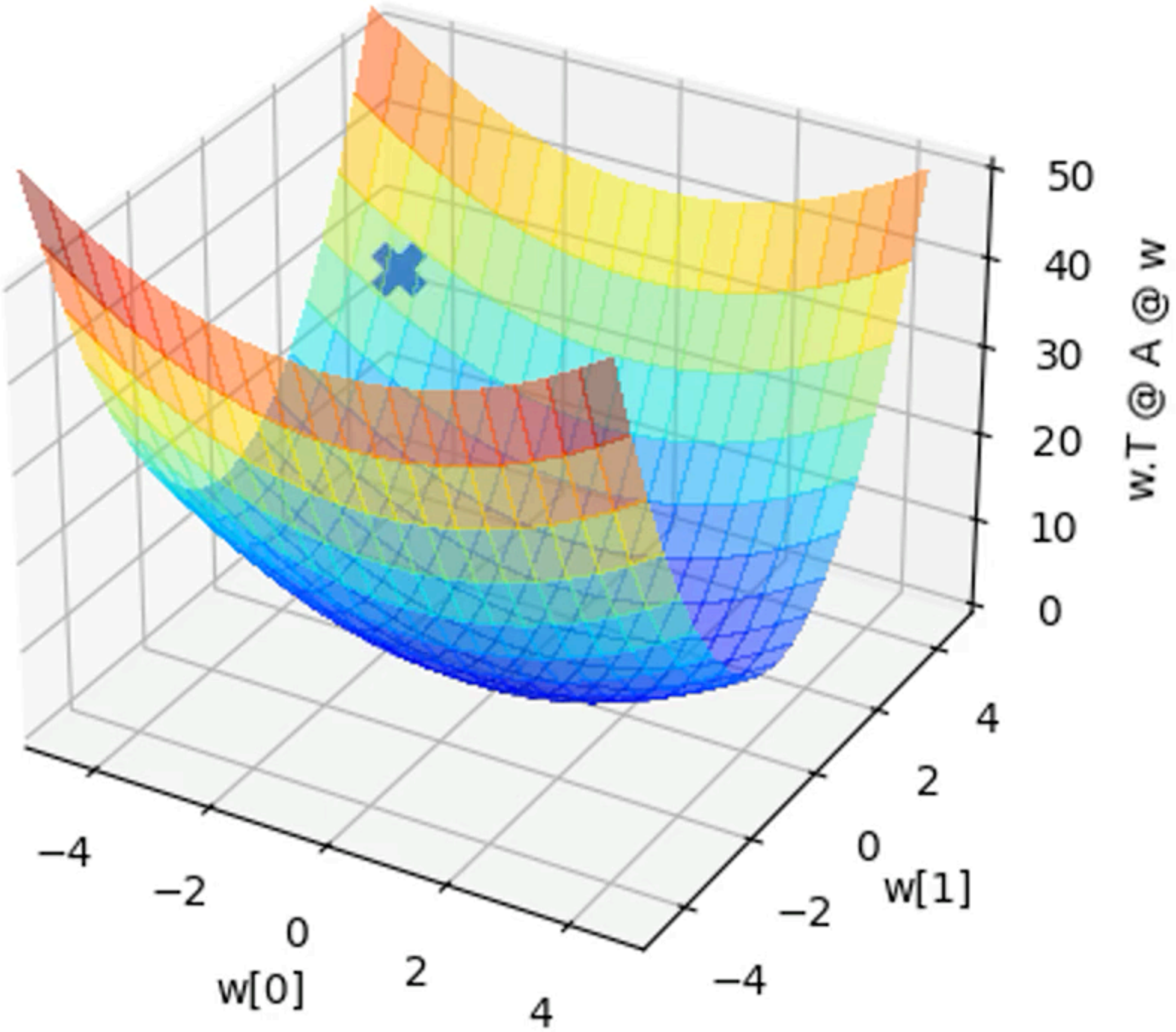
What is the disadvantage of GD on close-to-infinite dataset?

$$\mathbf{w}^k = \mathbf{w}^{k-1} - \alpha \left. \frac{\partial f^\top(\mathbf{w})}{\partial \mathbf{w}} \right|_{\mathbf{w}=\mathbf{w}^{k-1}}$$

Batches

$$f(\mathbf{w}) = \frac{1}{2}\mathbf{w}^\top \mathbf{A}\mathbf{w}$$

$$f(\mathbf{w}) = \frac{1}{2 \cdot 1000}\sum_{i=1}^{1000} (\mathbf{w} - \mathbf{w}_i)^\top \mathbf{A}(\mathbf{w} - \mathbf{w}_i)$$



What makes it different?

Gradient computation 1000x slower

Batches

$$f(\mathbf{w}) = \frac{1}{2}\mathbf{w}^\top \mathbf{A}\mathbf{w}$$

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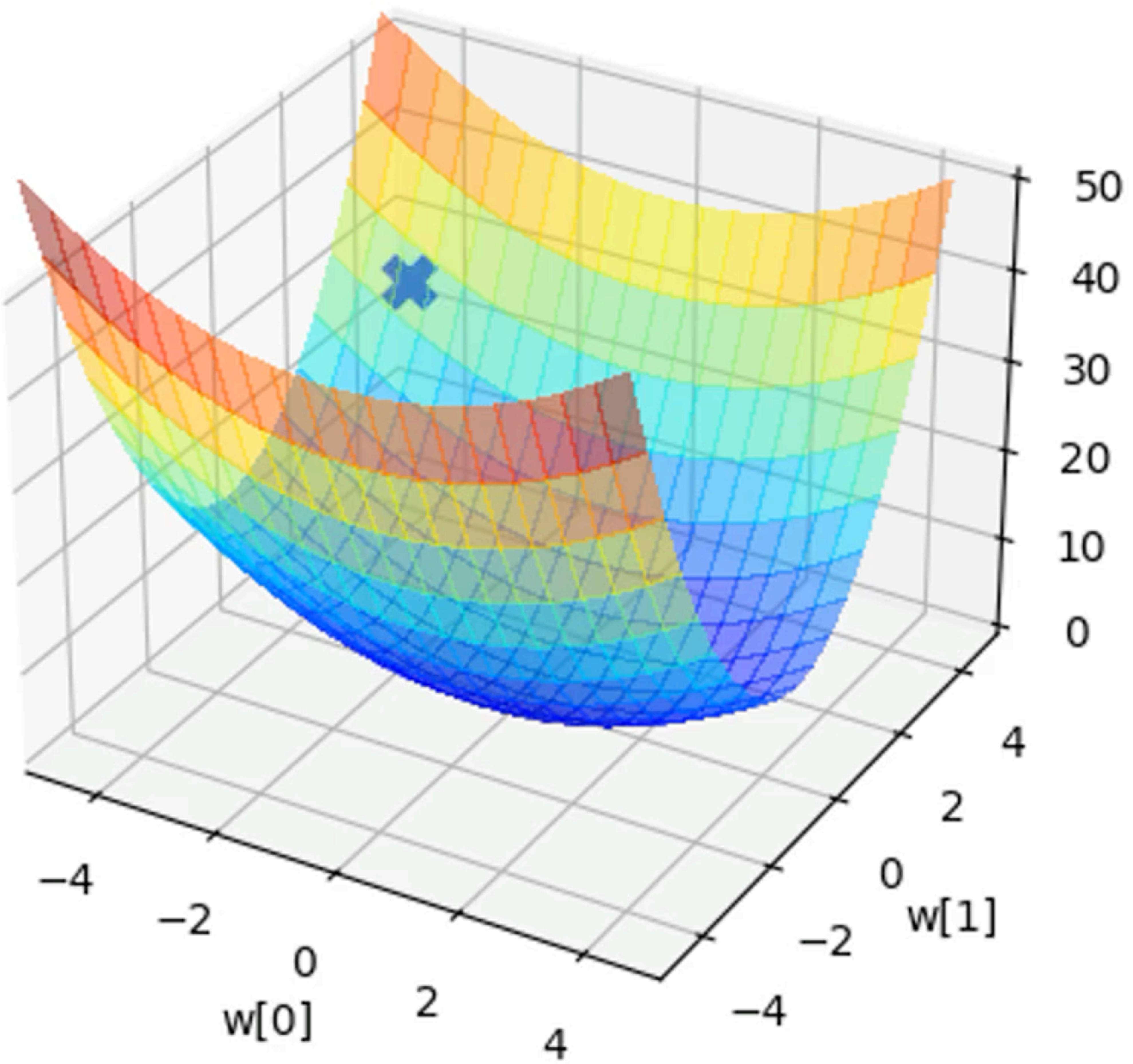

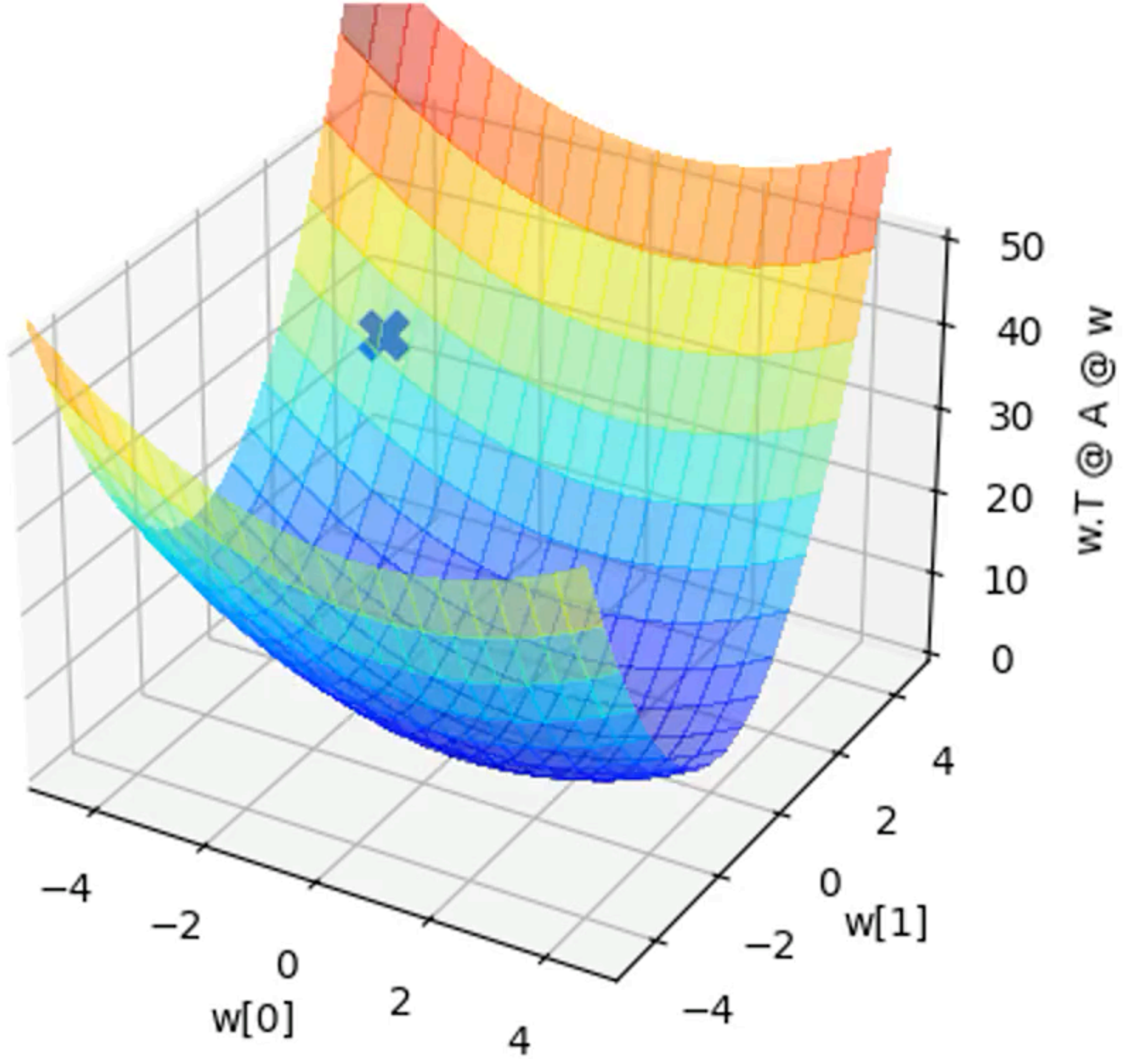

Does is worth to estimate the gradient from the full training set?

$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \mathbb{E}_{(\mathbf{x},y)\sim p_{\text{data}}}\left[\nabla_{\mathbf{w}} \log\big(p(y\,|\,\mathbf{x},\mathbf{w})\big)\right] \approx \frac{1}{N}\sum_i \nabla_{\mathbf{w}} \log\big(p(y_i\,|\,\mathbf{x}_i,\mathbf{w})\big)$$

- Standard error of the mean estimated from N samples is $\sigma/\sqrt{N}$, where σ^2 is true variance of input samples.
- "Estimate of the gradient" based on $N = 10000$ vs $N = 100$
  - standard error is $10\times$ better
  - number of computations is $100\times$ higher !!!
- Using the large training set for estimating the gradient may suffers diminishing returns.
- Convergence in the number of computations vs number of iterations.

How should I choose N?

$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \mathbb{E}_{(\mathbf{x},y)\sim p_{\text{data}}}\left[\nabla_{\mathbf{w}} \log\big(p(\mathbf{x}, y \,|\, \mathbf{w})\big)\right] \approx \frac{1}{N}\sum_i \nabla_{\mathbf{w}} \log\big(p(\mathbf{x}_i, y_i \,|\, \mathbf{w})\big)$$

- Large N => more accurate gradient with sub-linear returns.
- Runtime in multicore architectures is similar for small $N = 1,2,\ldots$
- Amount of required memory is linear in N (limiting factor for the most state-of-the-art hardware)
- GPU achieves better runtime with "power of 2" batch sizes.
- Small batches yields regularization.

Answer: $N \in \{4, 8, 16, 32, 64, 128, 256\}$ or anything else that works ;-)

$N = 1$ ………………… often called online learning

$1 < N <$ trn_size….. often called minibatch learning

SGD (Stochastic Gradient Descent) = GD over minibatches

$$\mathbf{w}^k = \mathbf{w}^{k-1} - \alpha \left. \frac{\partial f^\top(\mathbf{w})}{\partial \mathbf{w}} \right|_{\mathbf{w}=\mathbf{w}^{k-1}}$$

Drawbacks?

- Get stuck on flat regions
- Oscillates
- Noisy for small mini-batches

Advantages?

- Does not get stuck in saddle-points
- SGD is faster than GD

Stochastic Gradient Descent (SGD) = GD over minibatches

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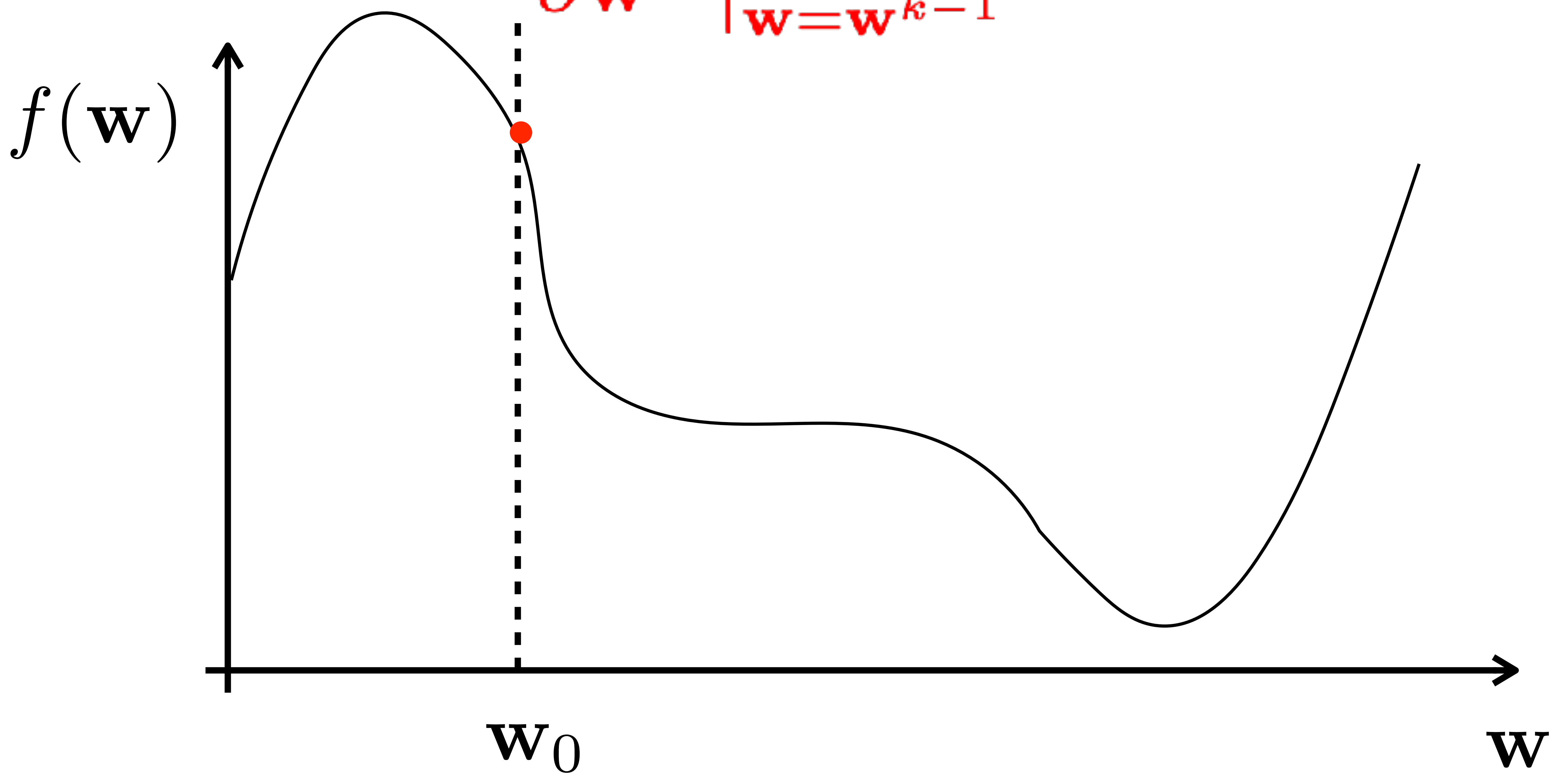
$$- \left. \frac{\partial f(\mathbf{w})}{\partial \mathbf{w}} \right|_{\mathbf{w}=\mathbf{w}^{k-1}} = ???$$



SGD drawbacks: can get stuck on flat regions

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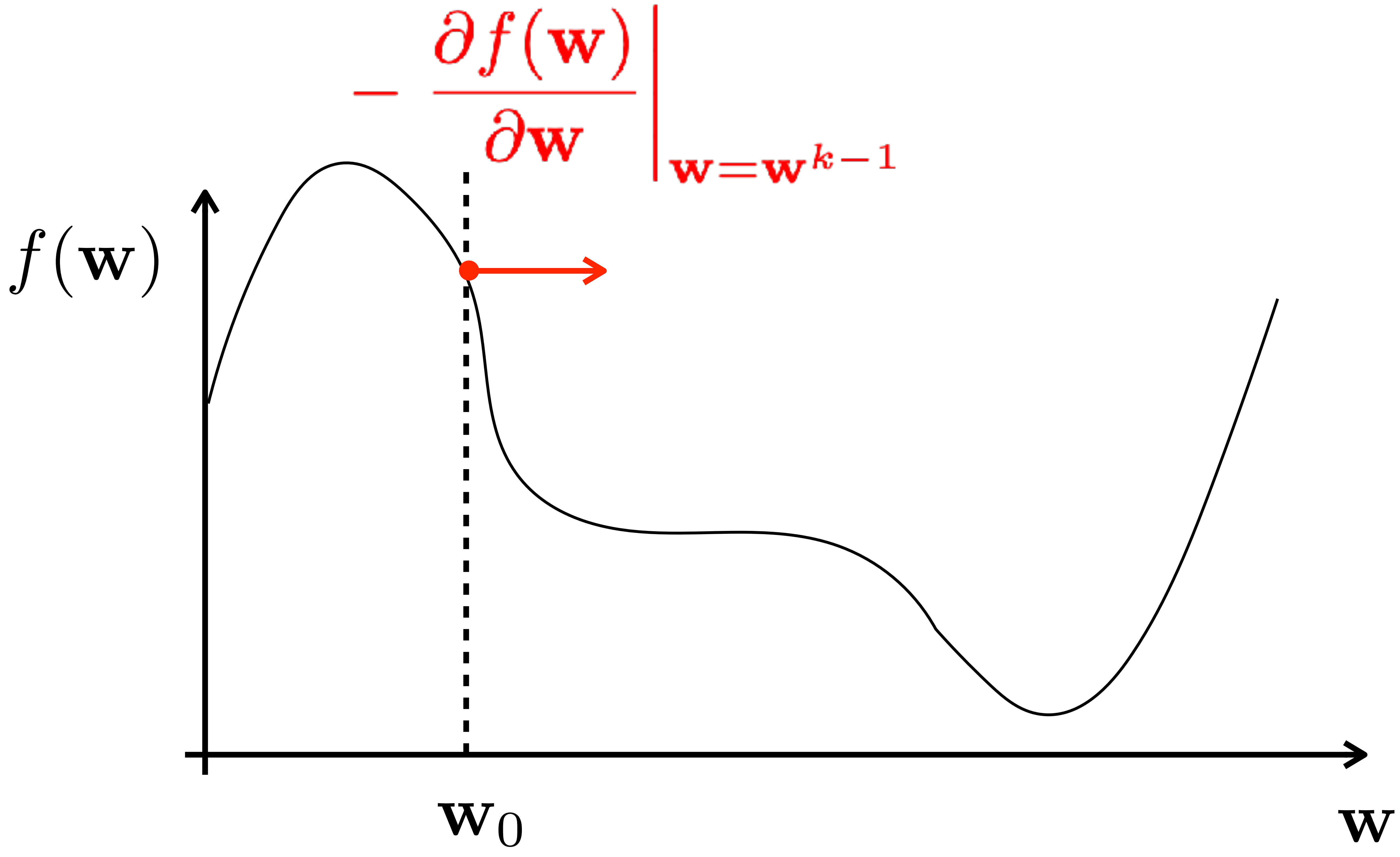

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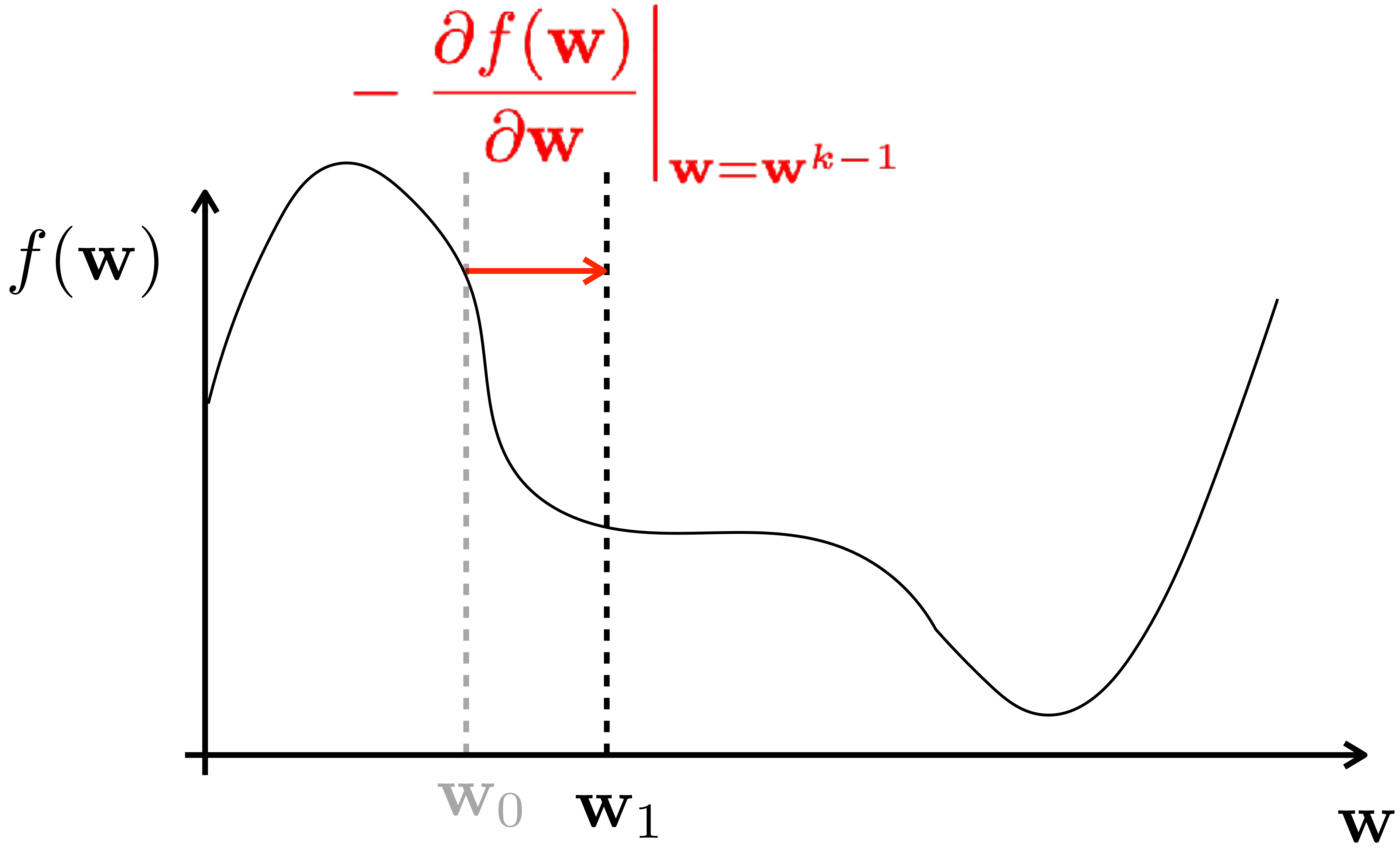

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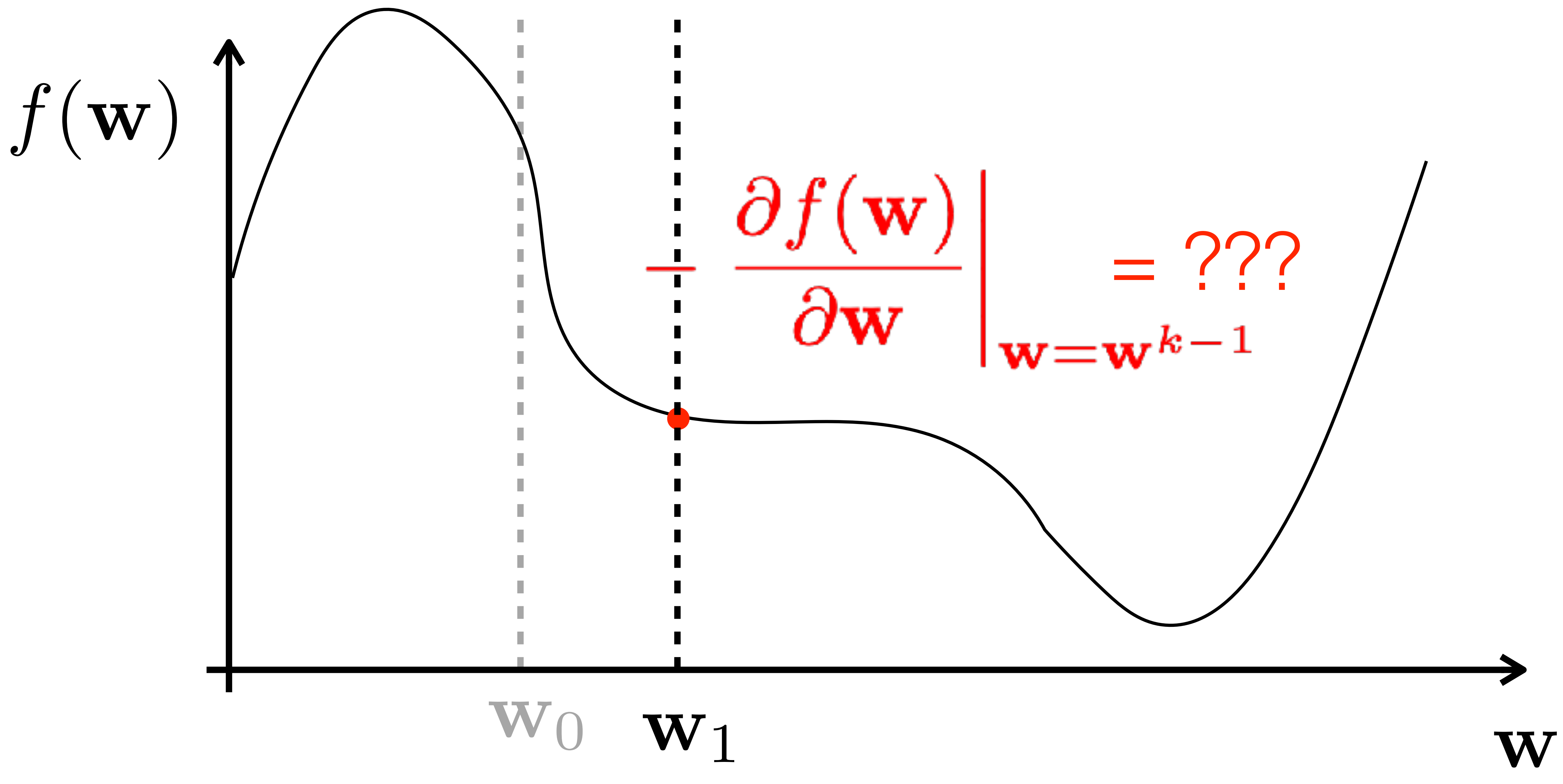

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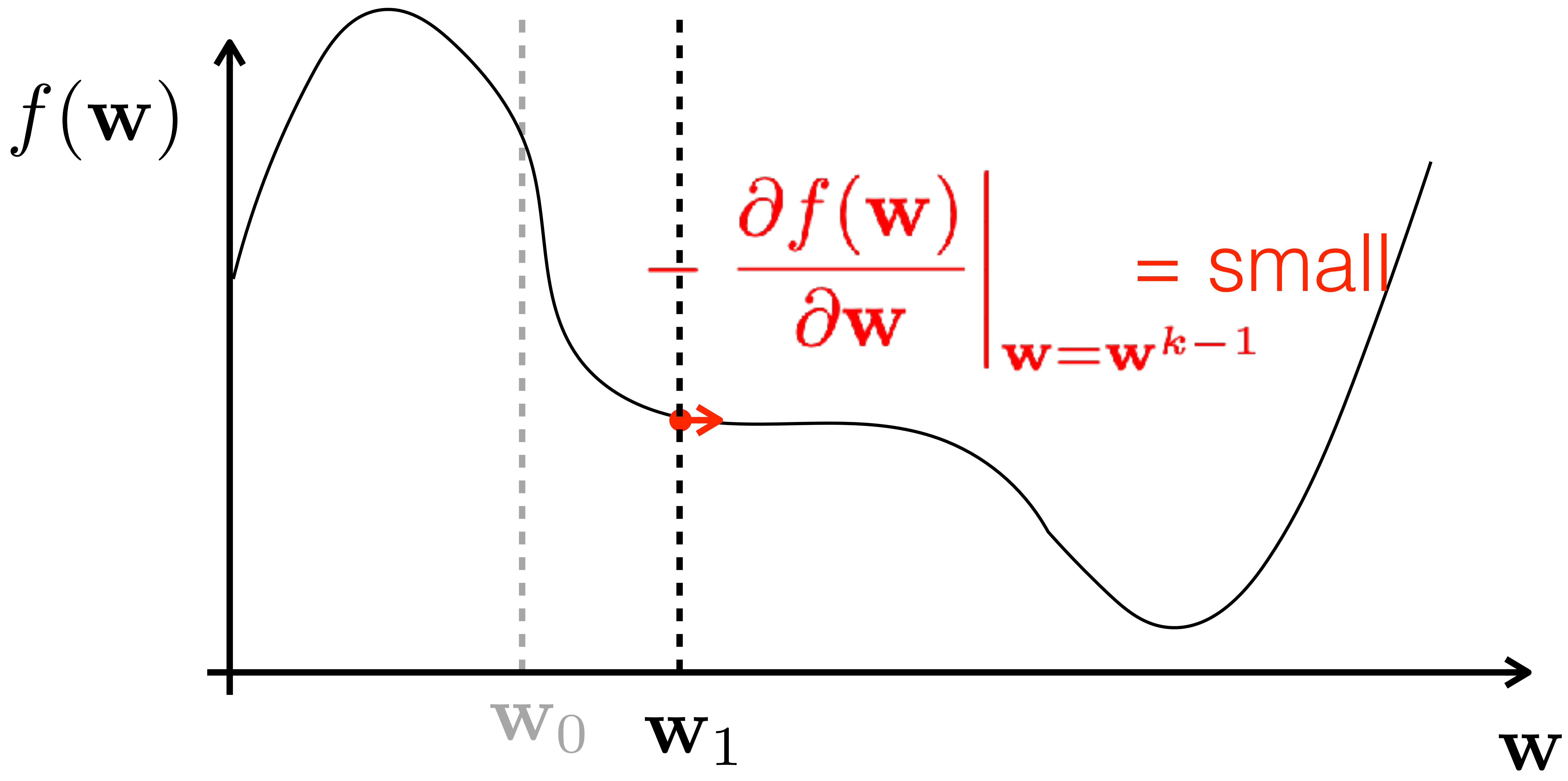

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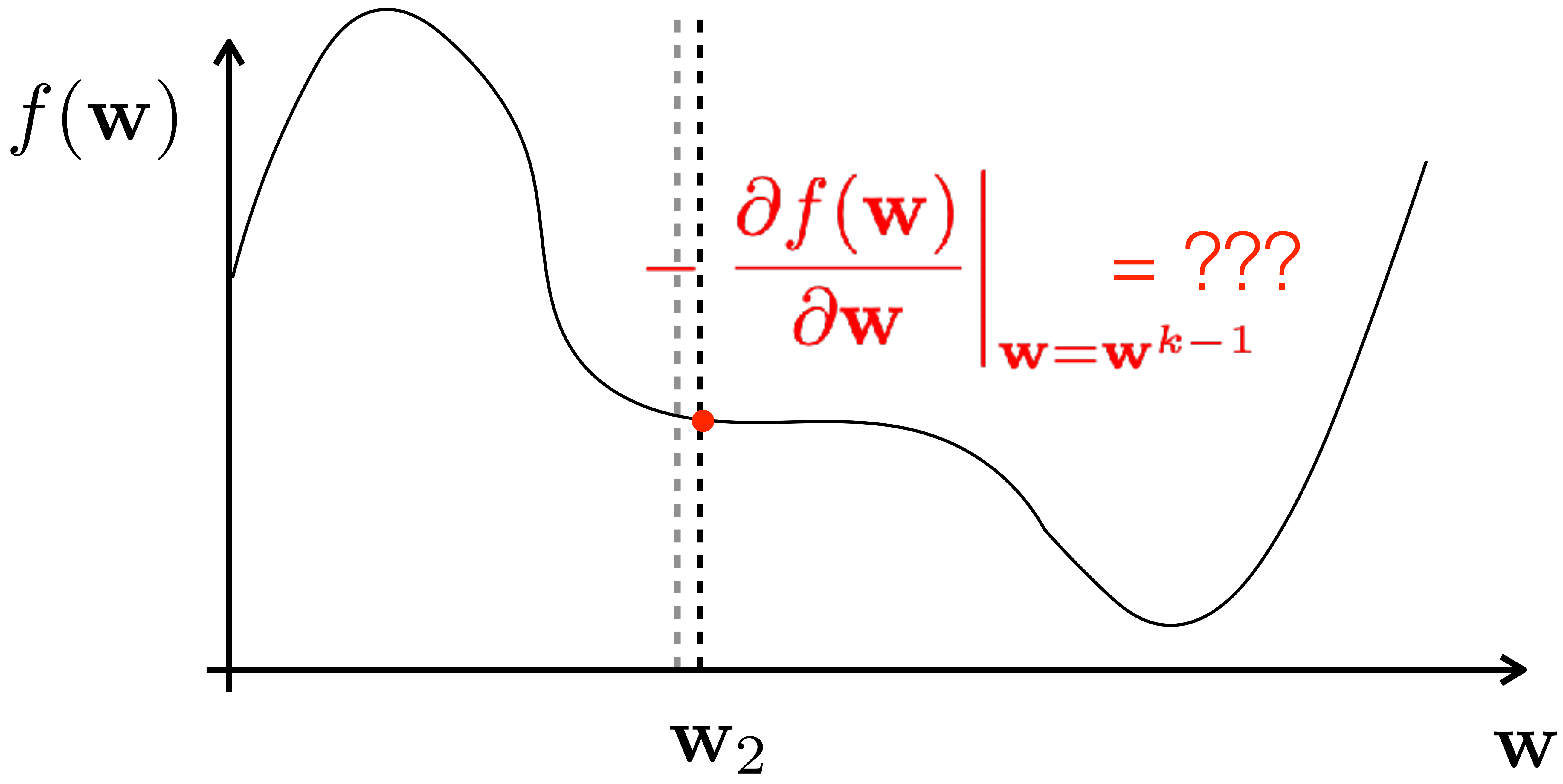

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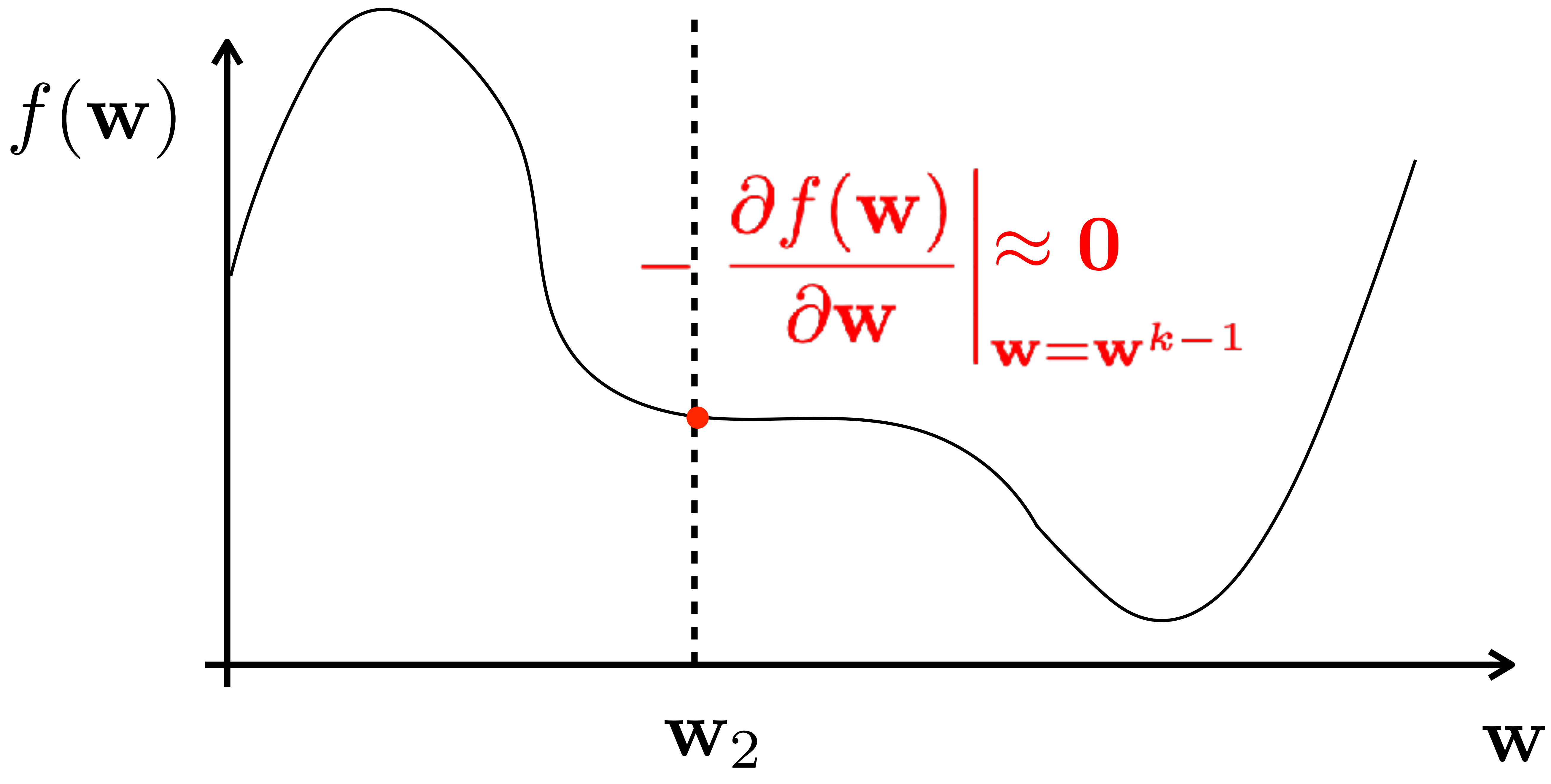
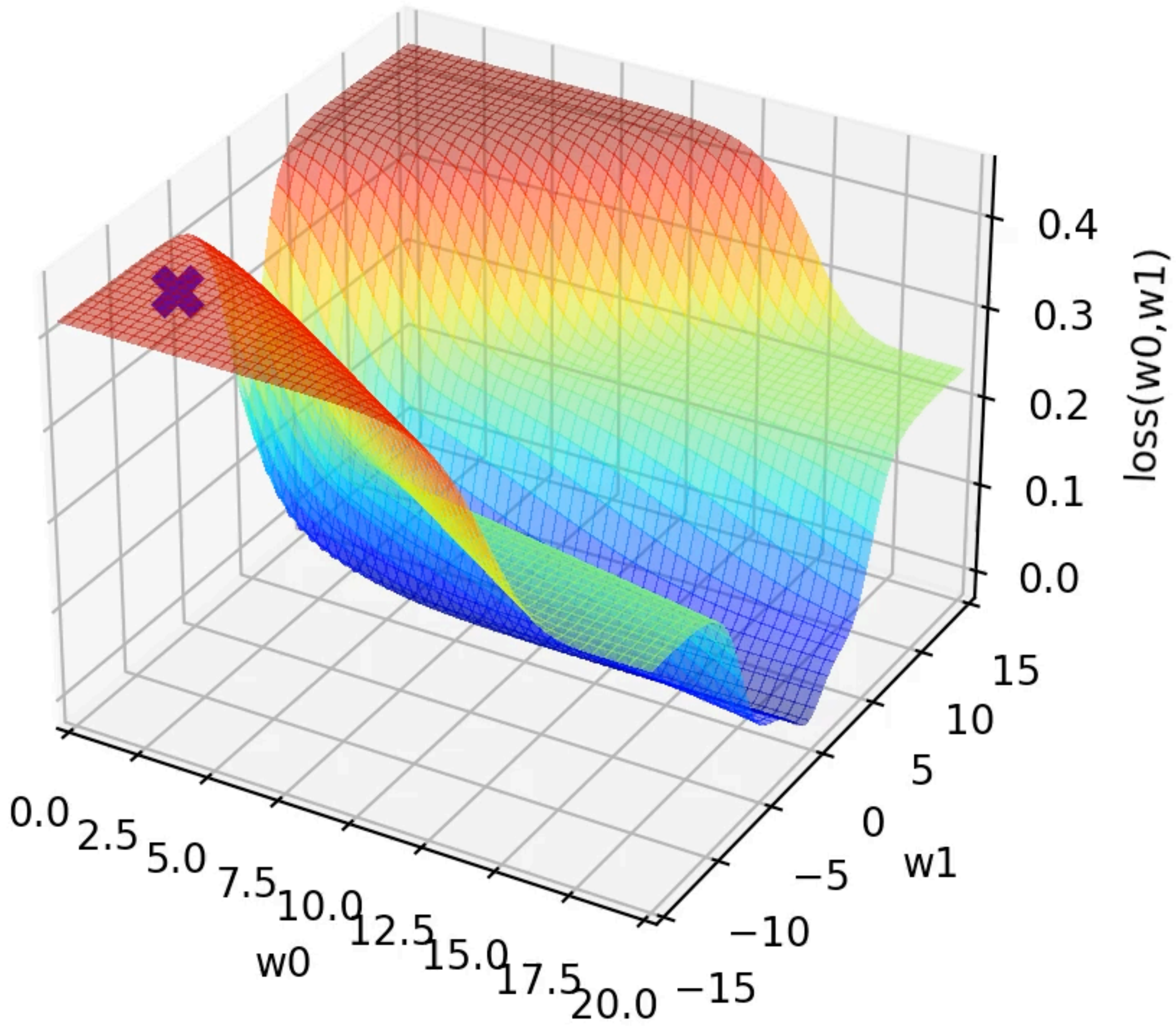


SGD drawbacks: Sigmoid fitting problem from labs



close-to-zero gradient plateaus

SGD drawbacks: oscillates

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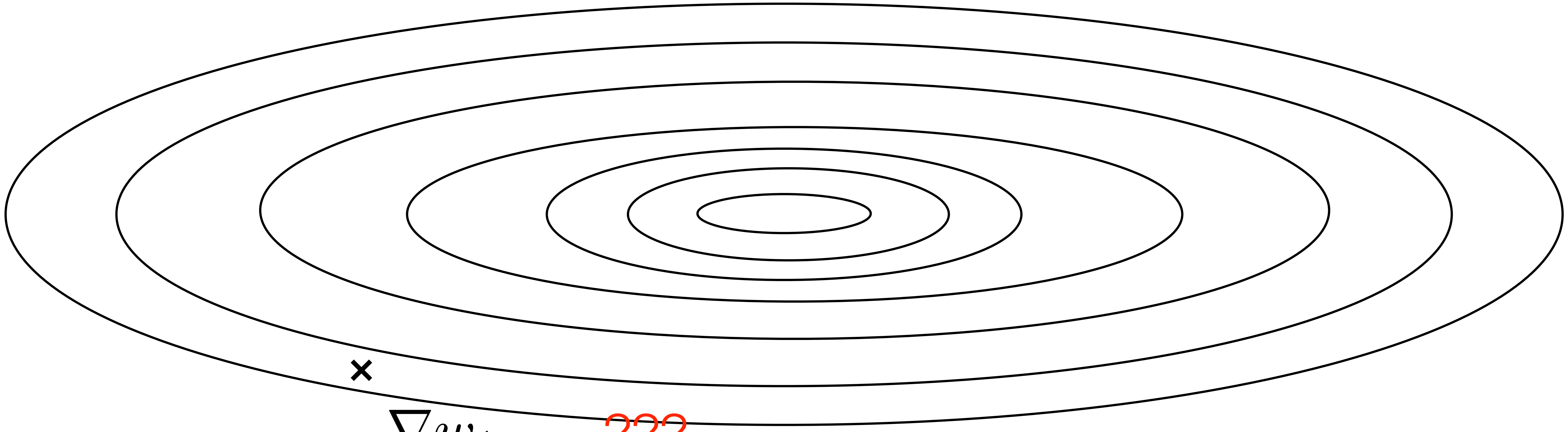

∇w_1 =???

∇w_2 =???

$$[\nabla w_1, \nabla w_2] = - \left.\frac{\partial f(\mathbf{w})}{\partial \mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}^{k-1}}$$

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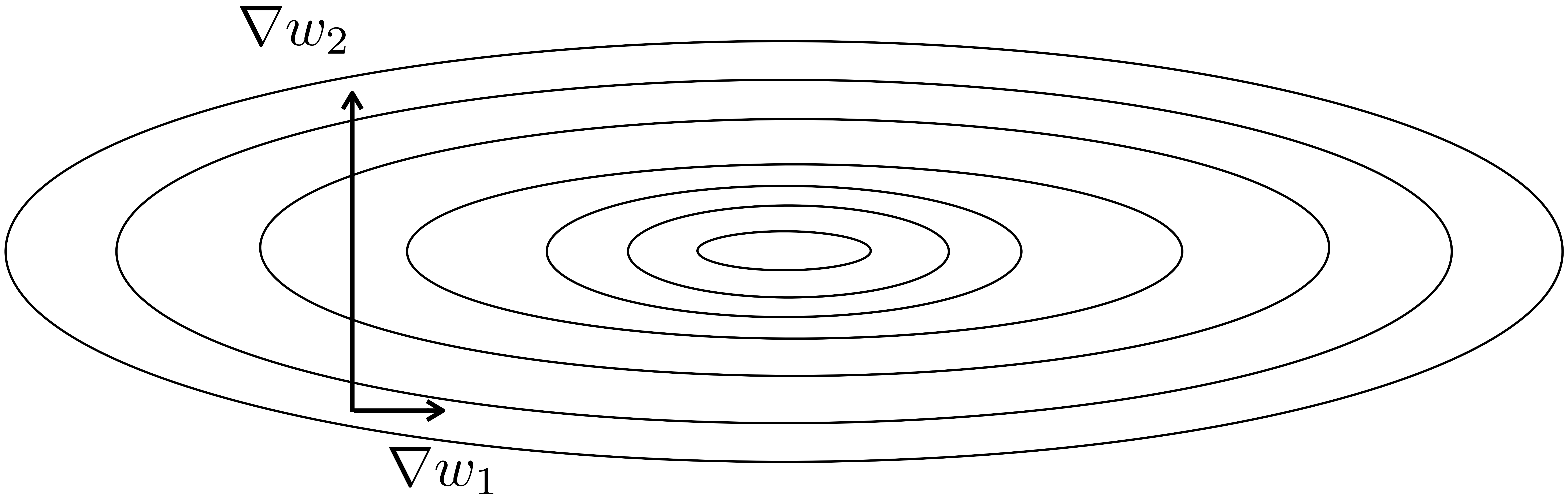

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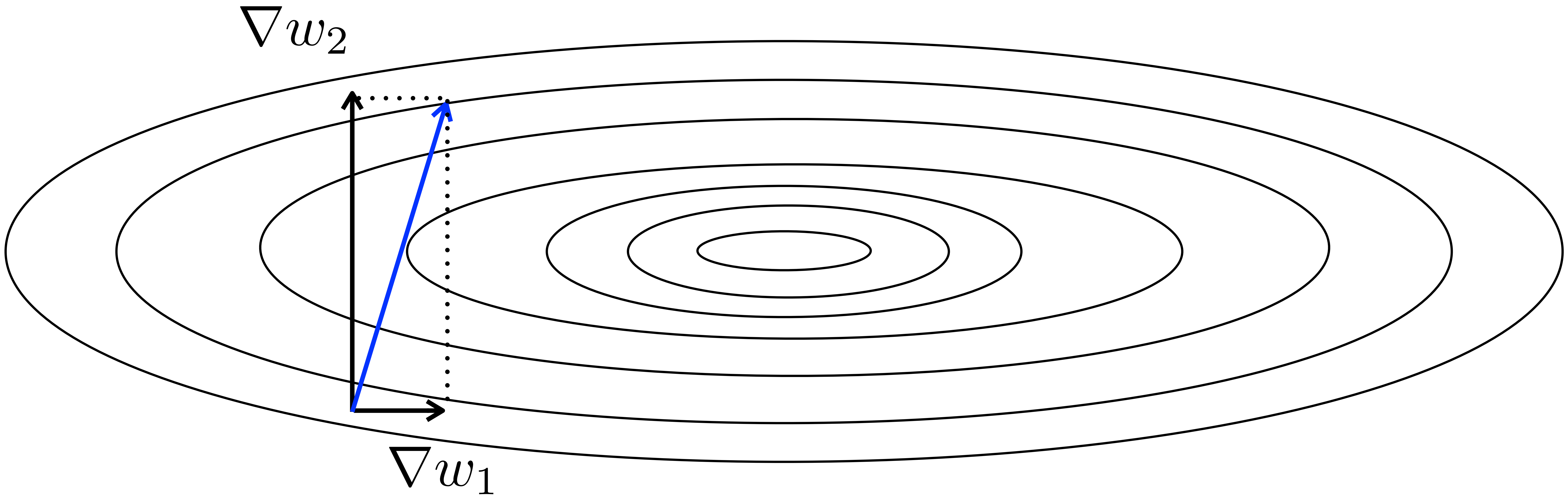

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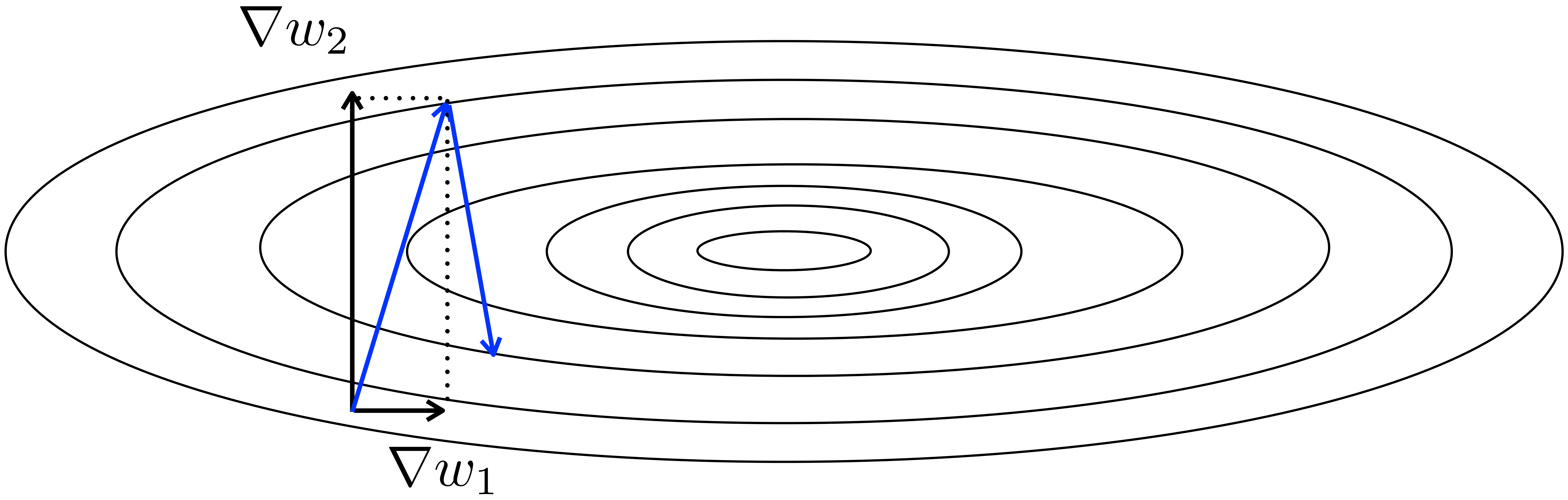

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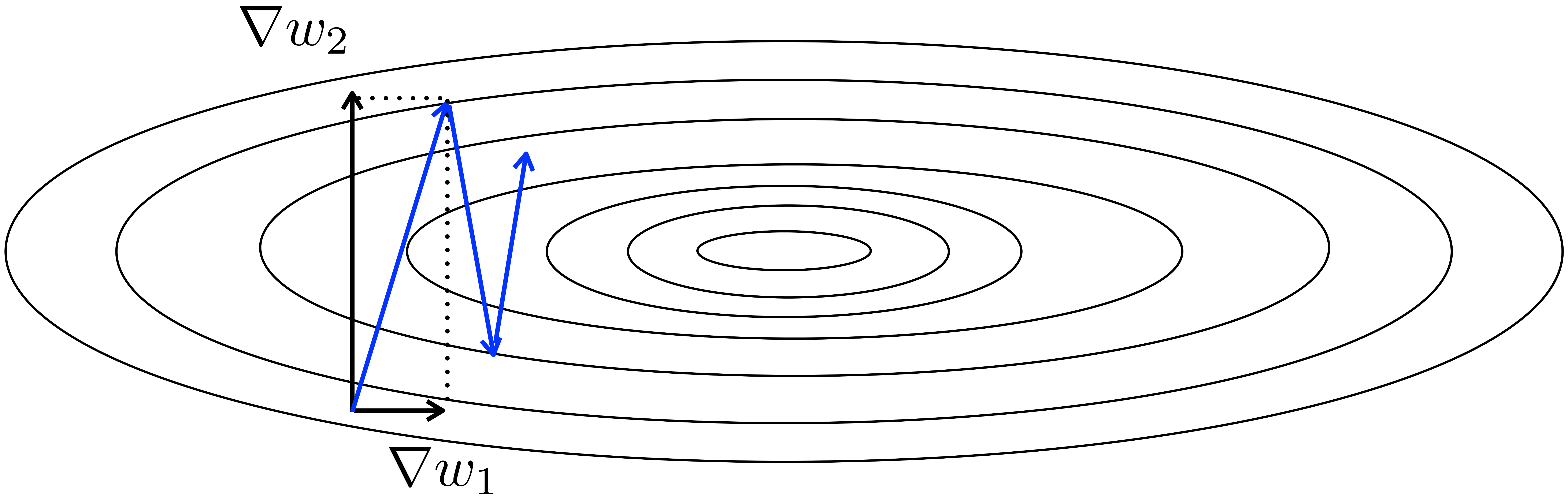

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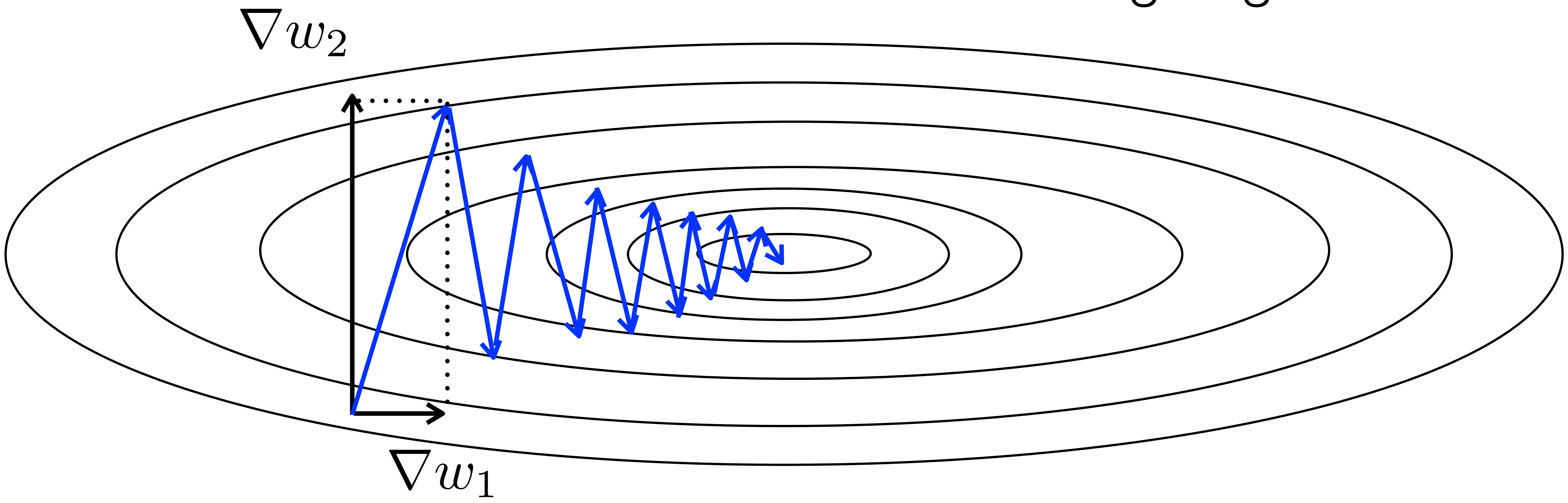
Undesired zig-zag behaviour



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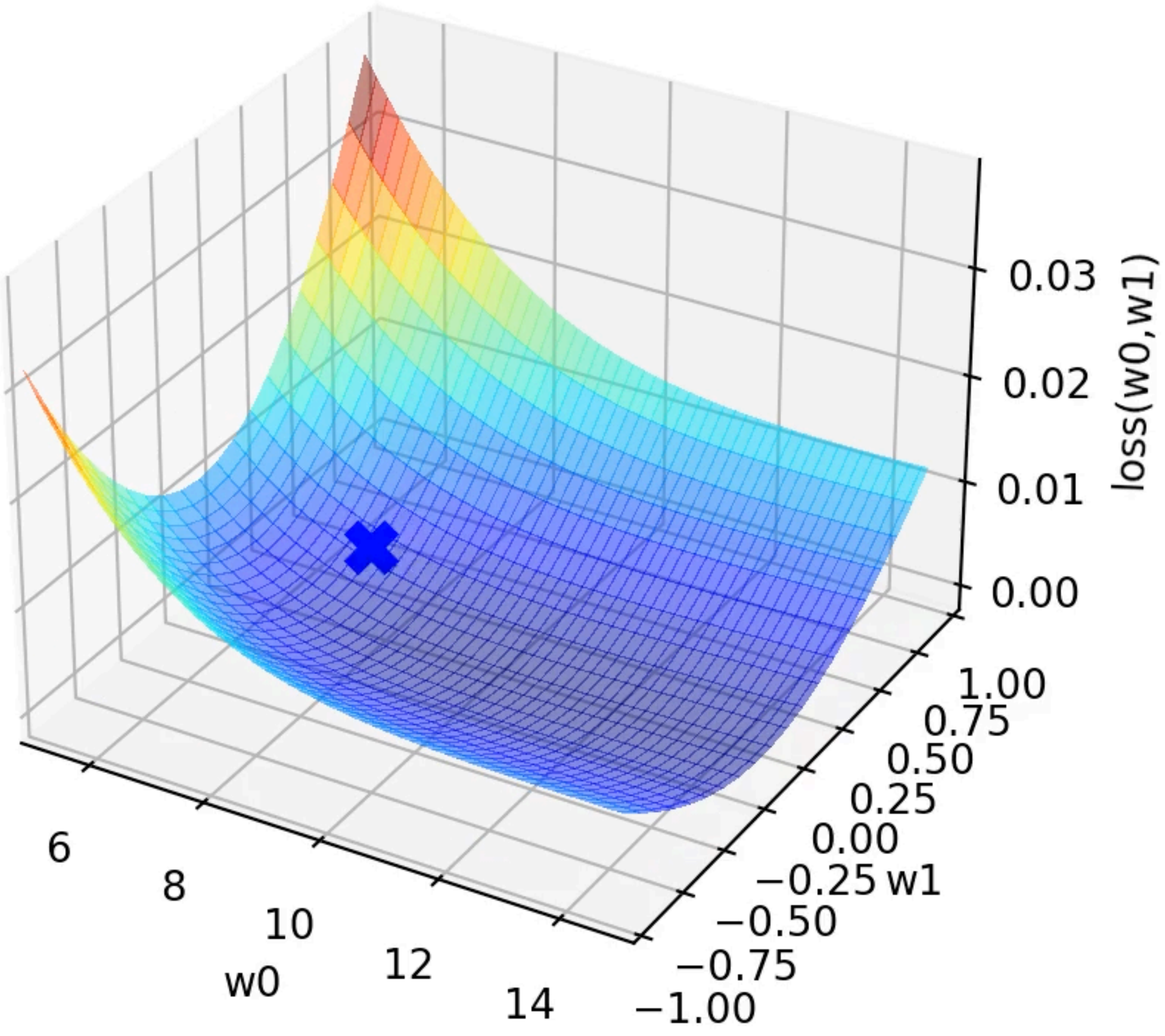
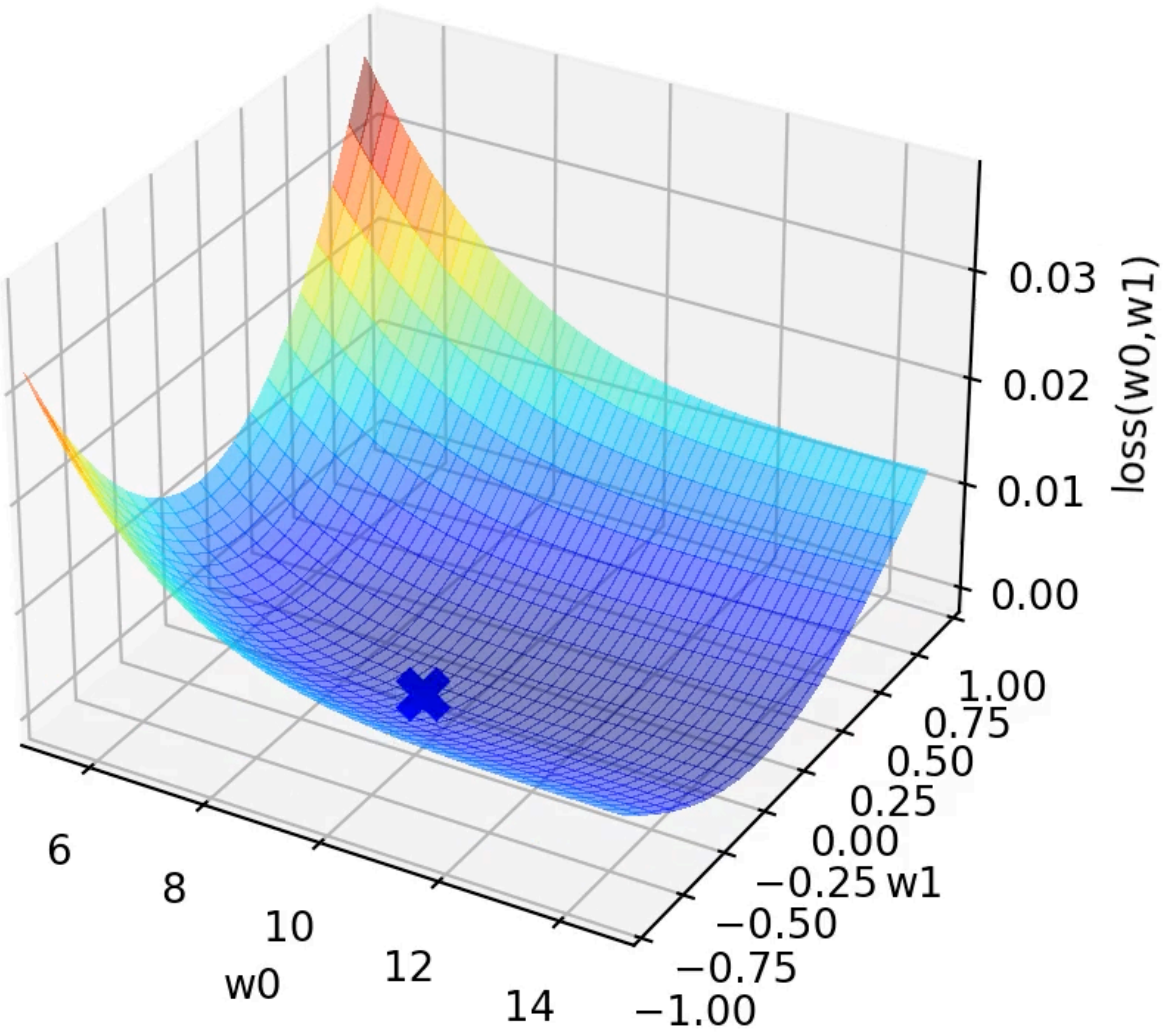


small learning rate



big learning rate

SGD drawbacks: oscillates

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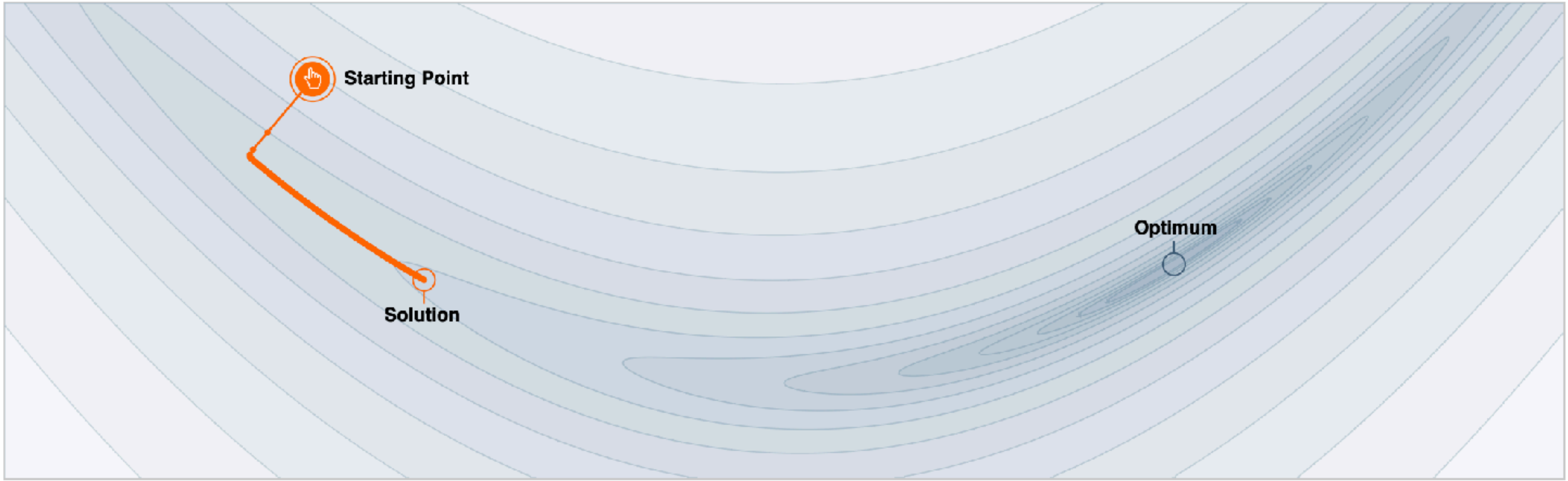
$\alpha =$ 1e-3



https://distill.pub/2017/momentum/

SGD drawbacks: oscillates

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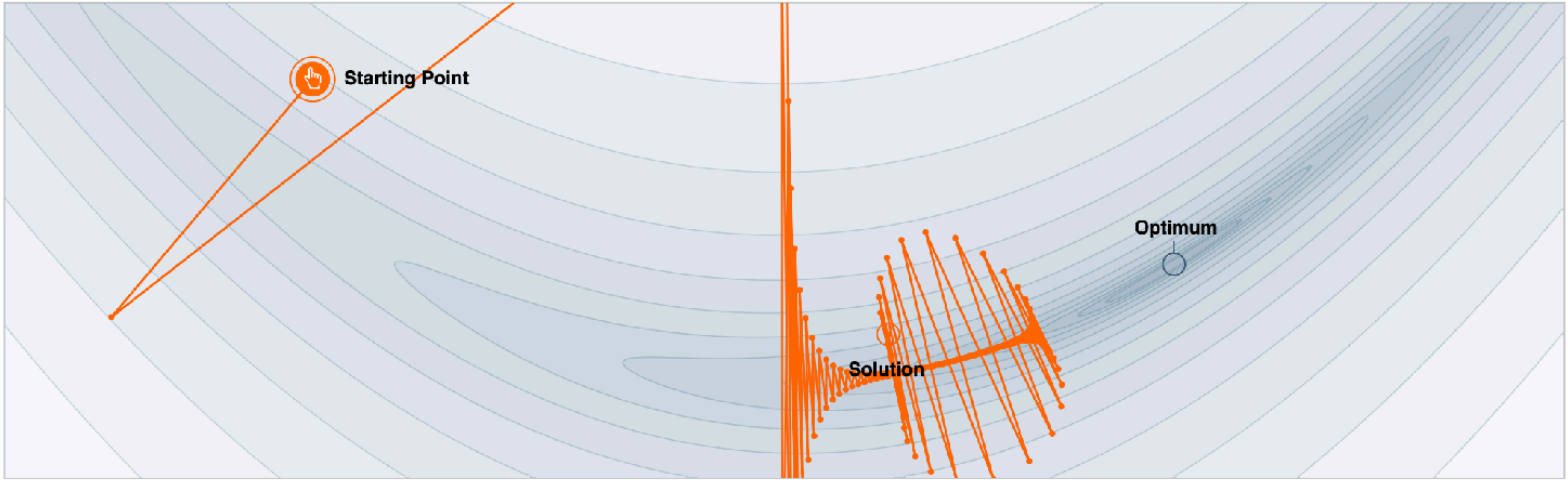
$\alpha =$ 5e-3



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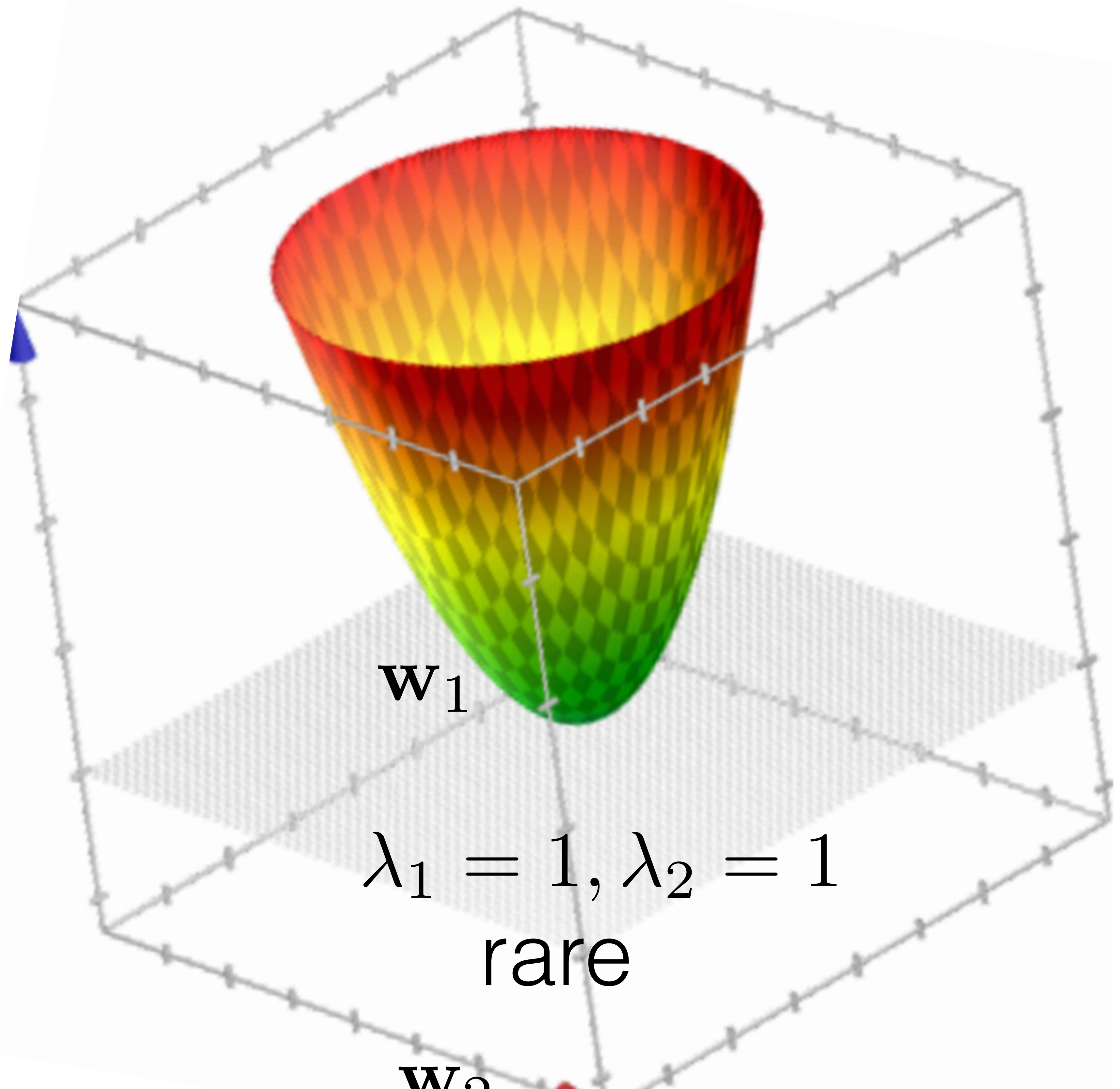
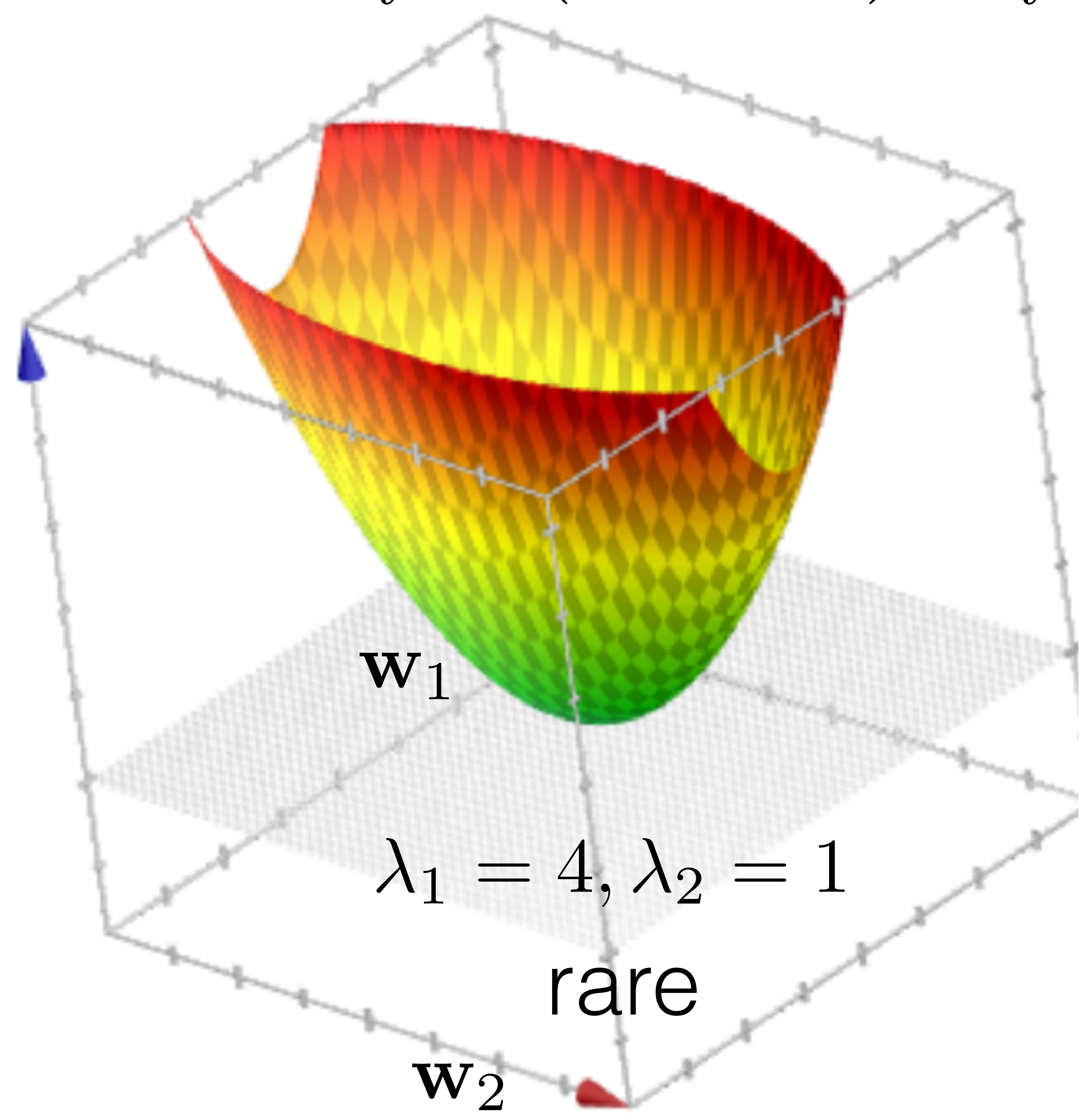
SGD on quadric

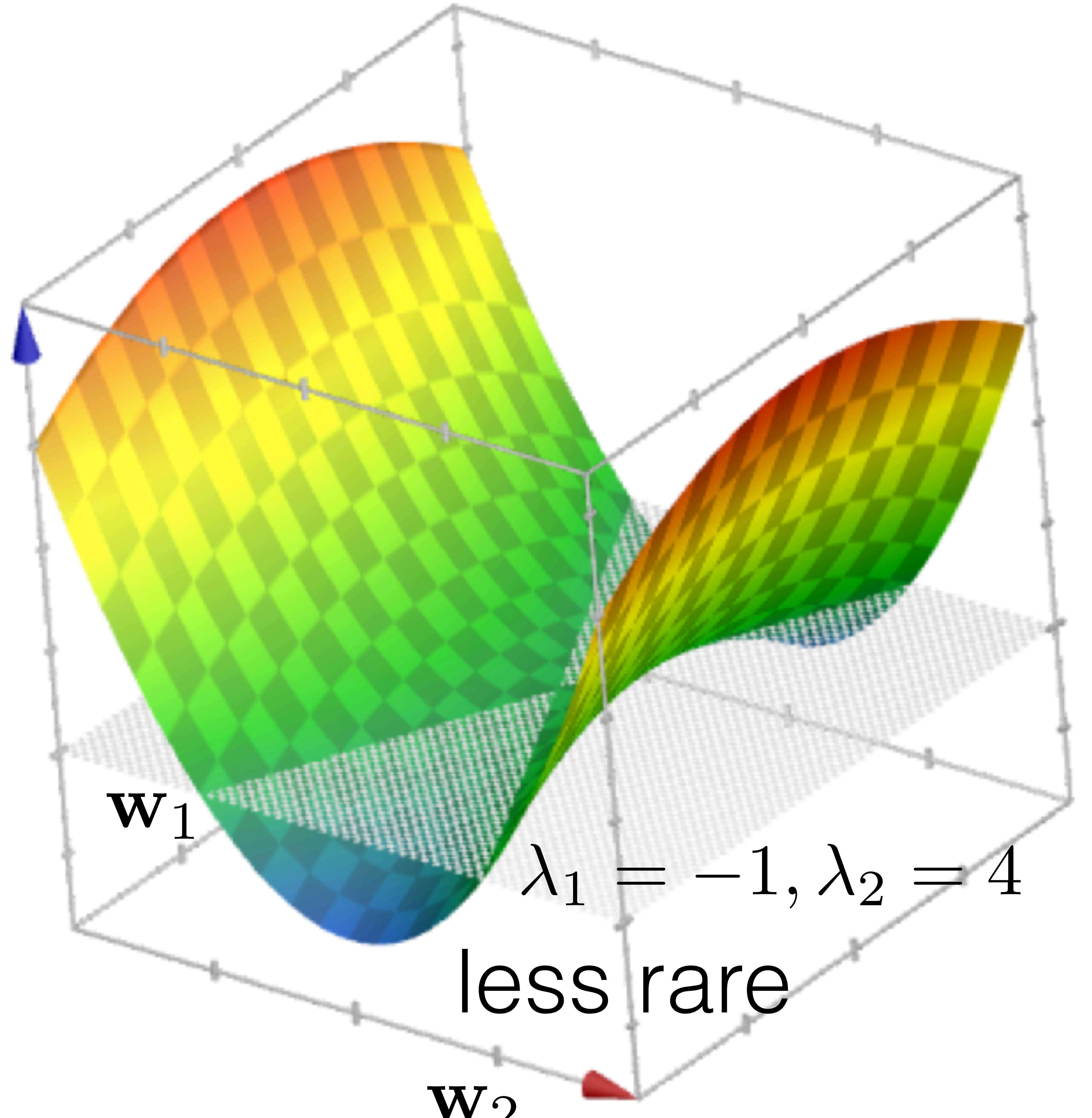
Criterion: $f(\mathbf{w}) = \frac{1}{2}\mathbf{w}^\top \mathtt{A}\mathbf{w}$ with $\mathtt{A} = \mathrm{diag}([\lambda_1, \dots, \lambda_n])$

Gradient: $\left.\frac{\partial f(\mathbf{w})}{\partial \mathbf{w}_i}\right|_{\mathbf{w}_i = \mathbf{w}_i^{k-1}} = \lambda_i \mathbf{w}_i^{k-1}$

SGD after k iterations: $\mathbf{w}_i^k = (1 - \alpha\lambda_i)^k \mathbf{w}_i^0$







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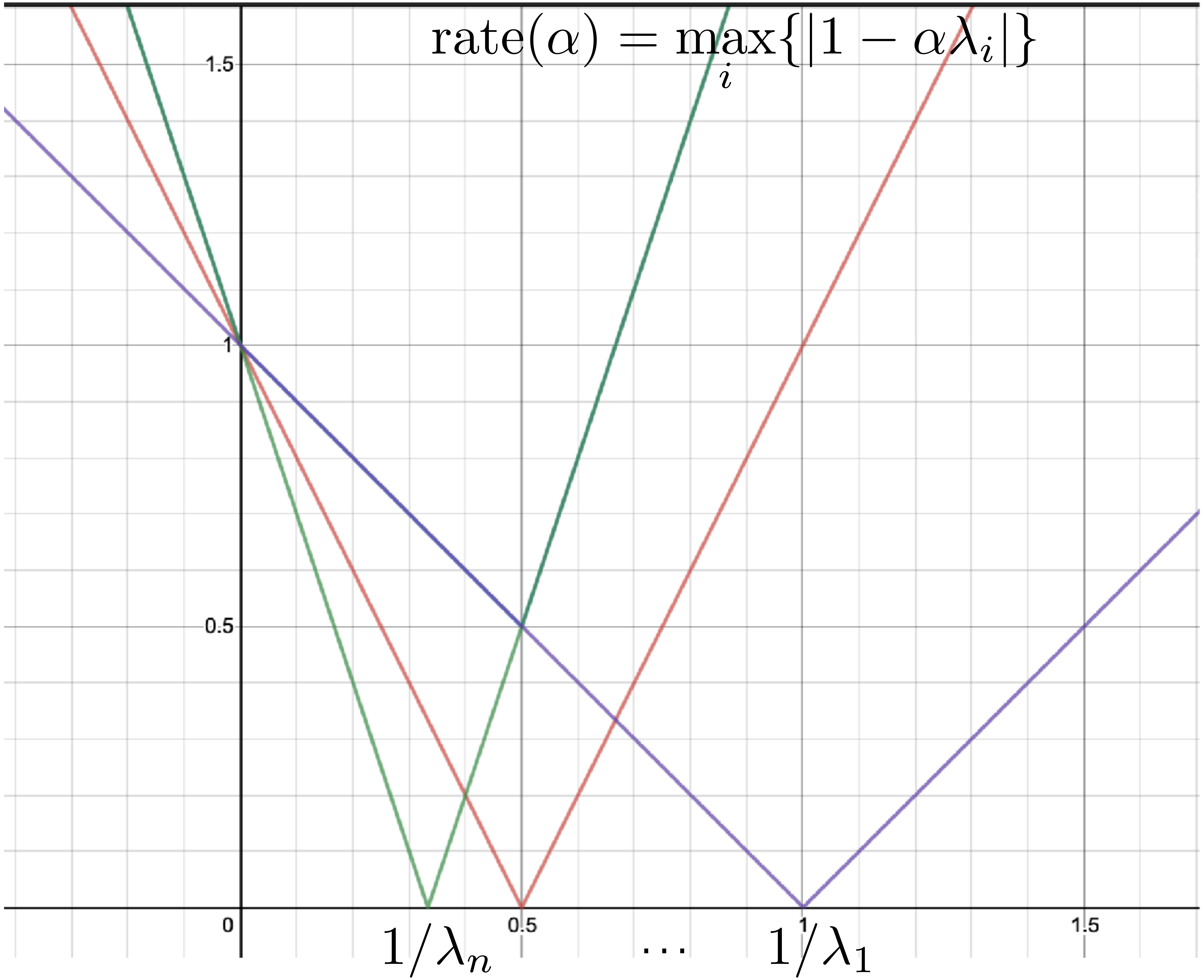
Gradient: $\left.\frac{\partial f(\mathbf{w})}{\partial \mathbf{w}_i}\right|_{\mathbf{w}_i = \mathbf{w}_i^{k-1}} = \lambda_i \mathbf{w}_i^{k-1}$

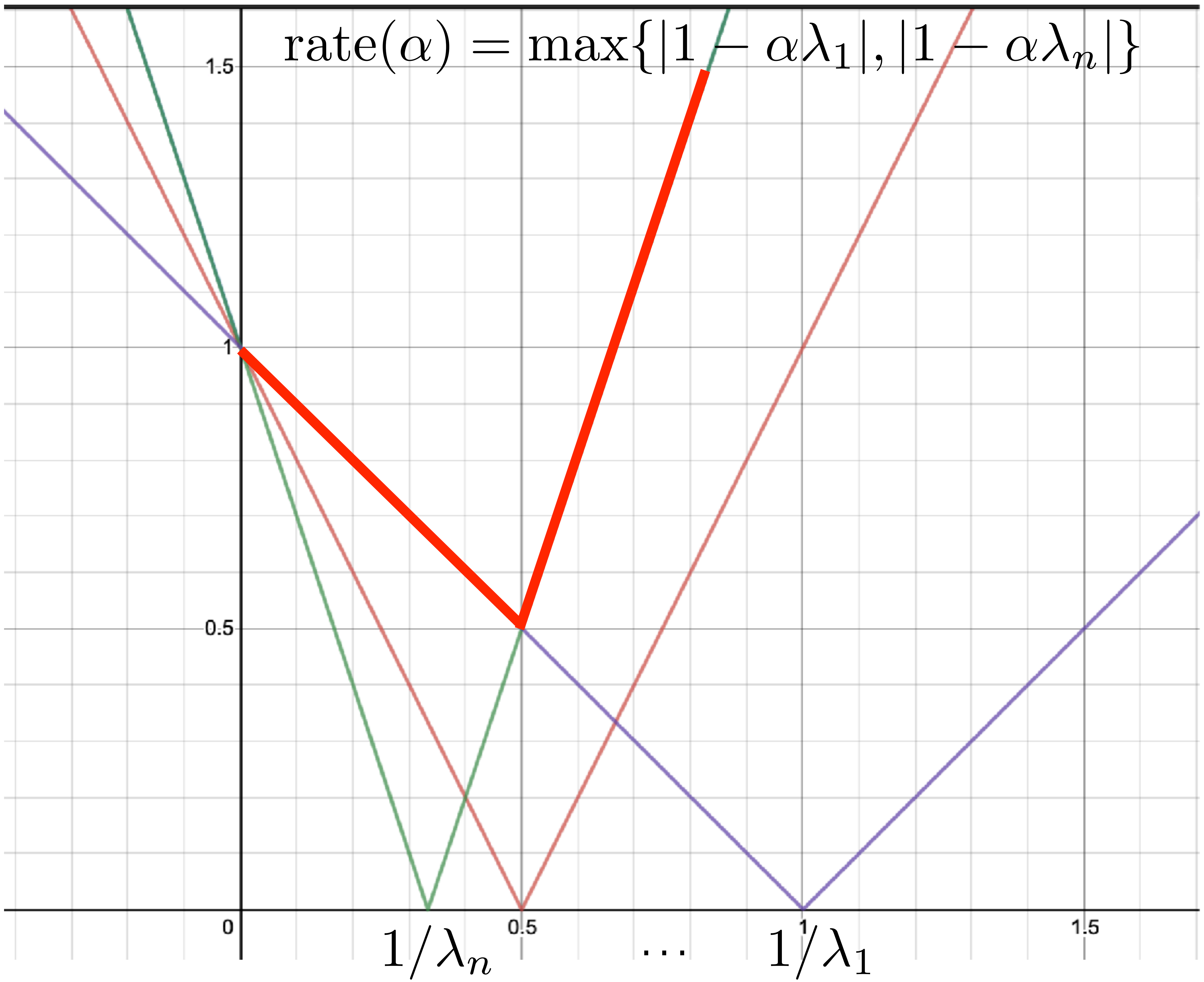
SGD after k iterations: $\mathbf{w}_i^k = (1 - \alpha\lambda_i)^k \mathbf{w}_i^0$

- Converges for: $0 < \alpha\lambda_i < 2$
- with convergence rate: $\mathrm{rate}(\alpha) = \max_i\{|1 - \alpha\lambda_i|\}$

SGD on quadric



SGD on quadric



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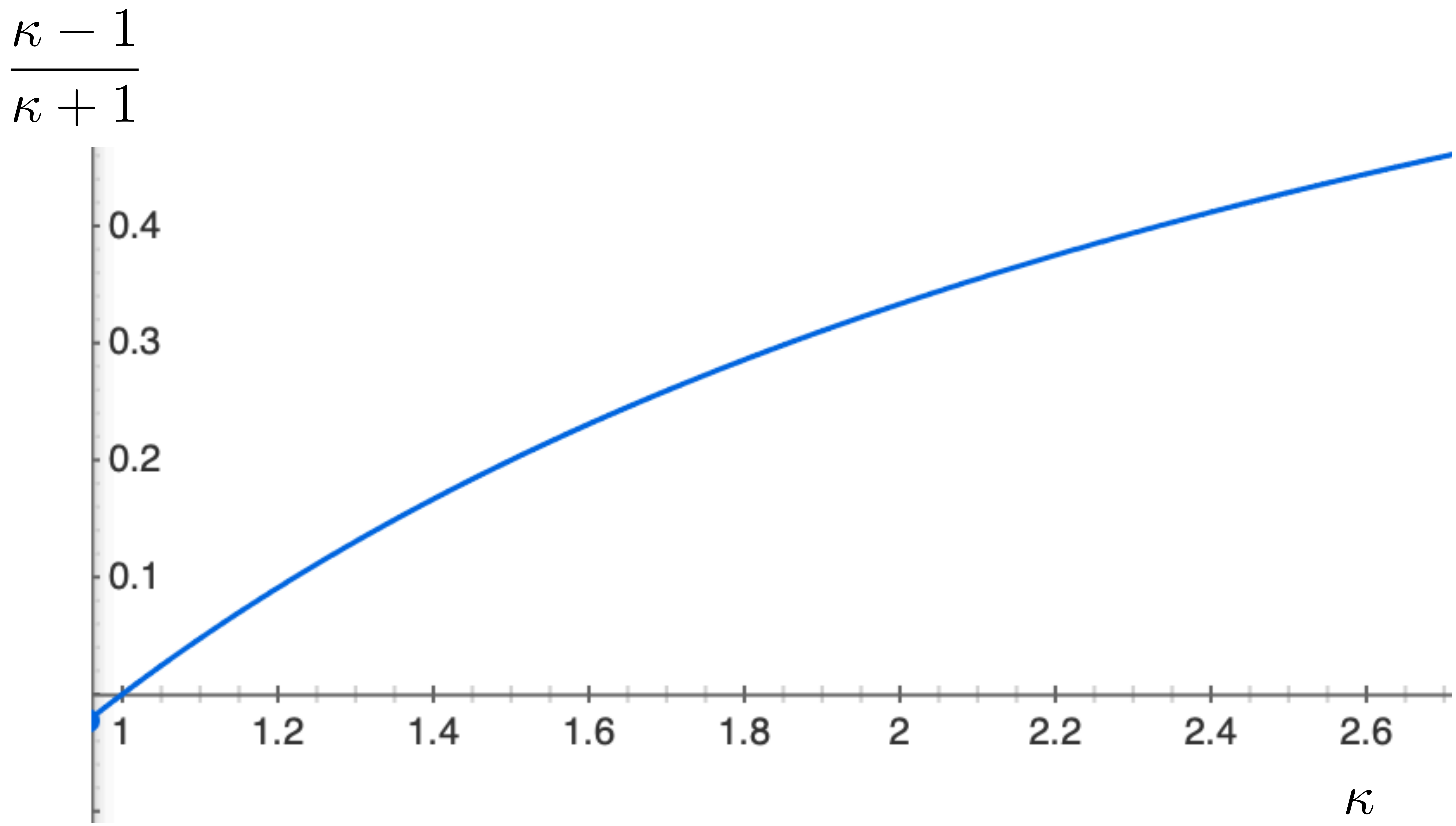
- Optimal conv. rate: $\mathrm{rate}(\alpha^*) = \min_\alpha \big(\mathrm{rate}(\alpha)\big) = \frac{\frac{\lambda_n}{\lambda_1} - 1}{\frac{\lambda_n}{\lambda_1} + 1}$
  where $\kappa = \frac{\lambda_n}{\lambda_1}$ is condition number

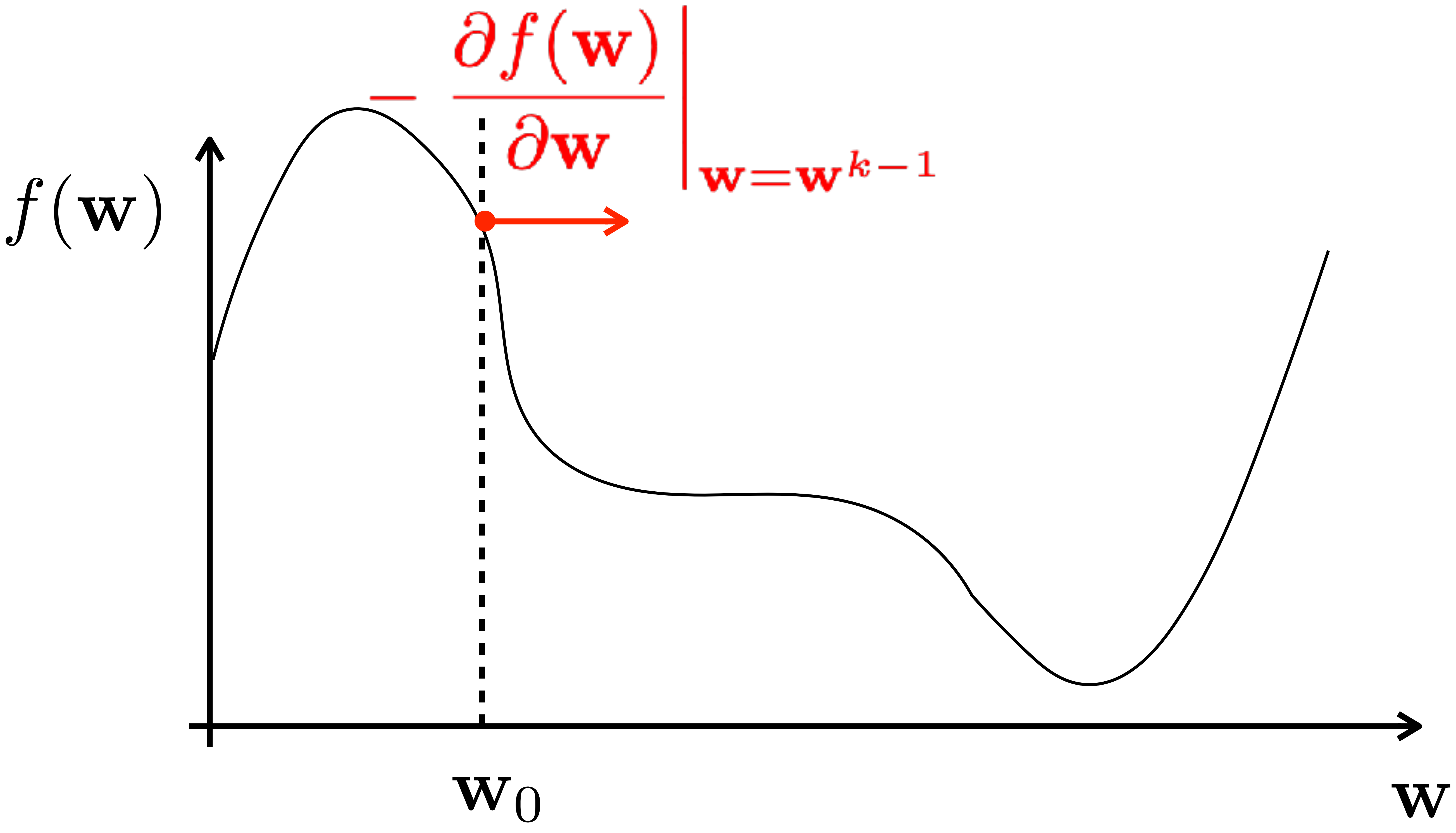
SGD on quadric



SGD + momentum

$$\mathbf{v}^k = \beta \mathbf{v}^{k-1} - \frac{\partial f^\top(\mathbf{w})}{\partial \mathbf{w}}\bigg|_{\mathbf{w}=\mathbf{w}^{k-1}}$$

$$\mathbf{w}^k = \mathbf{w}^{k-1} + \alpha \mathbf{v}^k$$



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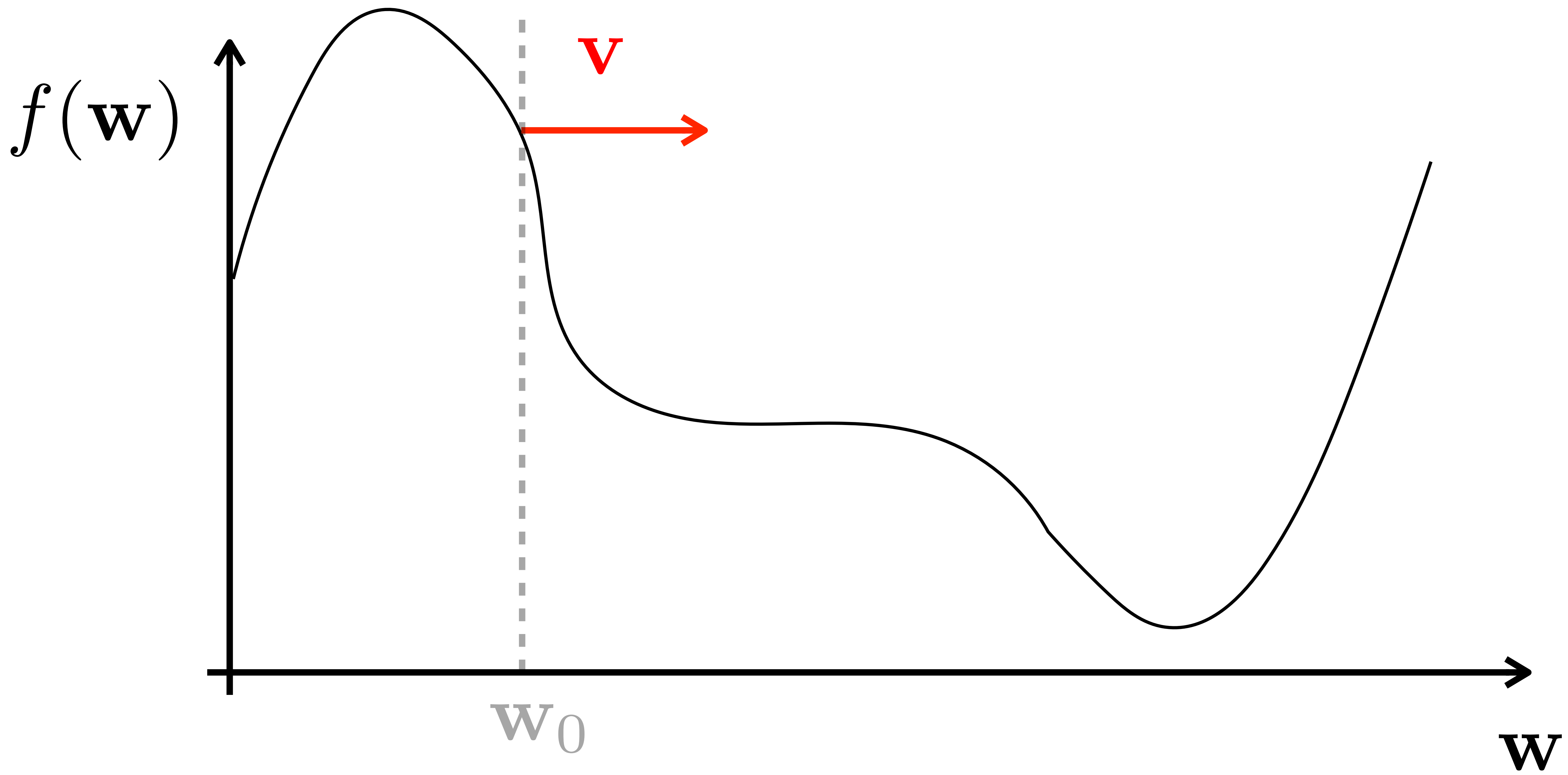

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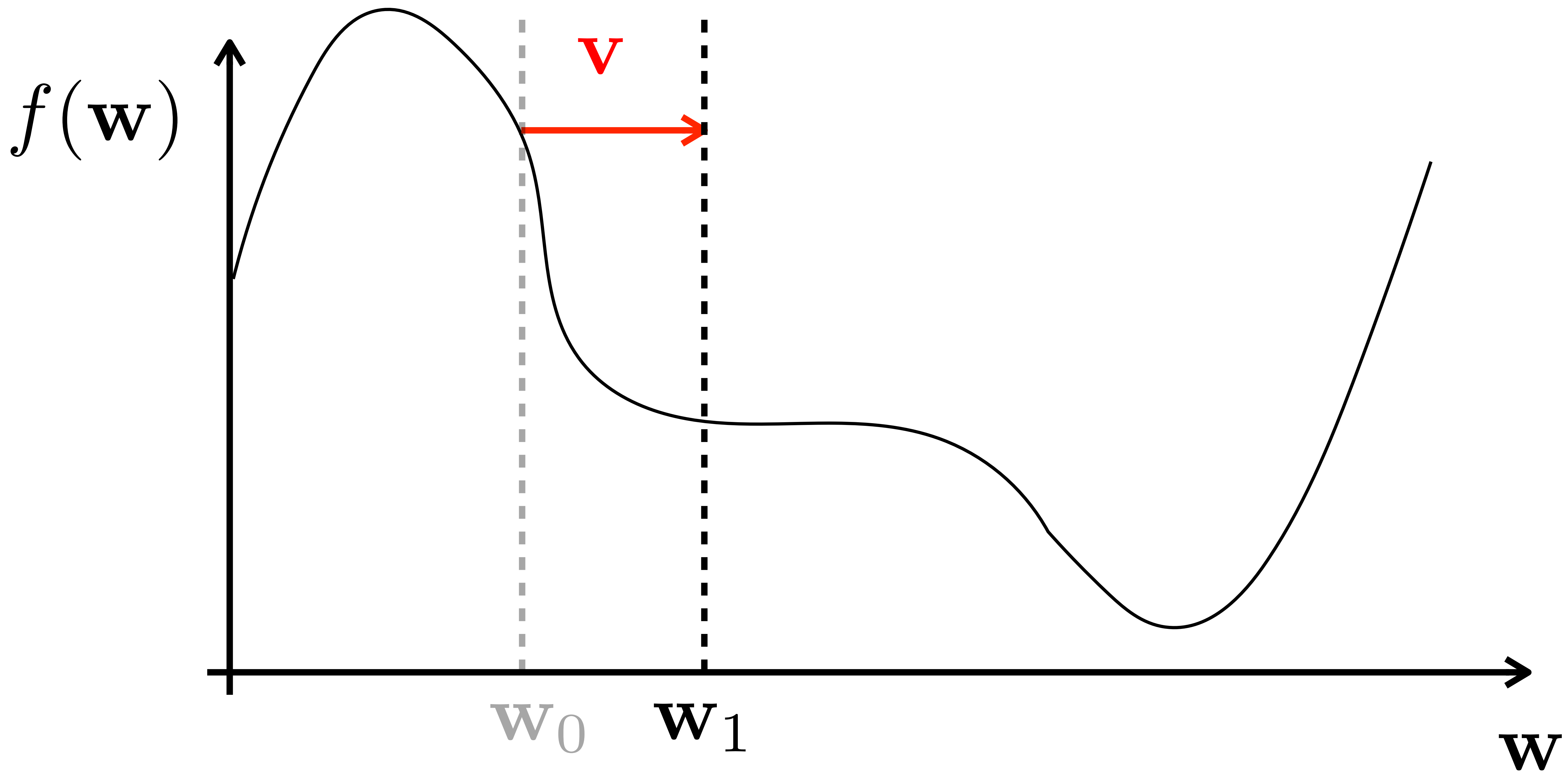

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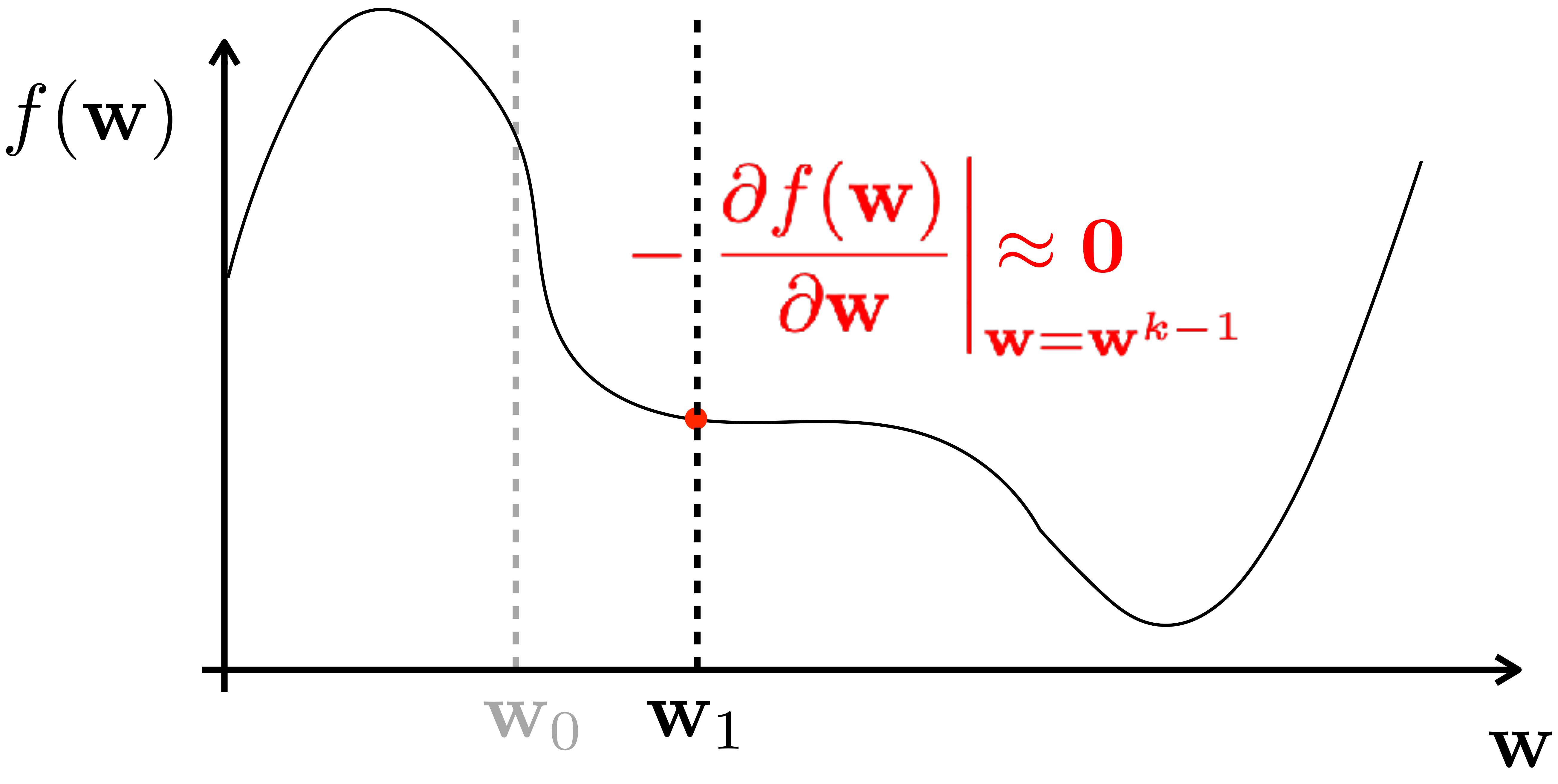

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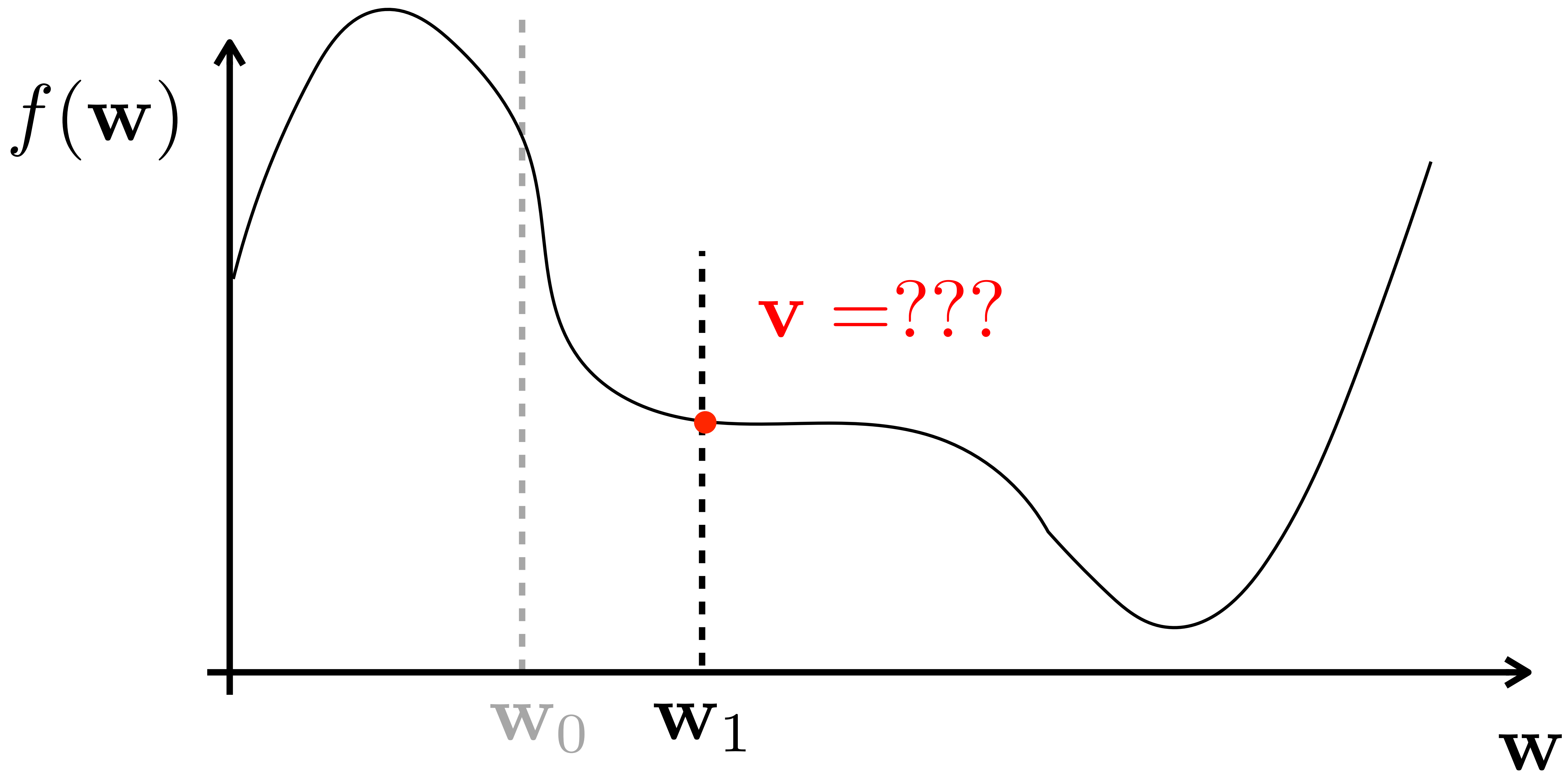
- Build velocity $\mathbf{v}$ as running average of gradients
- Rolling ball with velocity $\mathbf{v}$ and friction coeff β



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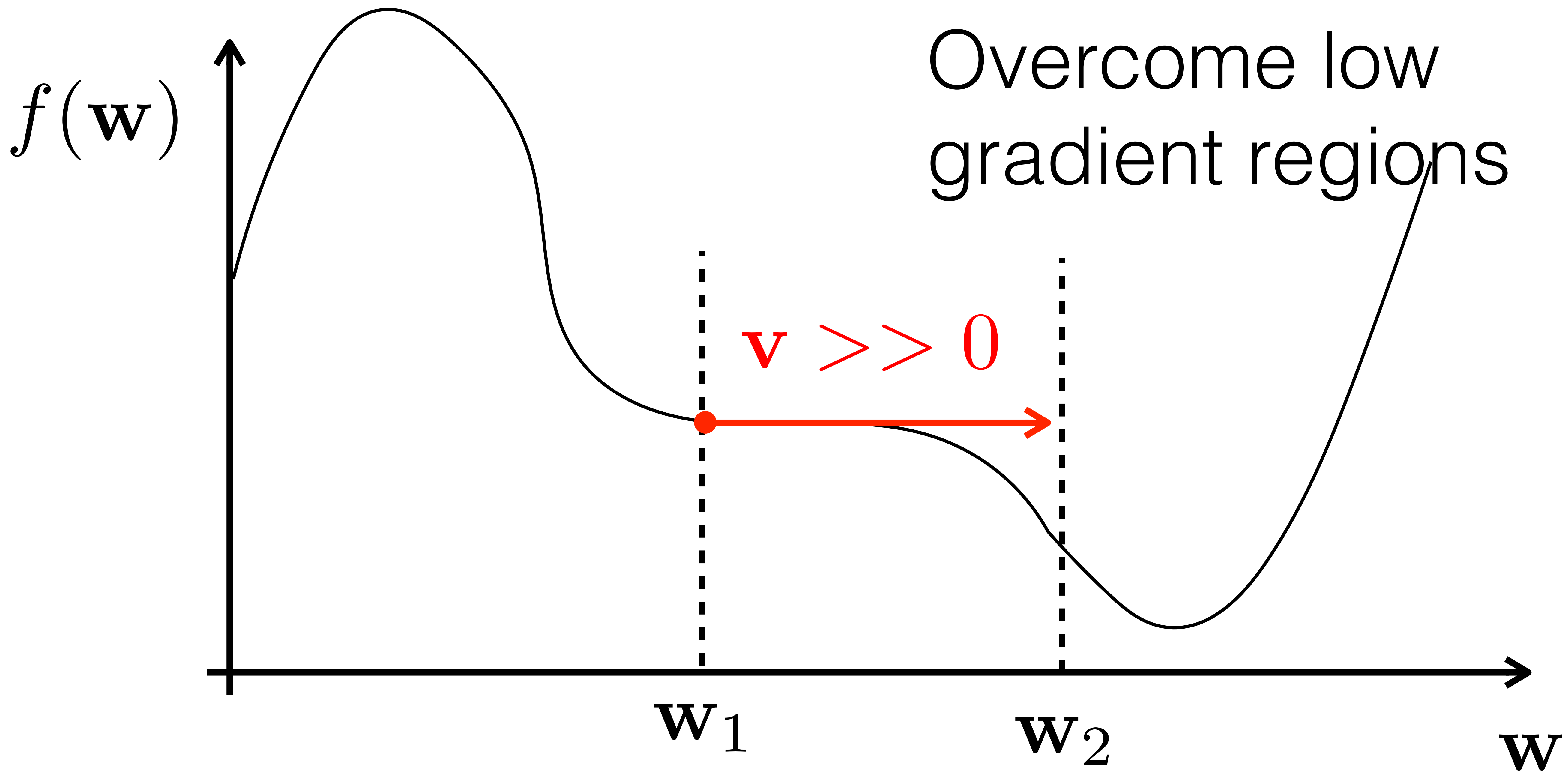

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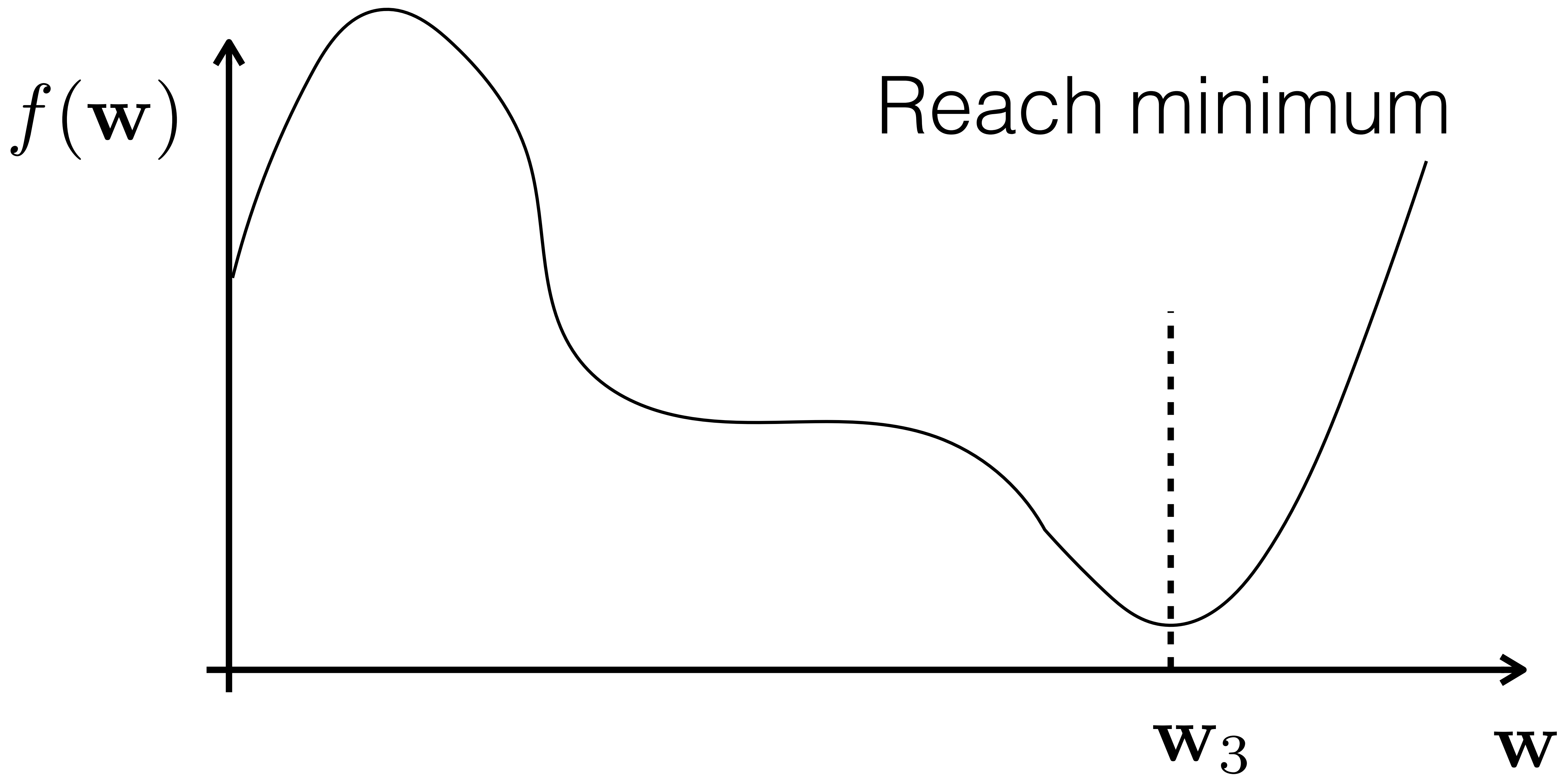

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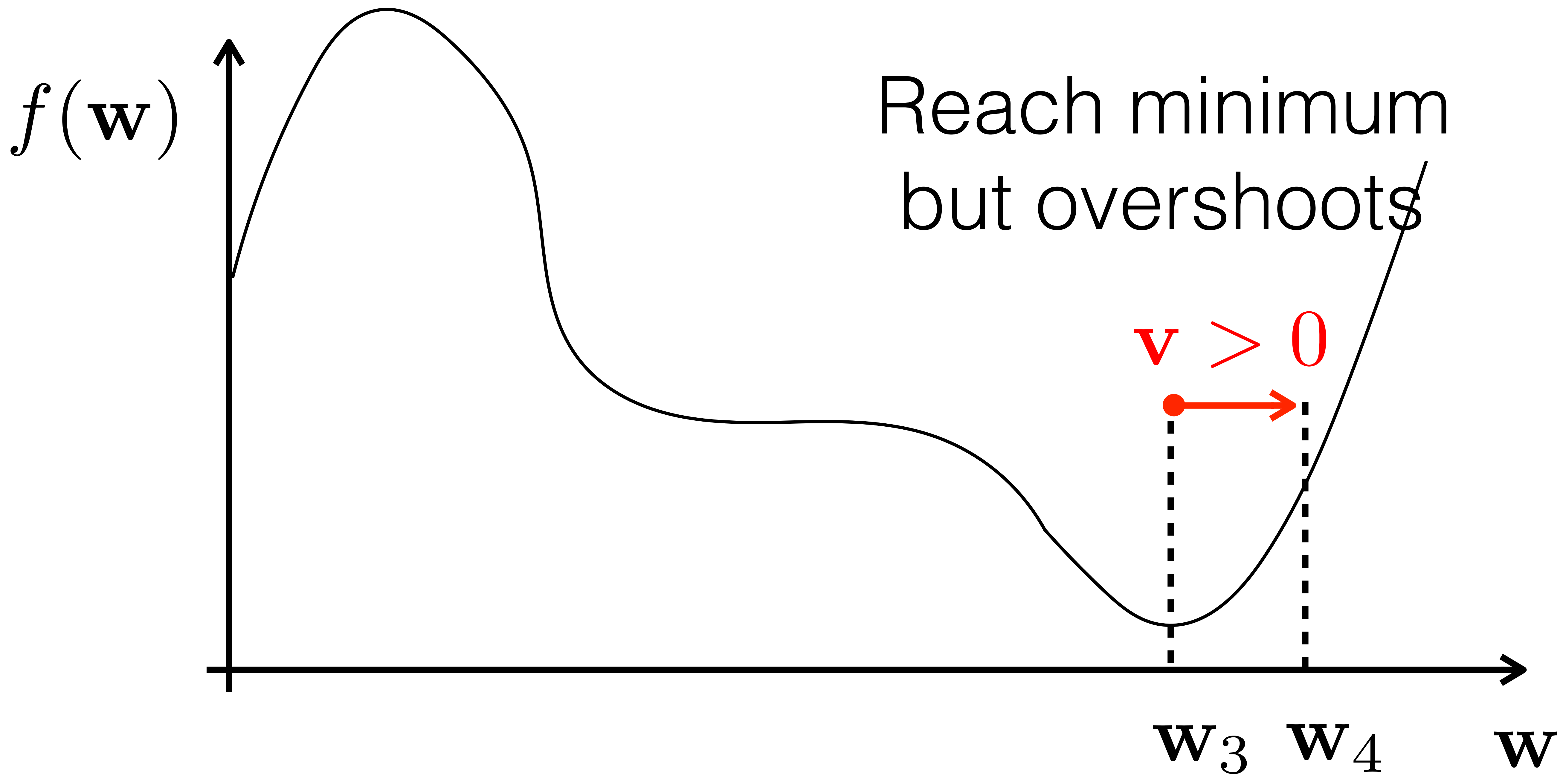

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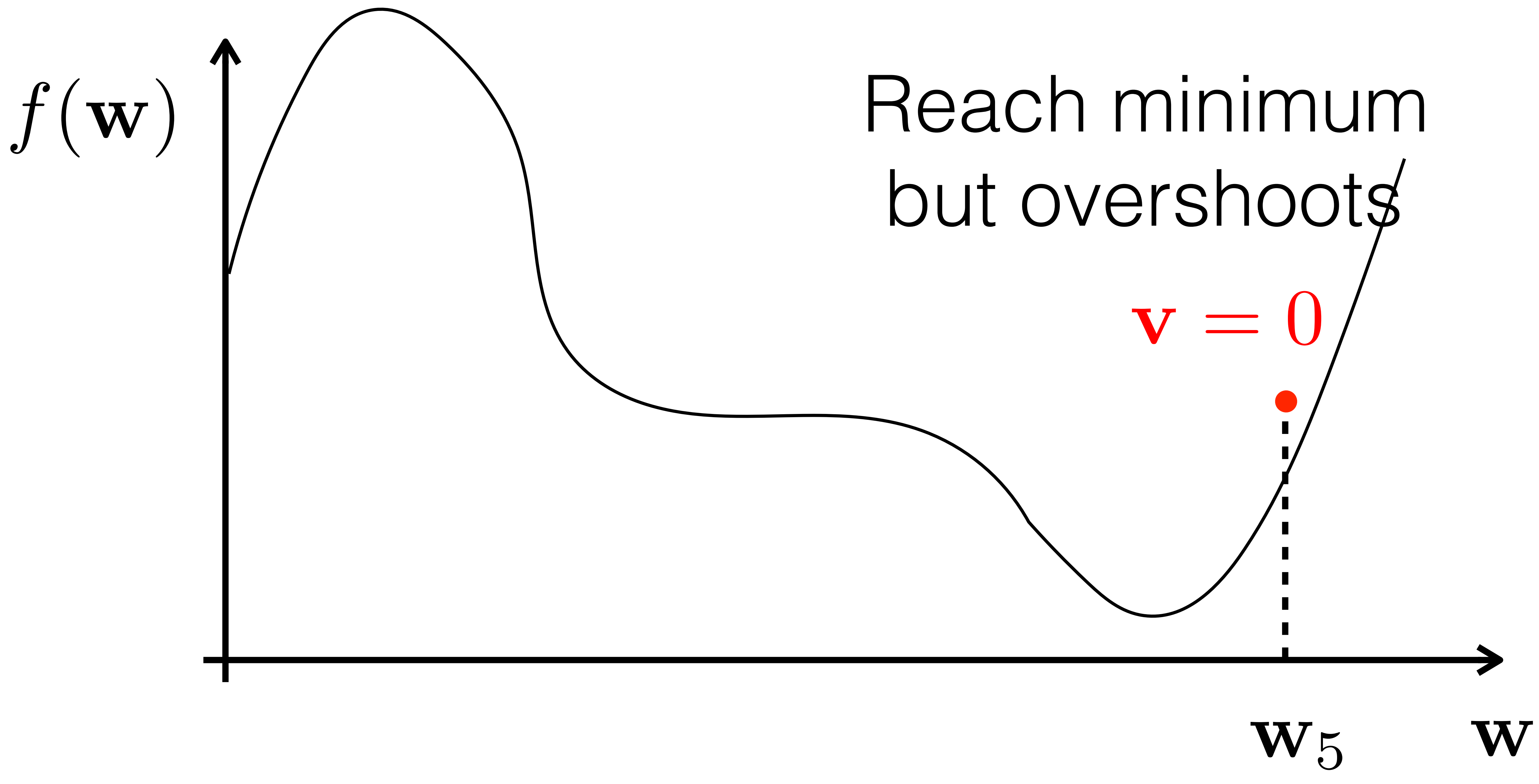

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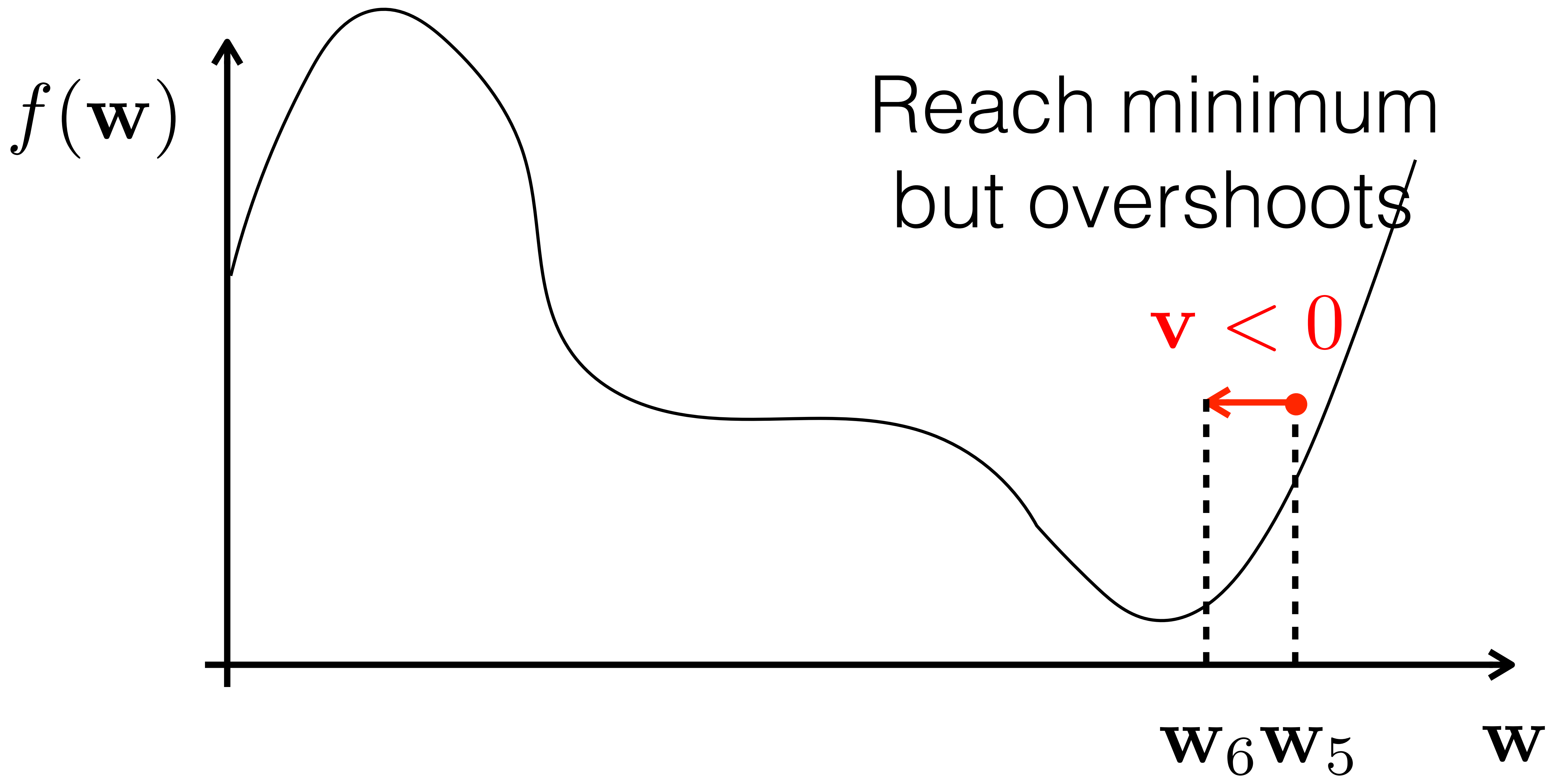

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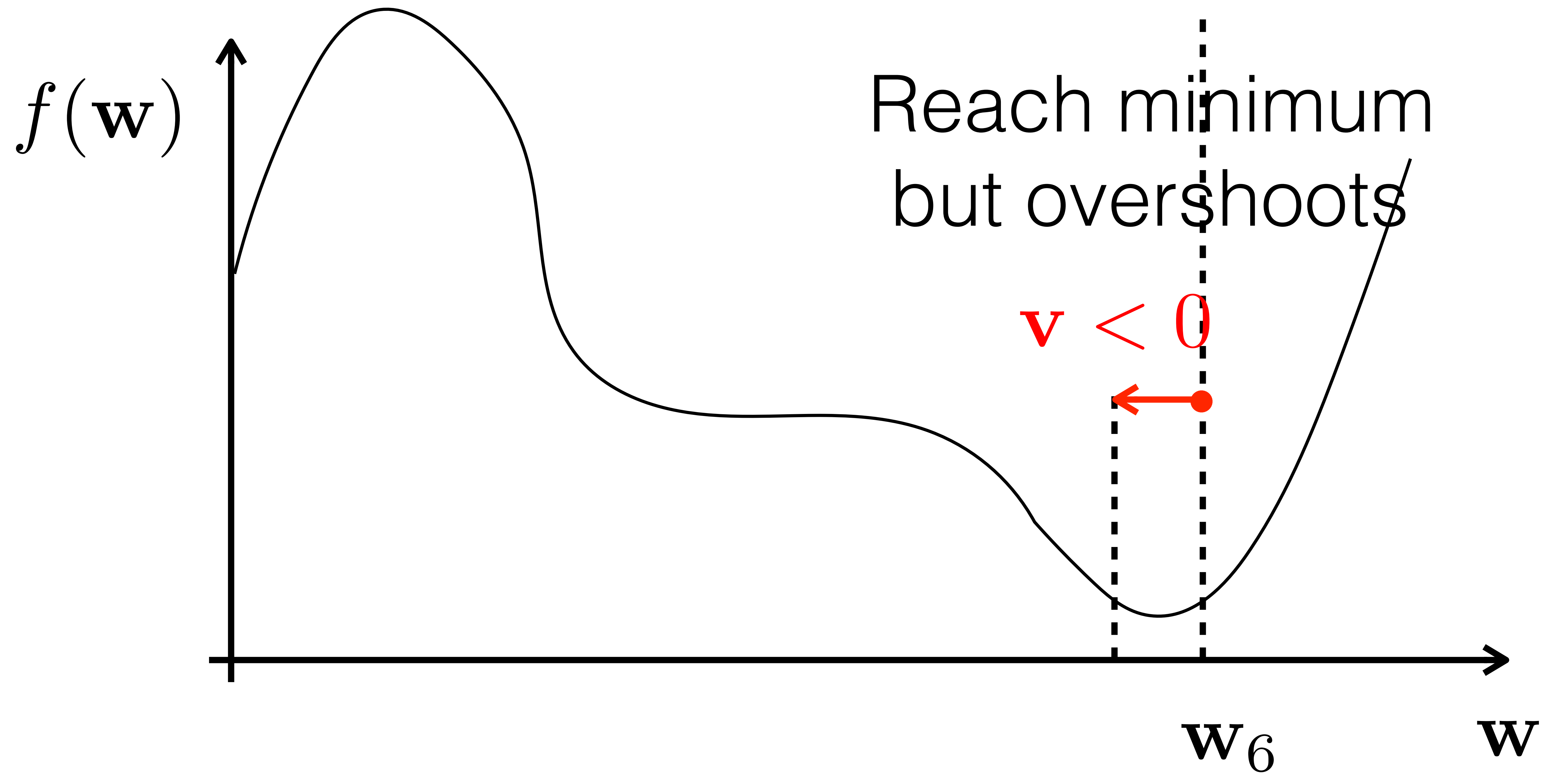

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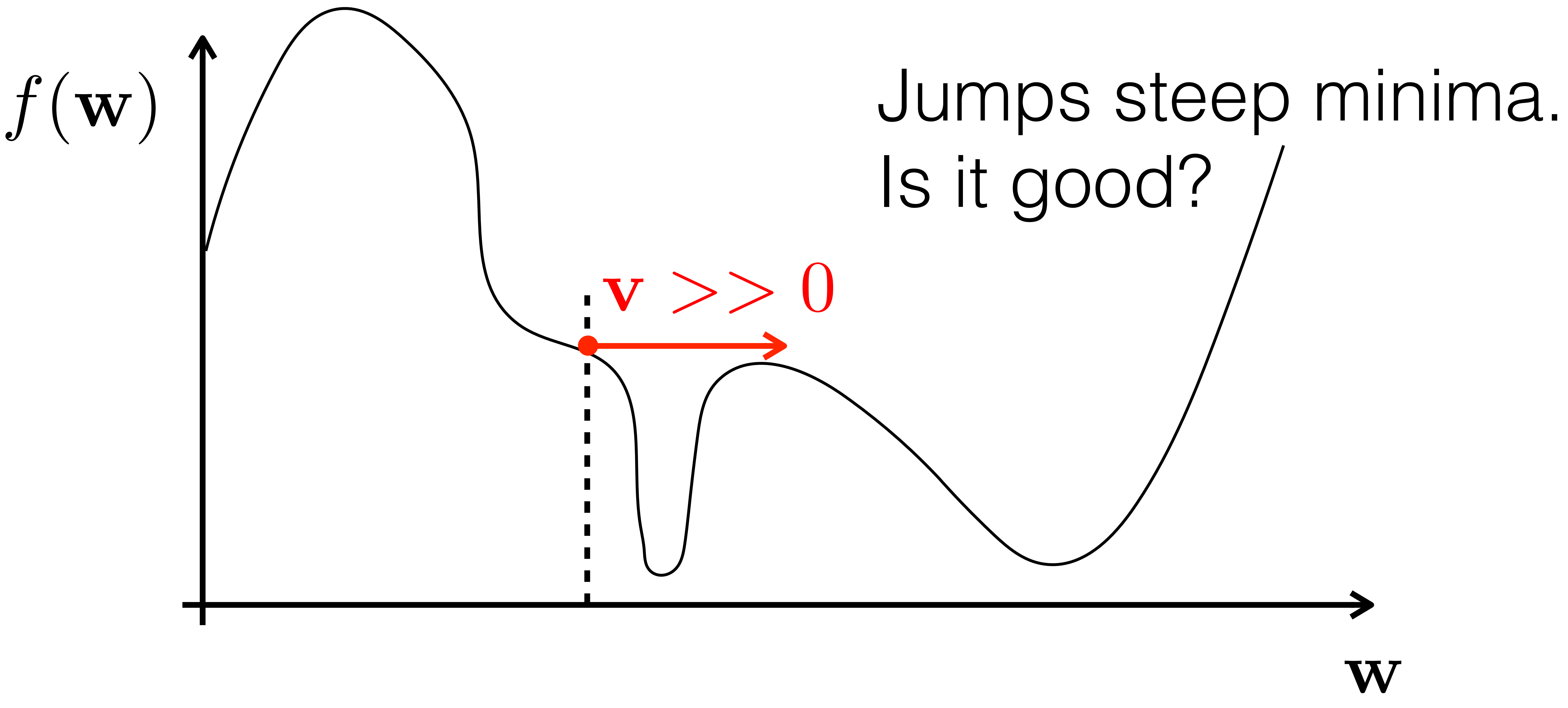
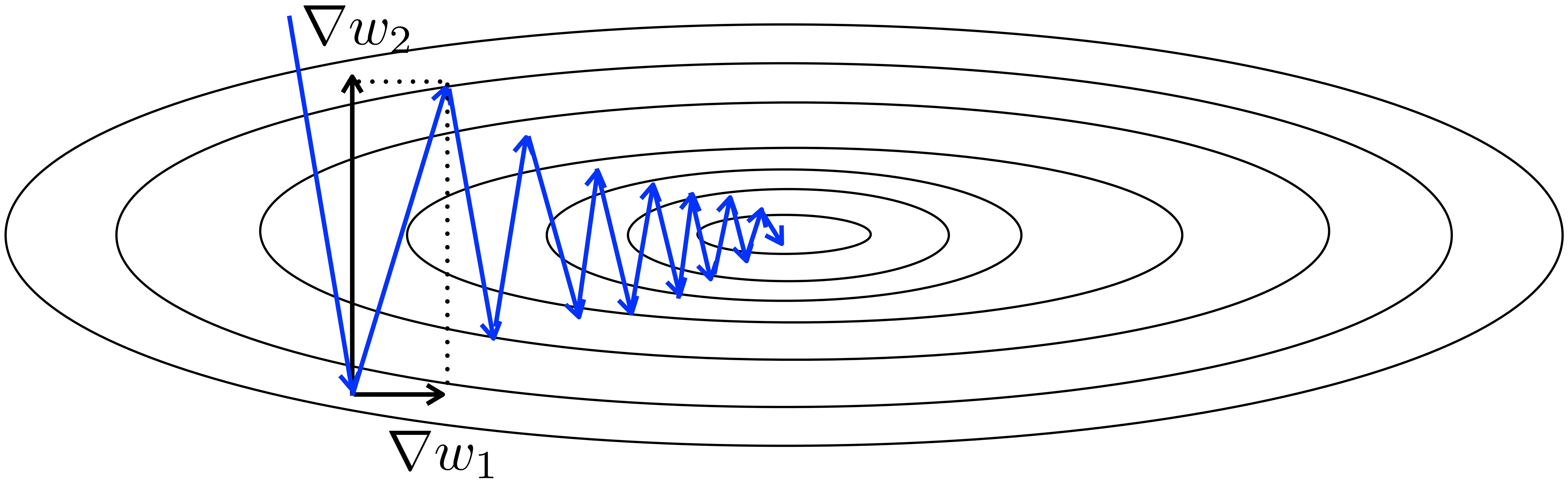


"SGD" vs "SGD + momentum" in 2D

$$\mathbf{w}^k = \mathbf{w}^{k-1} - \alpha \left. \frac{\partial f^\top(\mathbf{w})}{\partial \mathbf{w}} \right|_{\mathbf{w}=\mathbf{w}^{k-1}}$$

Undesired zig-zag behaviour



$$[\nabla w_1, \nabla w_2] = - \left. \frac{\partial f(\mathbf{w})}{\partial \mathbf{w}} \right|_{\mathbf{w}=\mathbf{w}^{k-1}}$$

"SGD" vs "SGD + momentum" in 2D

$$\mathbf{v}^k = \beta \mathbf{v}^{k-1} - \left.\frac{\partial f^\top(\mathbf{w})}{\partial \mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}^{k-1}}$$

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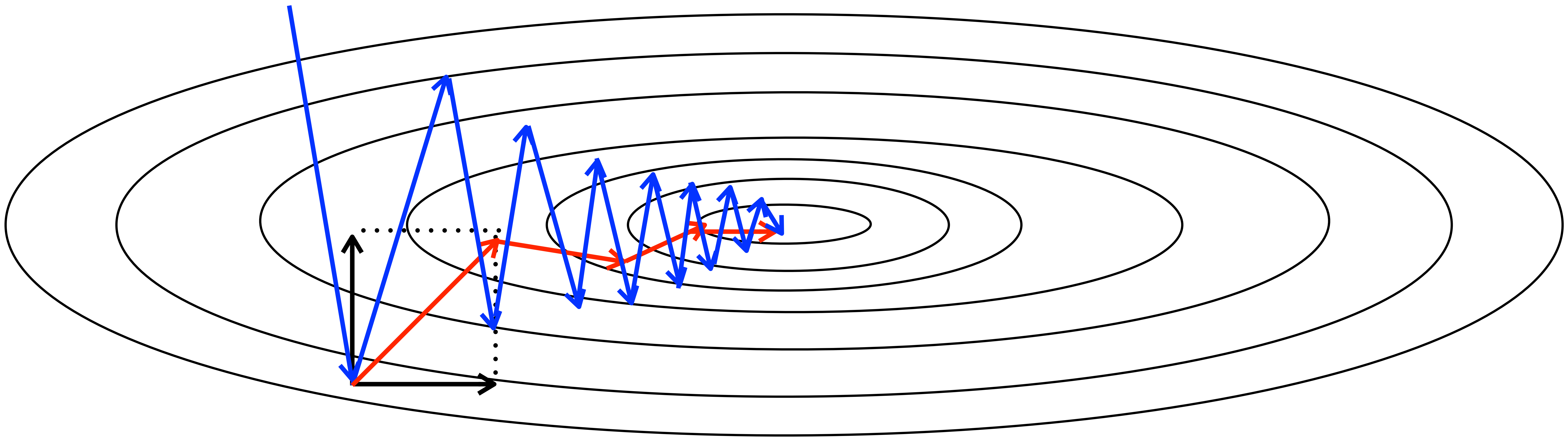


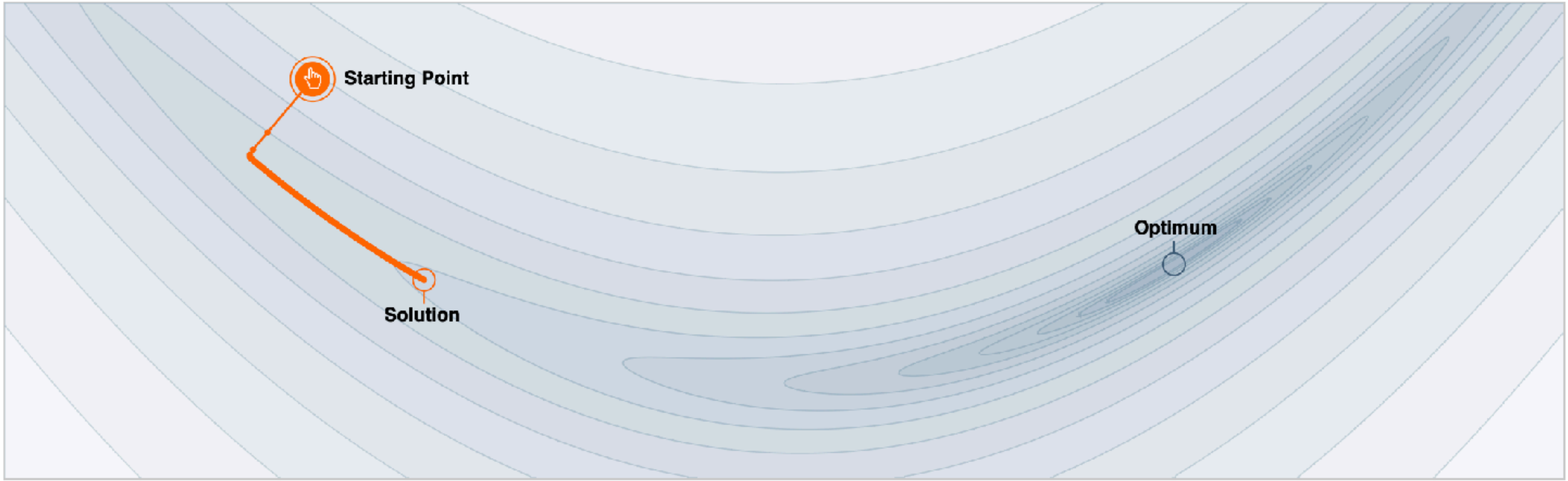
Momentum suppresses this problem partially by averaging element-wise gradients

“SGD” vs “SGD + momentum” in 2D

$$\mathbf{v}^k = \beta \mathbf{v}^{k-1} - \left.\frac{\partial f^\top(\mathbf{w})}{\partial \mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}^{k-1}}$$

$$\mathbf{w}^k = \mathbf{w}^{k-1} + \alpha \mathbf{v}^k$$

$\alpha =$ 1e-3 $\beta =$ 0



https://distill.pub/2017/momentum/

“SGD” vs “SGD + momentum” in 2D

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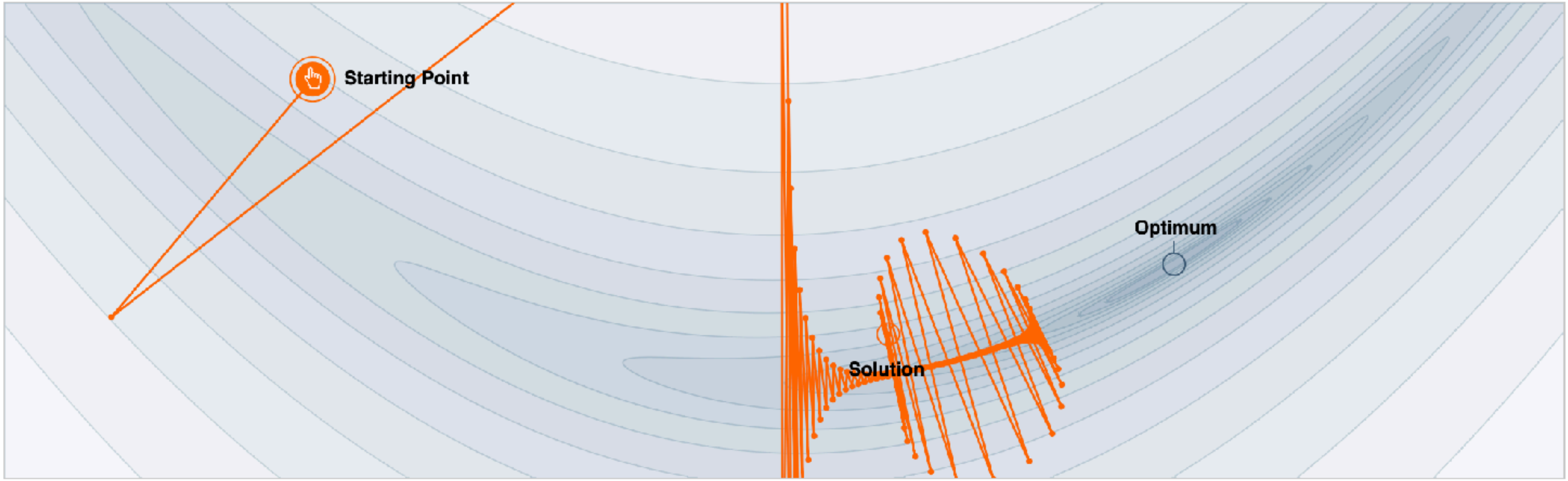
$$\mathbf{w}^k = \mathbf{w}^{k-1} + \alpha \mathbf{v}^k$$

$\alpha =$ 5e-3 $\beta =$ 0



https://distill.pub/2017/momentum/

"SGD" vs "SGD + momentum" in 2D

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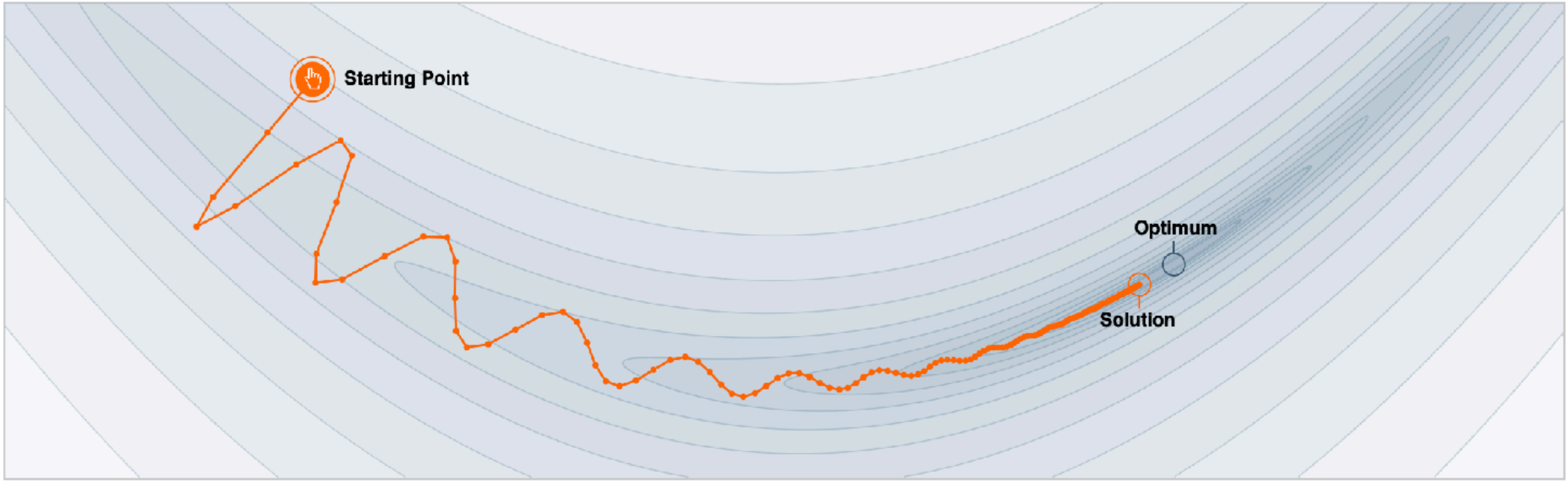
$$\mathbf{w}^k = \mathbf{w}^{k-1} + \alpha \mathbf{v}^k$$

$\alpha =$ 1e-3 $\beta =$ 0.9



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"SGD + momentum" on quadric

Criterion: $f(\mathbf{w}) = \frac{1}{2}\mathbf{w}^\top \mathtt{A}\mathbf{w}$ with $\mathtt{A} = \mathrm{diag}([\lambda_1, \dots, \lambda_n])$

Gradient: $\frac{\partial f(\mathbf{w}_i)}{\partial \mathbf{w}_i} = \lambda_i \mathbf{w}_i$

SGD+momentum after k iterations:

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$$\begin{bmatrix}\mathbf{v}_i^k \\ \mathbf{w}_i^k\end{bmatrix} = \begin{bmatrix}\beta & \lambda_i \\ -\alpha\beta & 1-\alpha\lambda_i\end{bmatrix}\begin{bmatrix}\mathbf{v}_i^{k-1} \\ \mathbf{w}_i^{k-1}\end{bmatrix} = \begin{bmatrix}\beta & \lambda_i \\ -\alpha\beta & 1-\alpha\lambda_i\end{bmatrix}^k \begin{bmatrix}\mathbf{v}_i^0 \\ \mathbf{w}_i^0\end{bmatrix}$$

[Flammarion, Bach COLT 2017]
https://arxiv.org/pdf/1504.01577.pdf
https://distill.pub/2017/momentum/

"SGD + momentum" on quadric

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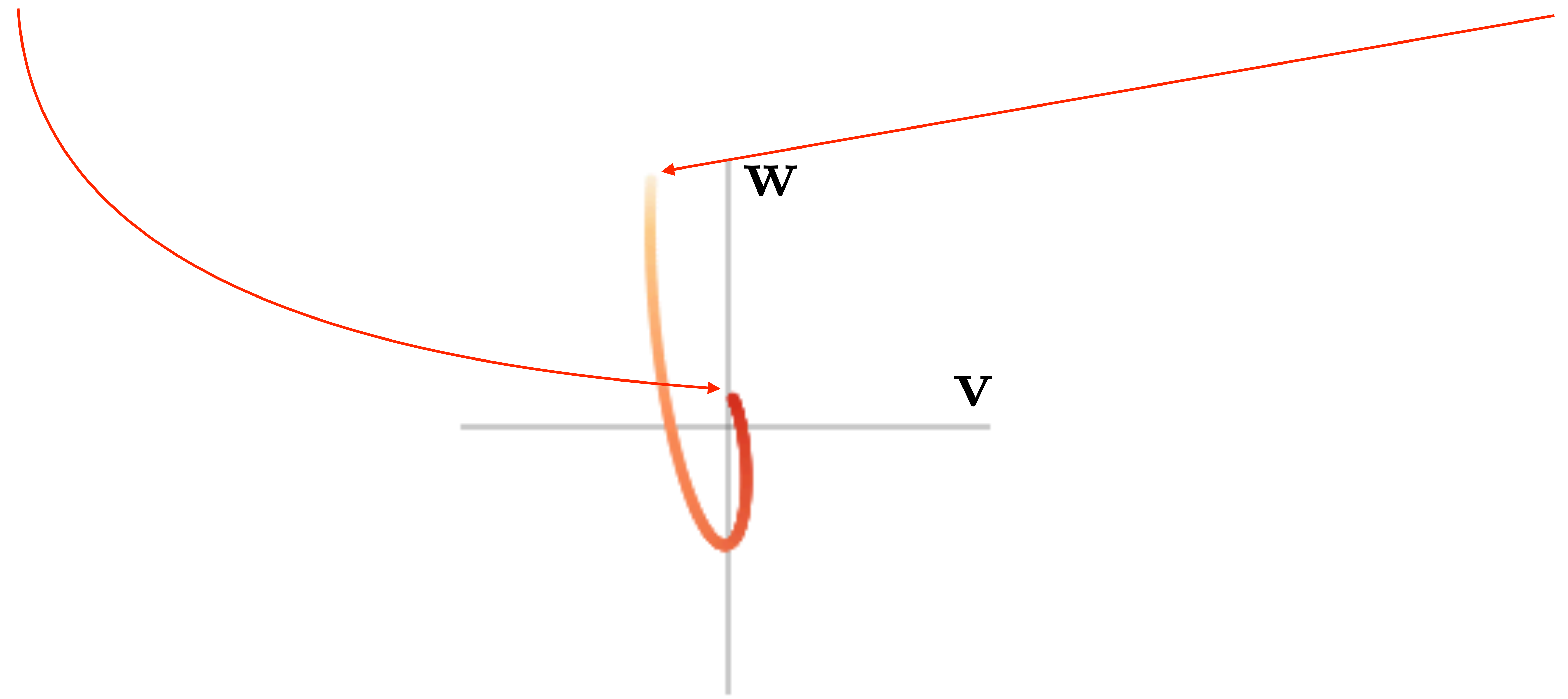

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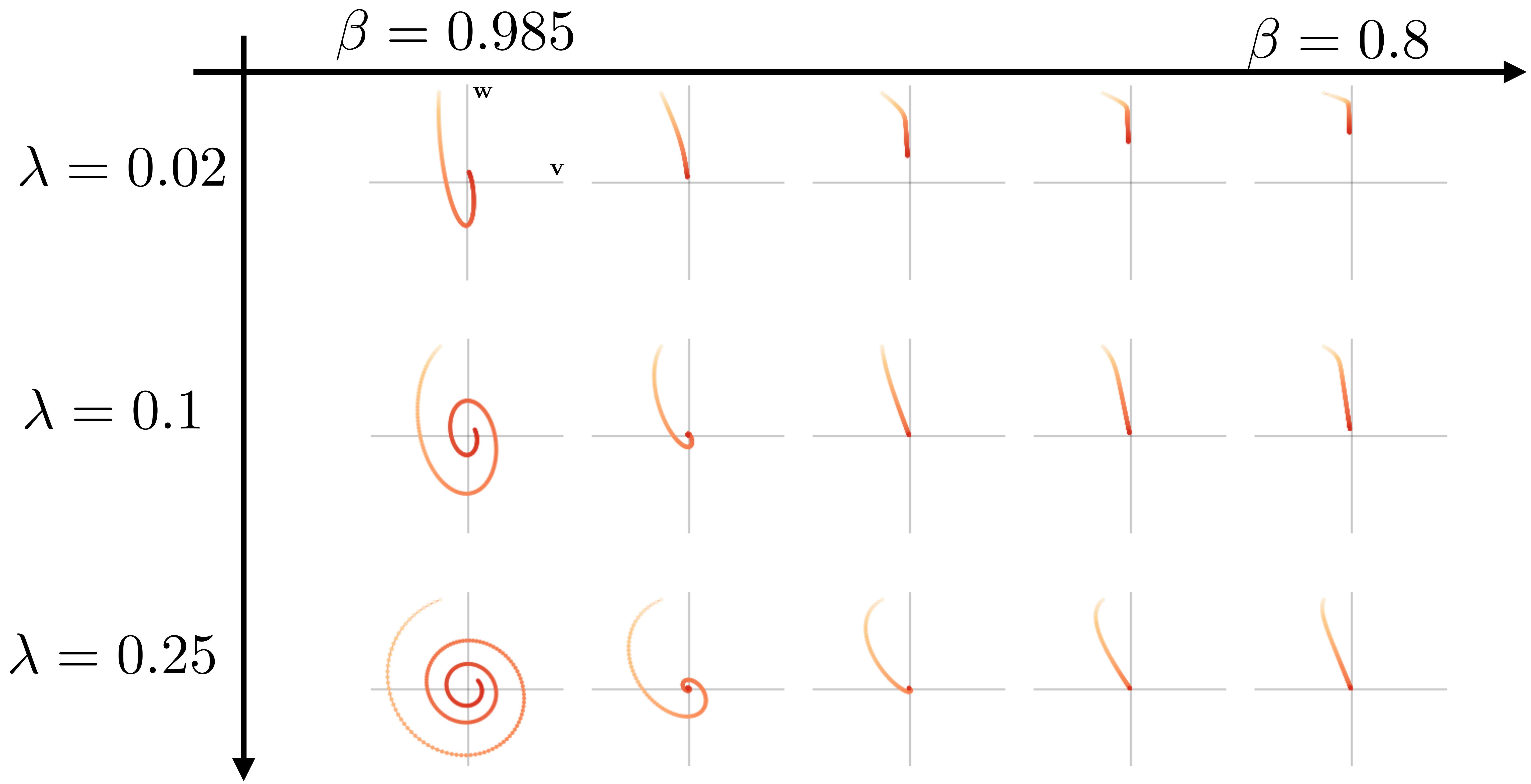

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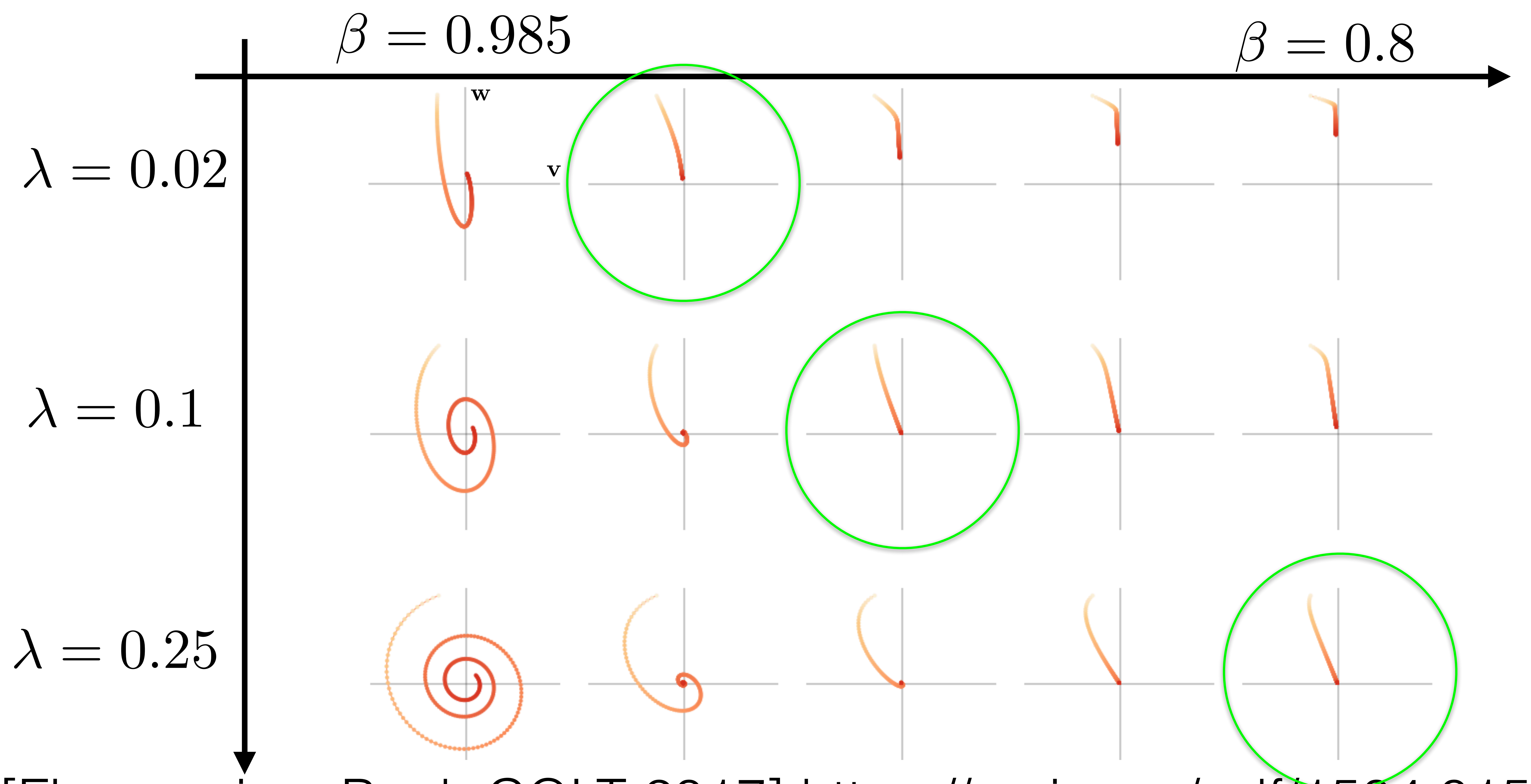

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- Converg. rate: $\mathrm{rate}_i(\alpha, \beta) = \max\{|\sigma_1(\alpha, \beta, \lambda_i)|, |\sigma_2(\alpha, \beta, \lambda_i)|\}$

[Flammarion, Bach COLT 2017] https://arxiv.org/pdf/1504.01577.pdf
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“SGD + momentum” on quadric

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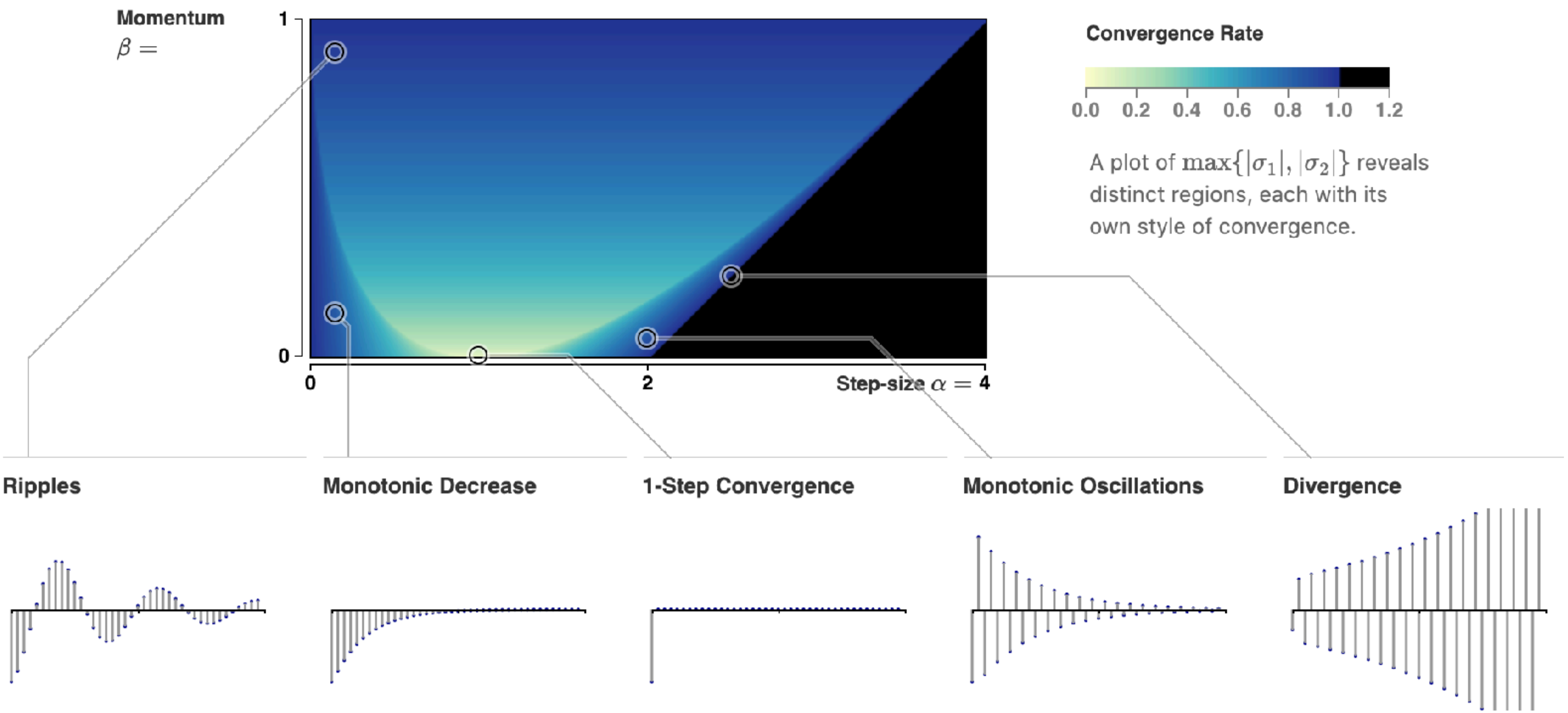

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- Converg. rate: $\mathrm{rate}_i(\alpha, \beta) = \max\{|\sigma_1(\alpha, \beta, \lambda_i)|, |\sigma_2(\alpha, \beta, \lambda_i)|\}$
- Optimal parameters:

$$\alpha^* = \Big(\frac{2}{\sqrt{\lambda_1} + \sqrt{\lambda_n}}\Big)^2 \qquad \beta^* = \Big(\frac{\sqrt{\lambda_n} - \sqrt{\lambda_1}}{\sqrt{\lambda_n} + \sqrt{\lambda_1}}\Big)^2$$

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- Optimal parameters:

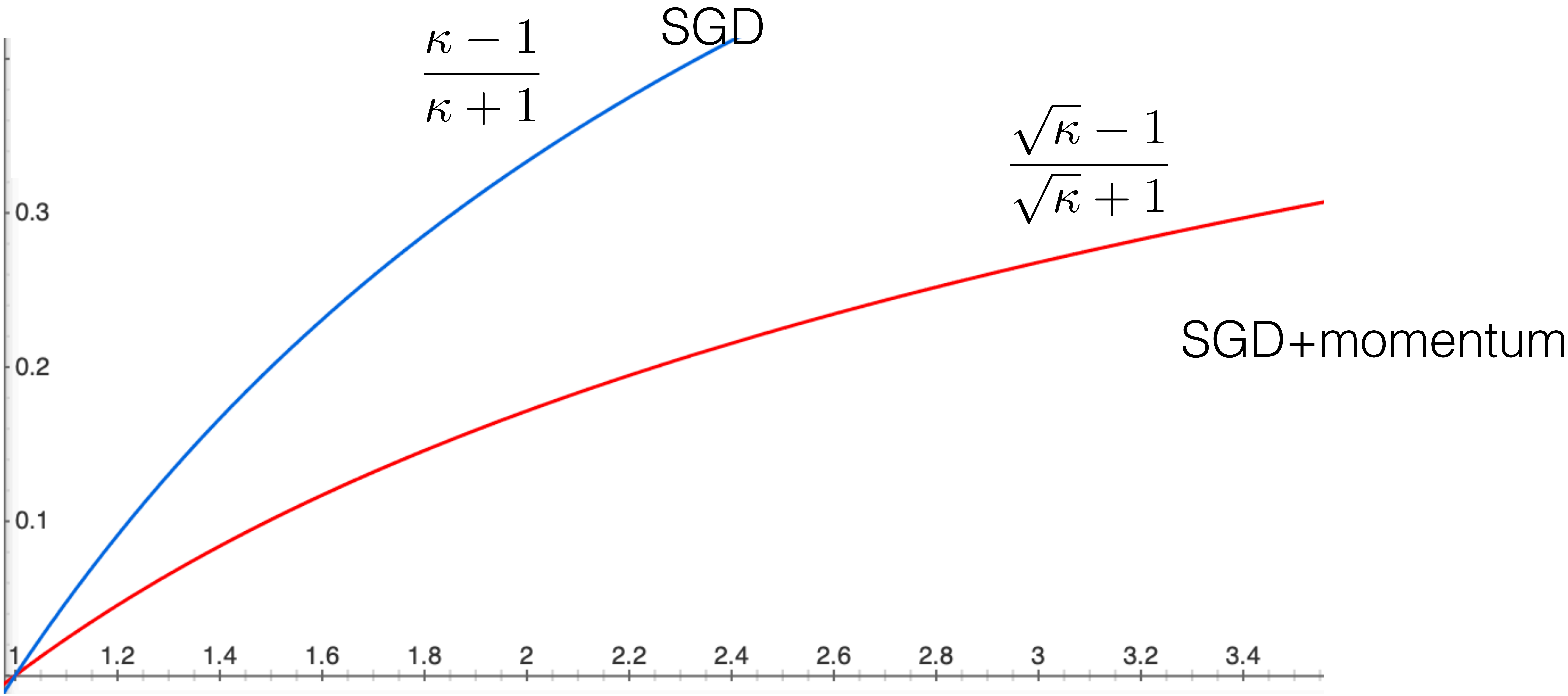
$$\alpha^* = \left(\frac{2}{\sqrt{\lambda_1} + \sqrt{\lambda_n}}\right)^2 \qquad \beta^* = \left(\frac{\sqrt{\lambda_n} - \sqrt{\lambda_1}}{\sqrt{\lambda_n} + \sqrt{\lambda_1}}\right)^2$$

- Optimal convergence rate: $$\mathrm{rate}(\alpha^*, \beta^*) = \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}$$

[Flammarion, Bach COLT 2017] https://arxiv.org/pdf/1504.01577.pdf
https://distill.pub/2017/momentum/

“SGD + momentum” on quadric

Convergence rate




```
torch.optim.SGD(params, lr=0.001, momentum=0.9)
```

PyTorch

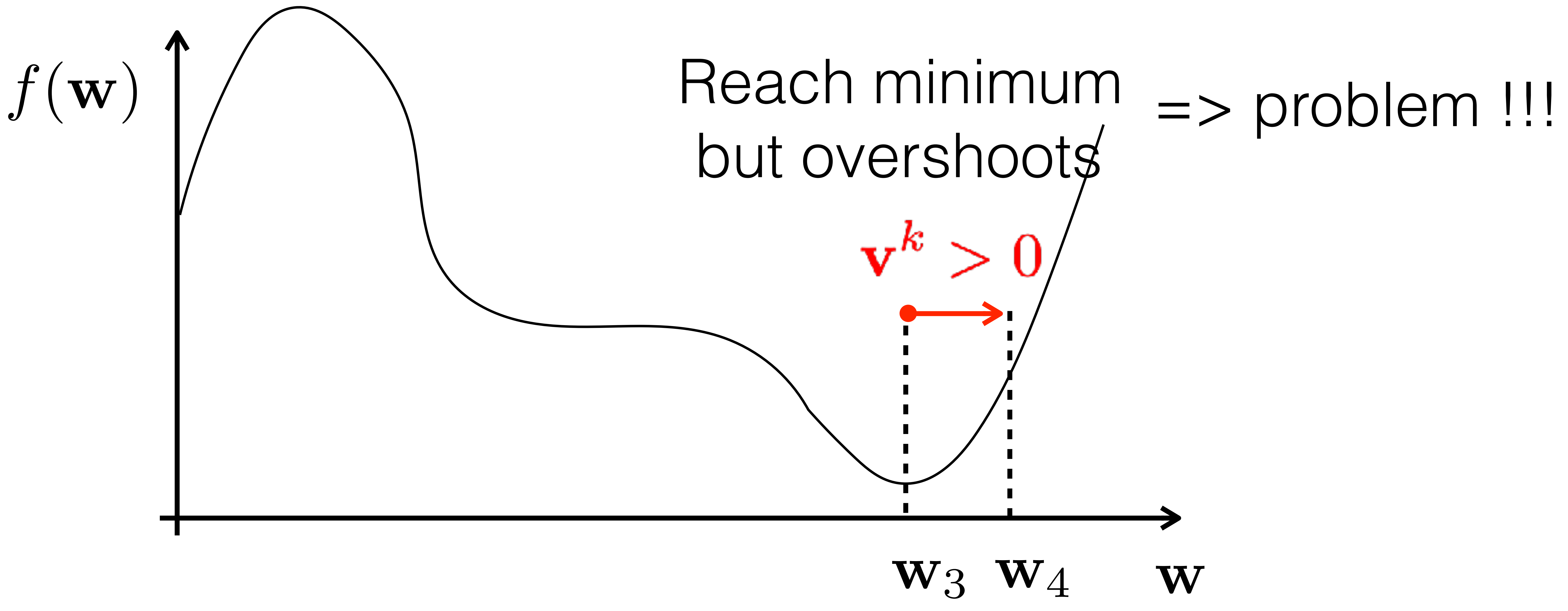
```
# initialise
import torch.nn as nn
import torch.optim as optim

# initialize optimizer
optimizer = optim.SGD(conv_net.parameters(), lr=1e-2)

# define ConvNet model
conv_net = …

# define criterion function
loss = loss_fn(conv_net(images), labels)

# compute gradient
loss.backward()

# update weights of the model
optimizer.step()
```

SGD + momentum - drawback

$$\mathbf{v}^k = \beta \mathbf{v}^{k-1} - \frac{\partial f^\top(\mathbf{w})}{\partial \mathbf{w}}\Big|_{\mathbf{w}=\mathbf{w}^{k-1}}$$

$$\mathbf{w}^k = \mathbf{w}^{k-1} + \alpha \mathbf{v}^k$$

- Build velocity $\mathbf{v}$ as running average of gradients
- Rolling ball with velocity $\mathbf{v}$ and friction coeff $\rho = 0.95$

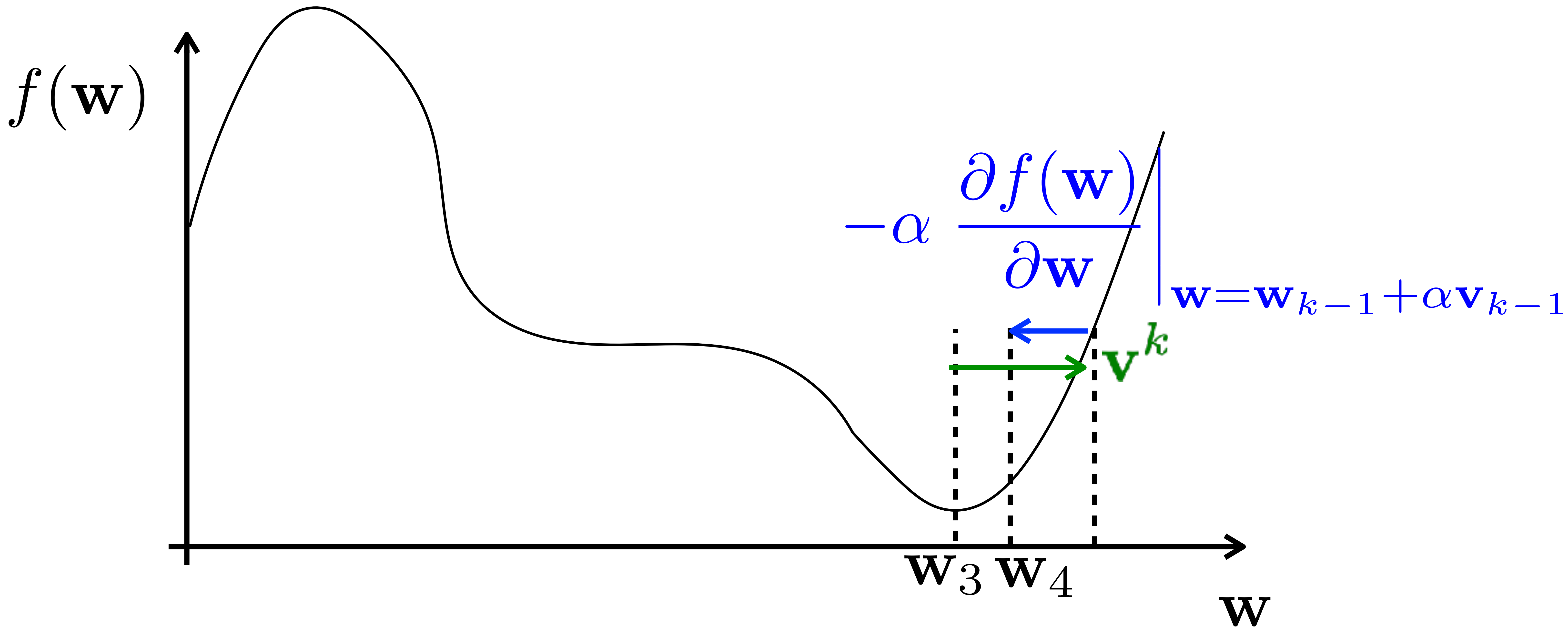


SGD with Nesterov momentum

$$\mathbf{v}^k = \beta \mathbf{v}^{k-1} - \left.\frac{\partial f^\top(\mathbf{w})}{\partial \mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}^{k-1}+\alpha\mathbf{v}^{k-1}}$$

$$\mathbf{w}^k = \mathbf{w}^{k-1} + \alpha \mathbf{v}^k$$

- Look one step ahead and reduce velocity by future gradient
- Partially prevents overshooting



http://www.cs.toronto.edu/~fritz/absps/momentum.pdf

SGD with Nesterov momentum

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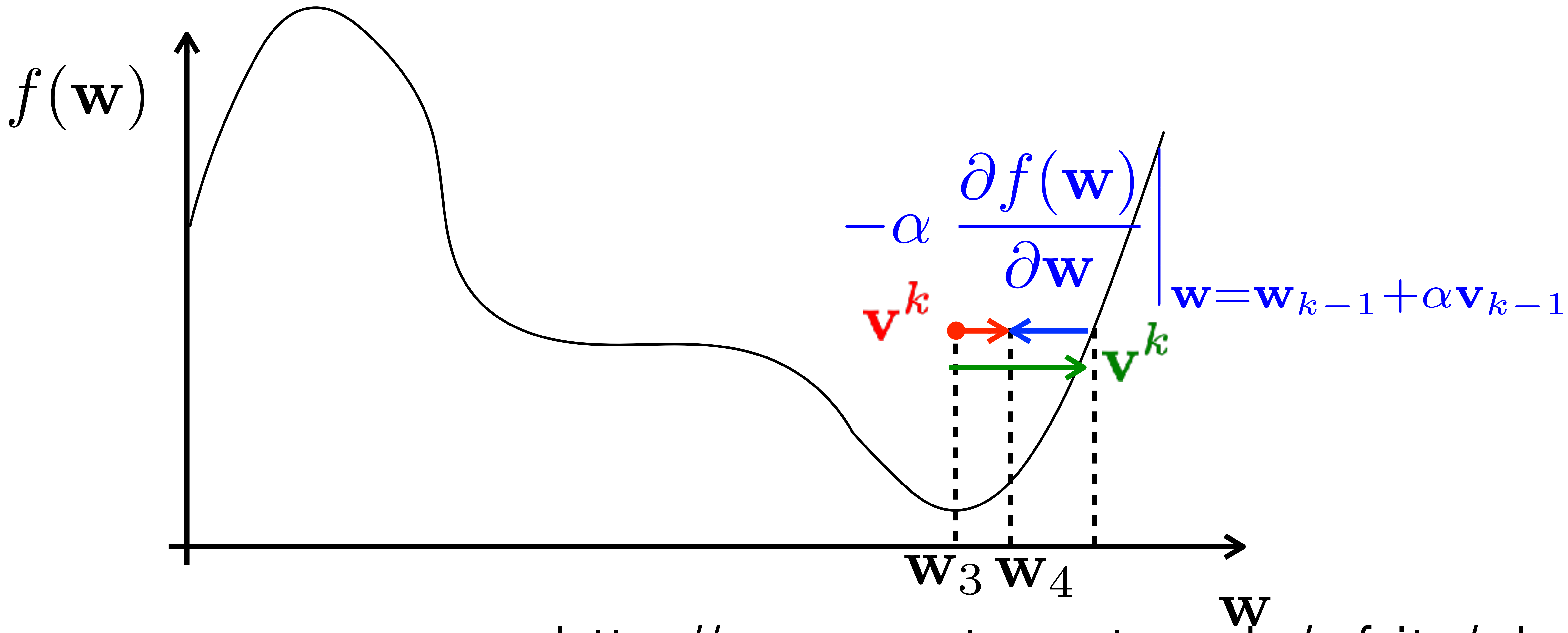
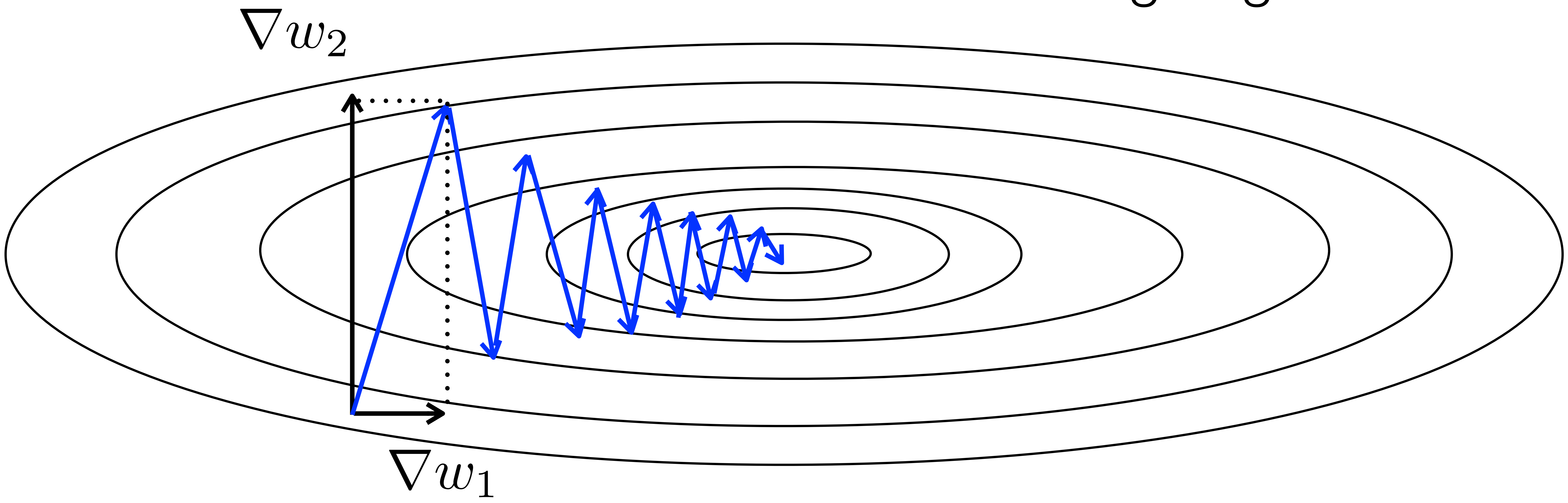


http://www.cs.toronto.edu/~fritz/absps/mon

Beyond first order methods

$$\mathbf{w}^k = \mathbf{w}^{k-1} - \alpha \left. \frac{\partial f^\top(\mathbf{w})}{\partial \mathbf{w}} \right|_{\mathbf{w}=\mathbf{w}^{k-1}}$$

Undesired zig-zag behaviour

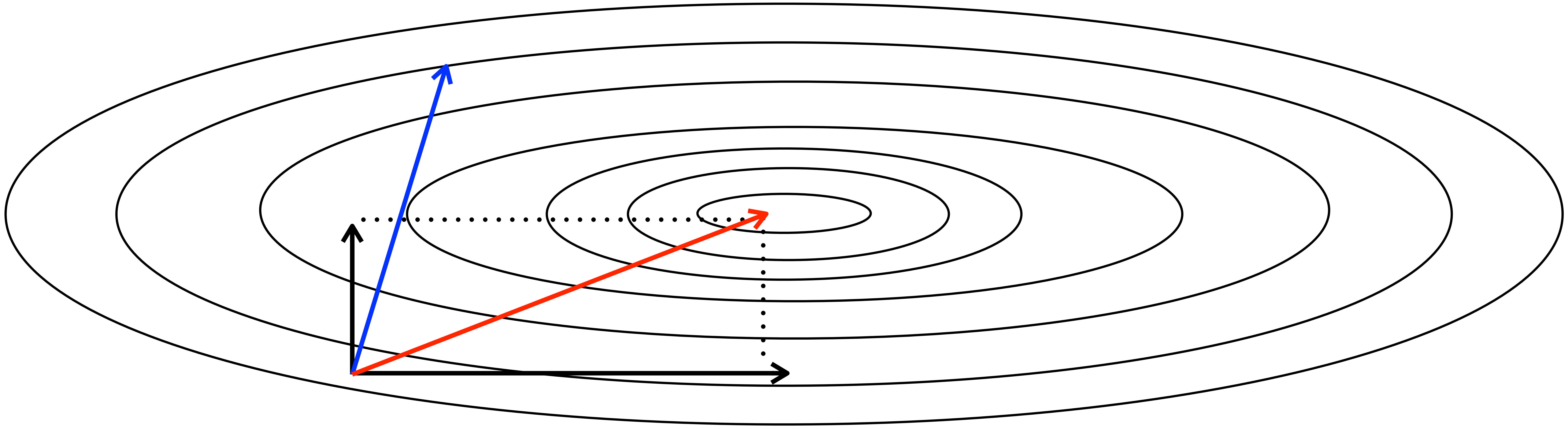


Momentum helps, but the zig-zag behaviour remains.

Full Newton Method

$$\mathbf{w}^k = \mathbf{w}^{k-1} - \alpha\, H^{-1}\, \frac{\partial f(\mathbf{w})}{\partial \mathbf{w}}\bigg|_{\mathbf{w}=\mathbf{w}^{k-1}}$$

Convergence rate for convex quadratic form is zero (converges within one step)



Hessian $H = \frac{\partial^2 f(\mathbf{w})}{\partial^2 \mathbf{w}}\bigg|_{\mathbf{w}=\mathbf{w}^{k-1}}$ adjusts the direction of the gradient.

Convergence rate of full Newton method on quadric case study

Criterion: $f(\mathbf{w}) = \frac{1}{2}\mathbf{w}^\top \mathtt{A}\mathbf{w}$ with $\mathtt{A} = \mathrm{diag}([\lambda_1, \ldots, \lambda_n])$

Gradient: $\left.\frac{\partial f(\mathbf{w})}{\partial \mathbf{w}_i}\right|_{\mathbf{w}_i = \mathbf{w}_i^{k-1}} = \lambda_i \mathbf{w}_i$ Hessian: $H = \left.\frac{\partial^2 f(\mathbf{w})}{\partial^2 \mathbf{w_i}}\right|_{\mathbf{w}_i = \mathbf{w}_i^{k-1}} = \lambda_i$

SGD after k iterations: $\mathbf{w}_i^k = (1 - \alpha\lambda_i)^k \mathbf{w}_i^0$

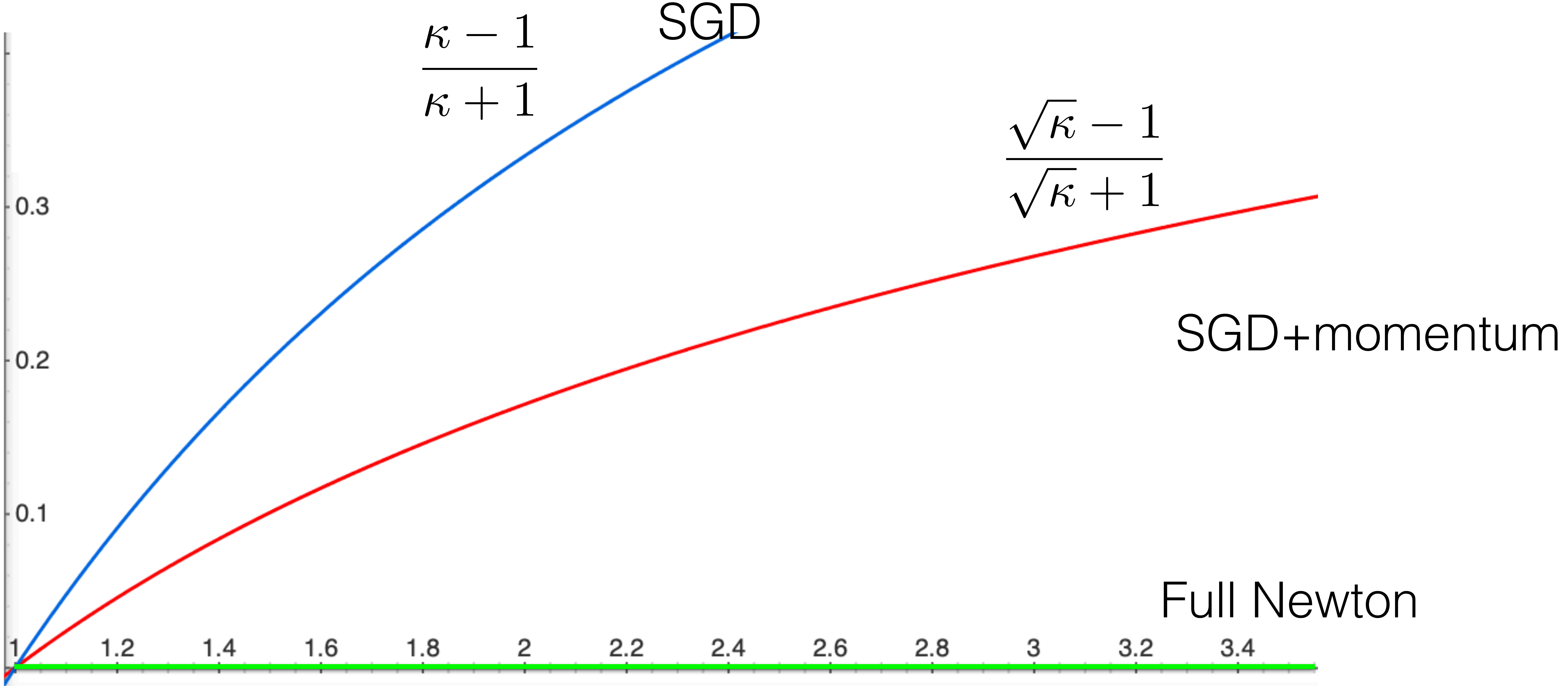
Full Newton after k iterations: $\mathbf{w}_i^k = (1 - \alpha)^k \mathbf{w}_i^0$

Optimal convergence rate: $\alpha^* = 1$

$\mathrm{rate}(\alpha^*) = 0$

SGD + momentum on quadric

Convergence rate

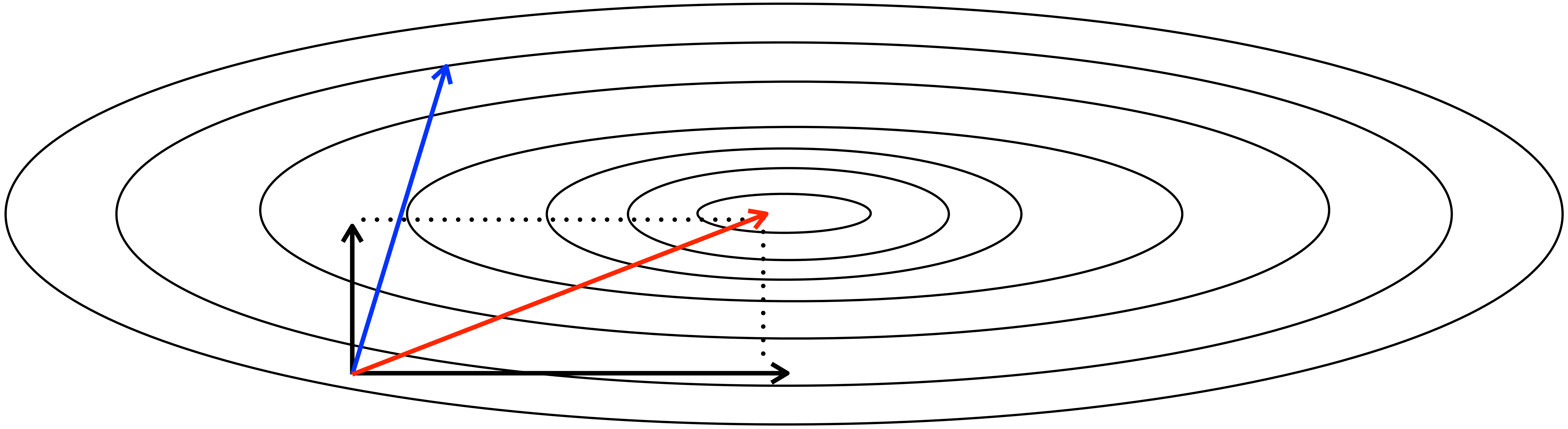


Full Newton Method

$$\mathbf{w}^k = \mathbf{w}^{k-1} - \alpha\, H^{-1} \left.\frac{\partial f(\mathbf{w})}{\partial \mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}^{k-1}}$$

$\mathbf{g}$

Convergence rate for convex quadratic form is zero (converges within one step)



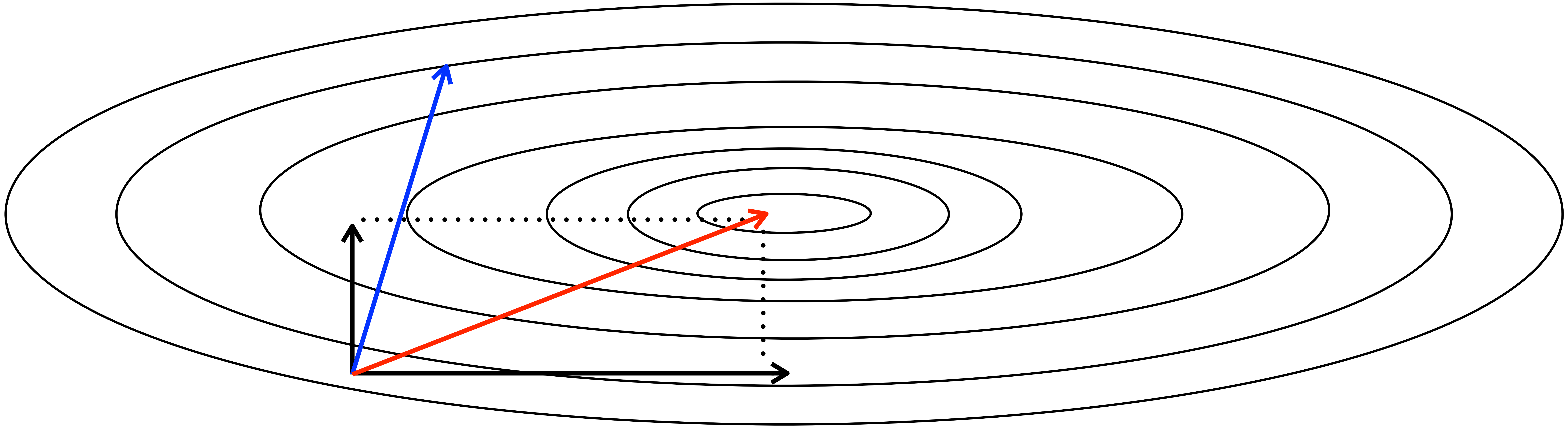
- Why not to use Hessian?
  - Hessian has $M \times M$ elements for M-dimensional parameters
  - Inverse of Hessian is $\mathcal{O}(M^3)$
  - Accurate estimate of $H^{-1} \cdot \mathbf{g}$ requiers significantly larger minibatches

Full Newton Method

$$\mathbf{w}^k = \mathbf{w}^{k-1} - \alpha\, {\color{red}H^{-1}} \left.\frac{\partial f(\mathbf{w})}{\partial \mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}^{k-1}}$$

$\mathbf{g}$

Convergence rate for convex quadratic form is zero (converges within one step)

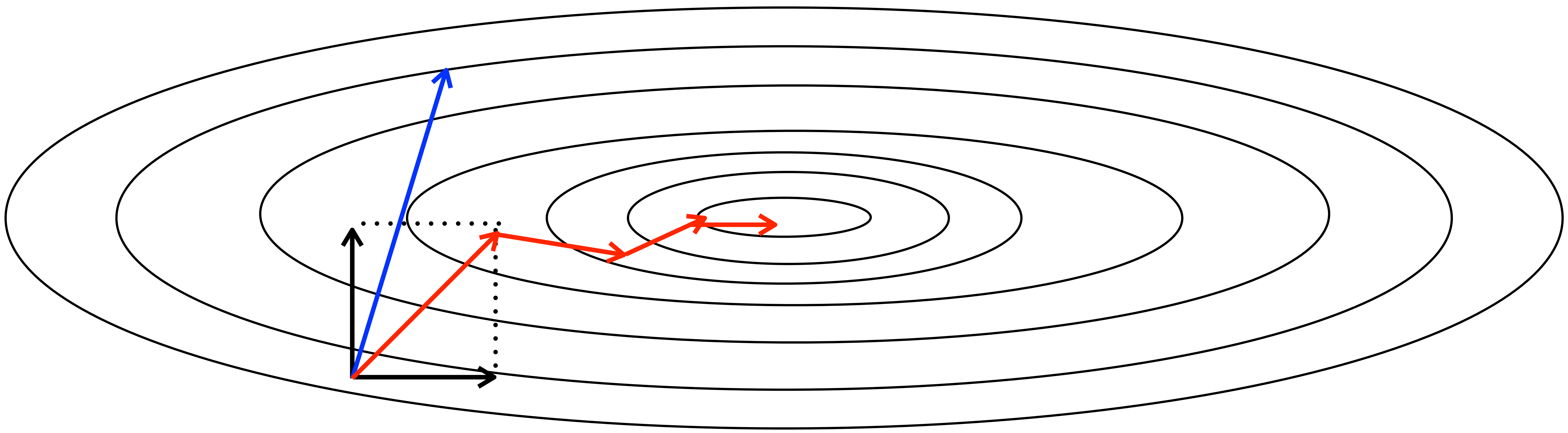


What does the Hessian actually do?

- It slows down each component by its eigenvalue
  (i.e. eigenvalue encodes steepness of the quadric in particular dimension)
- The faster the change the shorter the step

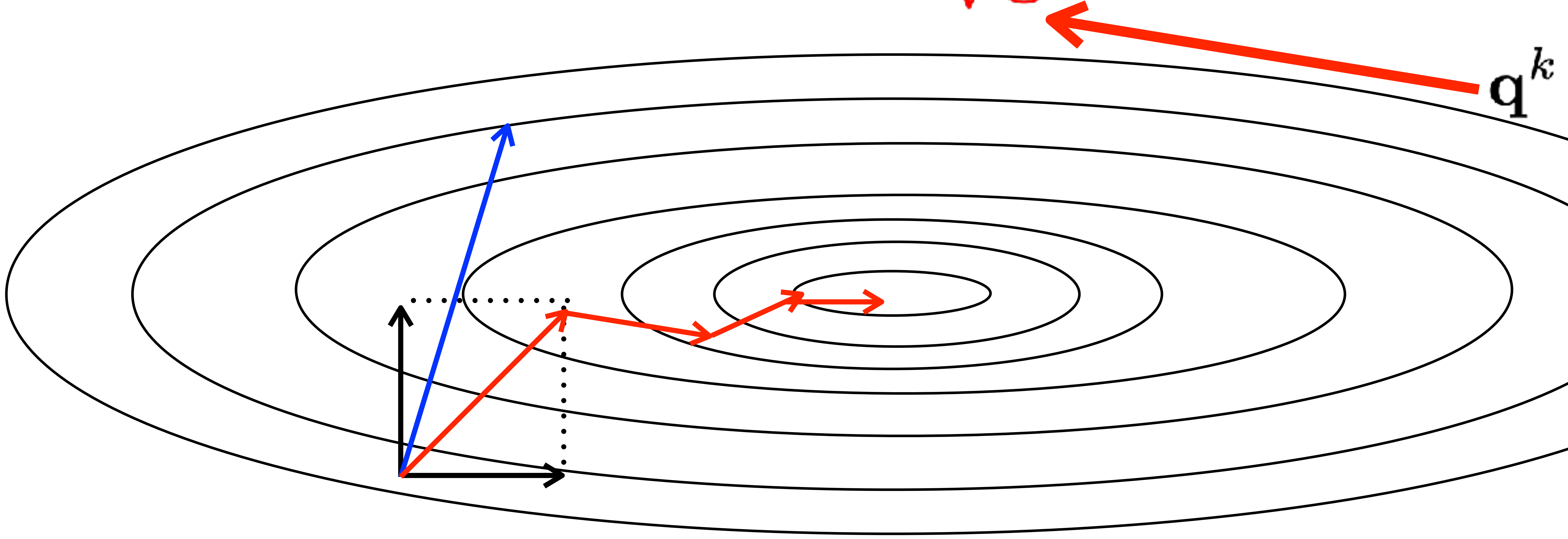
Full Newton method - approximation

$$\mathbf{w}^k \approx \mathbf{w}^{k-1} - \frac{\alpha}{\sqrt{\mathbf{g}^2 + \epsilon}} \odot \mathbf{g}$$



Full Newton method - approximation

$$\mathbf{w}^k \approx \mathbf{w}^{k-1} - \frac{\alpha}{\sqrt{\mathbf{g}^2 + \epsilon}} \odot \mathbf{g}$$



http://www.jmlr.org/papers/volume12/duchi11a/duchi11a.pdf

RMSprop

$$\mathbf{q}^k = \beta_2 \mathbf{q}^{k-1} + (1-\beta_2)\mathbf{g}^2$$

$$\mathbf{w}^k = \mathbf{w}^{k-1} - \frac{\alpha}{\sqrt{\mathbf{q}^k} + \epsilon} \odot \mathbf{g}$$

```
torch.optim.RMSprop(params, lr=0.01, alpha=0.99, eps=1e-08,
weight_decay=0, momentum=0, centered=False)
```

AdamOptimizer = AdaGrad + momentum in $\mathbf{g}$, $\mathbf{g}^2$

$$\mathbf{q}^k = \beta_2 \mathbf{q}^{k-1} + (1-\beta_2)\mathbf{g}^2$$

$$\mathbf{w}^k = \mathbf{w}^{k-1} - \frac{\alpha}{\sqrt{\mathbf{q}^k} + \epsilon} \odot \mathbf{g}$$

$\mathbf{v}^k$

AdamOptimizer = AdaGrad + momentum in $\mathbf{g},\ \mathbf{g}^2$

$$\mathbf{v}^k = \beta_1 \mathbf{v}^{k-1} + (1-\beta_1)\mathbf{g}$$

$$\mathbf{q}^k = \beta_2 \mathbf{q}^{k-1} + (1-\beta_2)\mathbf{g}^2$$

$$\mathbf{w}^k = \mathbf{w}^{k-1} - \frac{\alpha}{\sqrt{\mathbf{q}^k} + \epsilon} \odot \mathbf{v}^k$$

[Kingma ICLR 2015]

AdamOptimizer = AdaGrad + momentum in $\mathbf{g},\ \mathbf{g}^2$

$$\mathbf{v}^k = \beta_1 \mathbf{v}^{k-1} + (1-\beta_1)\mathbf{g}$$

$$\mathbf{q}^k = \beta_2 \mathbf{q}^{k-1} + (1-\beta_2)\mathbf{g}^2$$

$$\hat{\mathbf{v}}_k = \frac{\mathbf{v}_k}{1-\beta_1^k}$$

$$\hat{\mathbf{q}}^k = \frac{\mathbf{q}^k}{1-\beta_2^k}$$

$$\mathbf{w}^k = \mathbf{w}^{k-1} - \frac{\alpha}{\sqrt{\hat{\mathbf{q}}^k} + \epsilon} \odot \hat{\mathbf{v}}^k$$

[Kingma ICLR 2015]

AdamOptimizer = AdaGrad + momentum in $\mathbf{g}$, $\mathbf{g}^2$

$$\mathbf{v}^k = \beta_1 \mathbf{v}^{k-1} + (1-\beta_1)\mathbf{g}$$

$$\mathbf{q}^k = \beta_2 \mathbf{q}^{k-1} + (1-\beta_2)\mathbf{g}^2$$

$$\hat{\mathbf{v}}_k = \frac{\mathbf{v}_k}{1-\beta_1^k}$$

$$\hat{\mathbf{q}}^k = \frac{\mathbf{q}^k}{1-\beta_2^k}$$

$$\mathbf{w}^k = \mathbf{w}^{k-1} - \frac{\alpha}{\sqrt{\hat{\mathbf{q}}^k} + \epsilon} \odot \hat{\mathbf{v}}^k$$

Default values: $\alpha = 0.1$ $\beta_1 = 0.9$ $\beta_2 = 0.999$

```
torch.optim.Adam(params, lr=0.001, betas=(0.9, 0.999),
            eps=1e-08, weight_decay=0, amsgrad=False)
```

Summary

- Adam is the most popular choice, since it is not that sensitive to other hyper-parameters.

- PyTorch of all previously mentioned implementations available:

```
torch.optim.Adam(params, lr=0.001,
        betas=(0.9, 0.999),eps=1e-08,
        weight_decay=0, amsgrad=False)
```

- Anything more complex than Adam typically suffers from sub-linear returns in huge state-of-the-art networks https://arxiv.org/abs/1805.02338v1

- There is a whole family of Quasi-Newton methods, which make use of advanced Hessian approximations (L-BFGS).

```
torch.optim.LBFGS(params, lr=1, …)
```

BFGS: Where does the name came from?

Broyden

BFGS: Where does the name came from?

Broyden **F**letcher

BFGS: Where does the name came from?

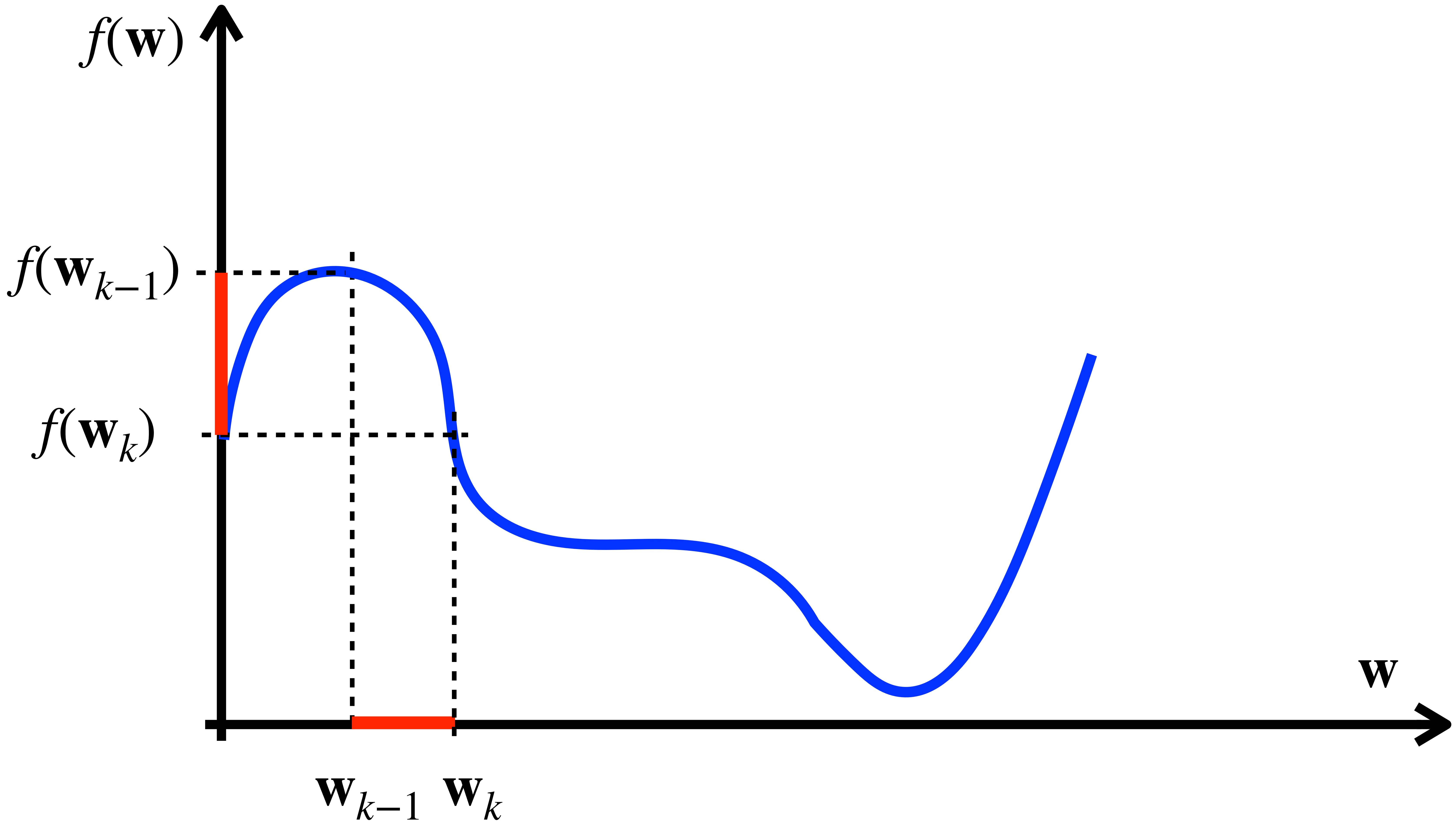
Broyden **F**letcher **G**oldfarb

BFGS: Where does the name came from?

Broyden **F**letcher **G**oldfarb **S**hanno

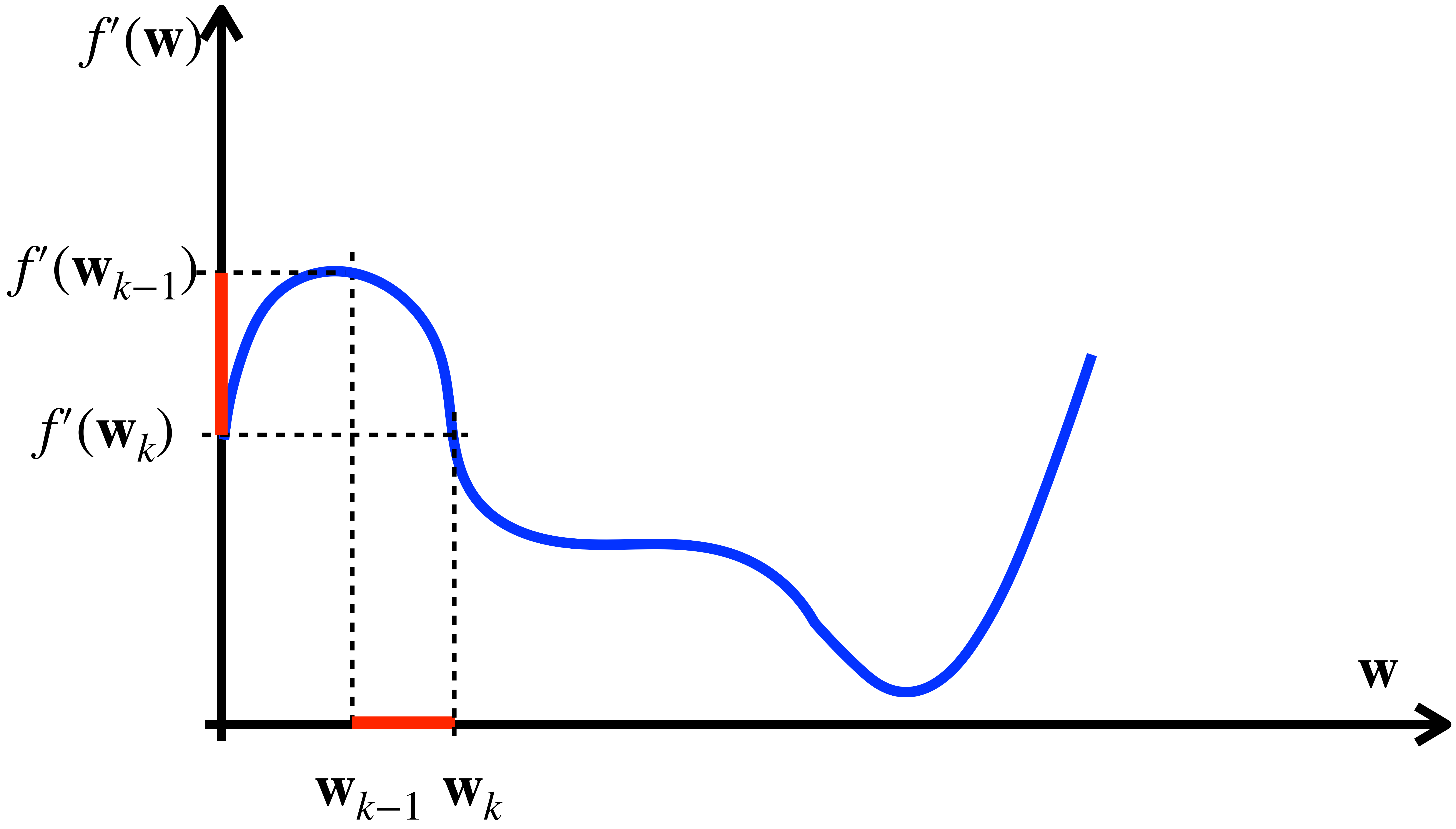
Broyden **F**letcher **G**oldfarb **S**hanno

Approximating 1D gradient: $$f'(\mathbf{w}_k) \approx \frac{f(\mathbf{w}_k) - f(\mathbf{w}_{k-1})}{\mathbf{w}_k - \mathbf{w}_{k-1}}$$



Broyden **F**letcher **G**oldfarb **S**hanno

Approximating 1D hessian: $f''(\mathbf{w}_k) \approx \dfrac{f'(\mathbf{w}_k) - f'(\mathbf{w}_{k-1})}{\mathbf{w}_k - \mathbf{w}_{k-1}}$



Broyden **F**letcher **G**oldfarb **S**hanno

Approximating 1D hessian: $f''(\mathbf{w}_k) \approx \dfrac{f'(\mathbf{w}_k) - f'(\mathbf{w}_{k-1})}{\mathbf{w}_k - \mathbf{w}_{k-1}}$

Approximating 1D Newton method (secant method):

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \frac{1}{f''(\mathbf{w}_k)} \cdot f'(\mathbf{w}_k) \approx \mathbf{w}_k - \frac{f'(\mathbf{w}_k) - f'(\mathbf{w}_{k-1})}{\mathbf{w}_k - \mathbf{w}_{k-1}} \cdot f'(\mathbf{w})$$

Broyden **F**letcher **G**oldfarb **S**hanno

Approximating 1D hessian: $f''(\mathbf{w}_k) \approx \dfrac{f'(\mathbf{w}_k) - f'(\mathbf{w}_{k-1})}{\mathbf{w}_k - \mathbf{w}_{k-1}} = \hat{\mathbf{H}}_k$

Approximating N-D hessian:

$\hat{\mathbf{H}}_k \cdot (\mathbf{w}_k - \mathbf{w}_{k-1}) = \nabla f_k - \nabla f_{k-1}$

Can I solve it?

(NxN)/2 unknowns, but only N equations

$\arg\min_{\hat{\mathbf{H}}_k} \|\hat{\mathbf{H}}_k - \hat{\mathbf{H}}_{k-1})\|_F$ .... close to previous hessian approximation

subject to : $\hat{\mathbf{H}}_k = \hat{\mathbf{H}}_k^\top$ .... symmetric

$\hat{\mathbf{H}}_k \cdot (\mathbf{w}_k - \mathbf{w}_{k-1}) = \nabla f_k - \nabla f_{k-1}$ ... approximate hessian via secan method

$$\hat{\mathbf{H}}_k^\star = \hat{\mathbf{H}}_{k-1} + \frac{(\nabla f_k - \nabla f_{k-1})(\nabla f_k - \nabla f_{k-1})^\top}{(\nabla f_k - \nabla f_{k-1})^\top \Delta \mathbf{w_k}} + \frac{\hat{\mathbf{H}}_{k-1}\Delta\mathbf{w}_k\Delta\mathbf{w}_k^\top\hat{\mathbf{H}}_{k-1}}{\Delta\mathbf{w}_k^\top\hat{\mathbf{H}}_{k-1}\Delta\mathbf{w}_k}$$ .... analytical solution

Approximating N-D Newton method (BFGS method):

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \mathbf{H}_k^{-1} \cdot \nabla f_k \approx \mathbf{w}_k - \hat{\mathbf{H}}_k^{\star\,-1} \cdot \nabla f_k$$

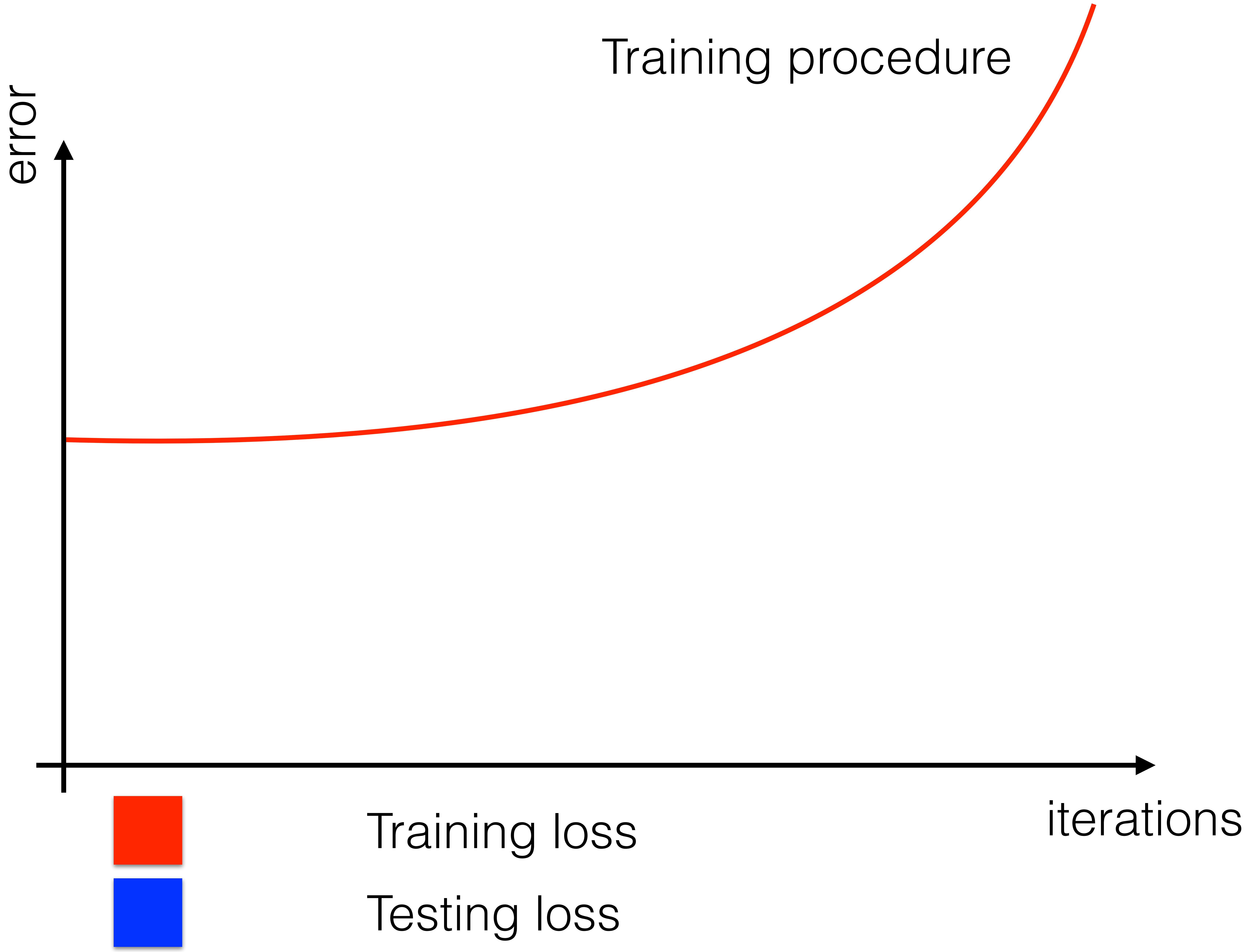
Broyden **F**letcher **G**oldfarb **S**hanno

Applications everywhere, where Hessian computation is too painful but GD suffers from slow convergence:

- Structural design (bridges, buildings, aerospace components) e.g. minimize material usage or structural properties
- Process optimization (chemistry)
- Tuning control system (automotive, aerospace, aircrafts, powerplants)
- Computer graphics (mesh fitting with structural priors)
- ….

Training procedure

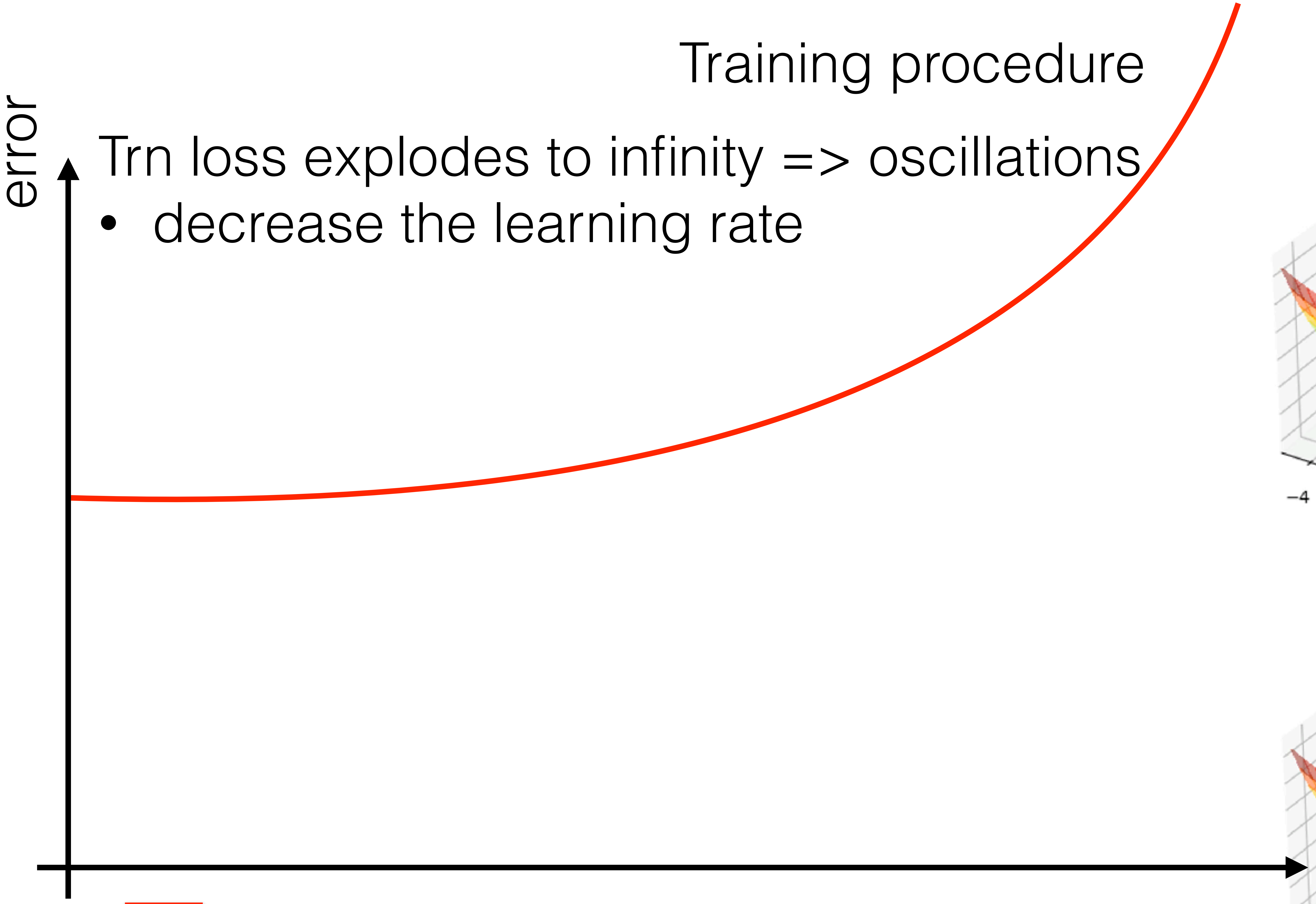
- Choose:
  - Network architecture (ideally re-use pre-trained net)
  - Weight initialization (Xavier)
  - Learning rate and other hyper-parameters.
  - Loss + regularization
- Divide data on three representative subsets:
  - Training data (the set on which the backprop is used to estimate weights)
  - Validation data (the set on which hyper-param are tuned)
  - Testing data (the set on which the error is reported)

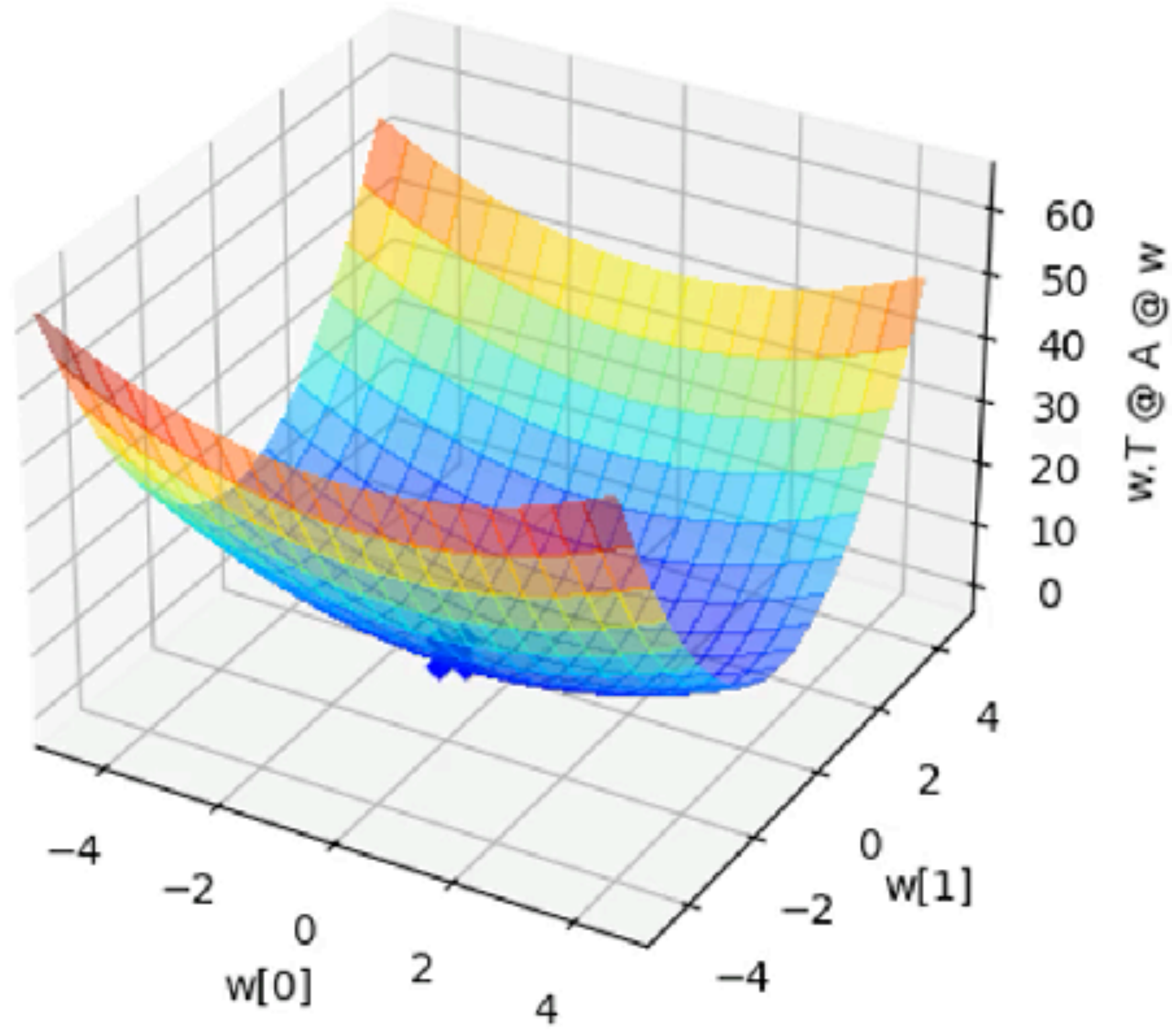

Training procedure
error
iterations
Training loss
Testing loss

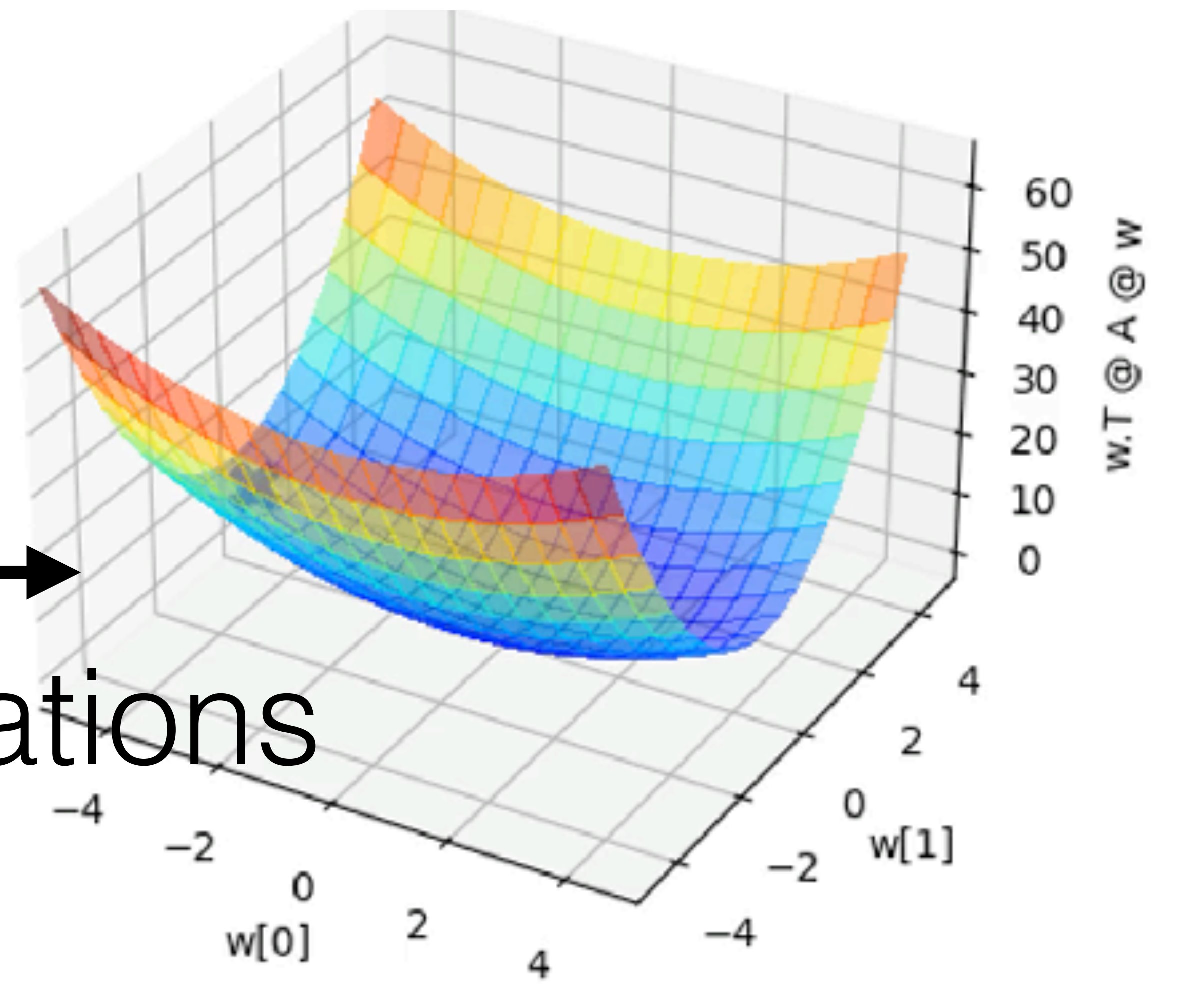
Training procedure

Trn loss explodes to infinity => oscillations

- decrease the learning rate

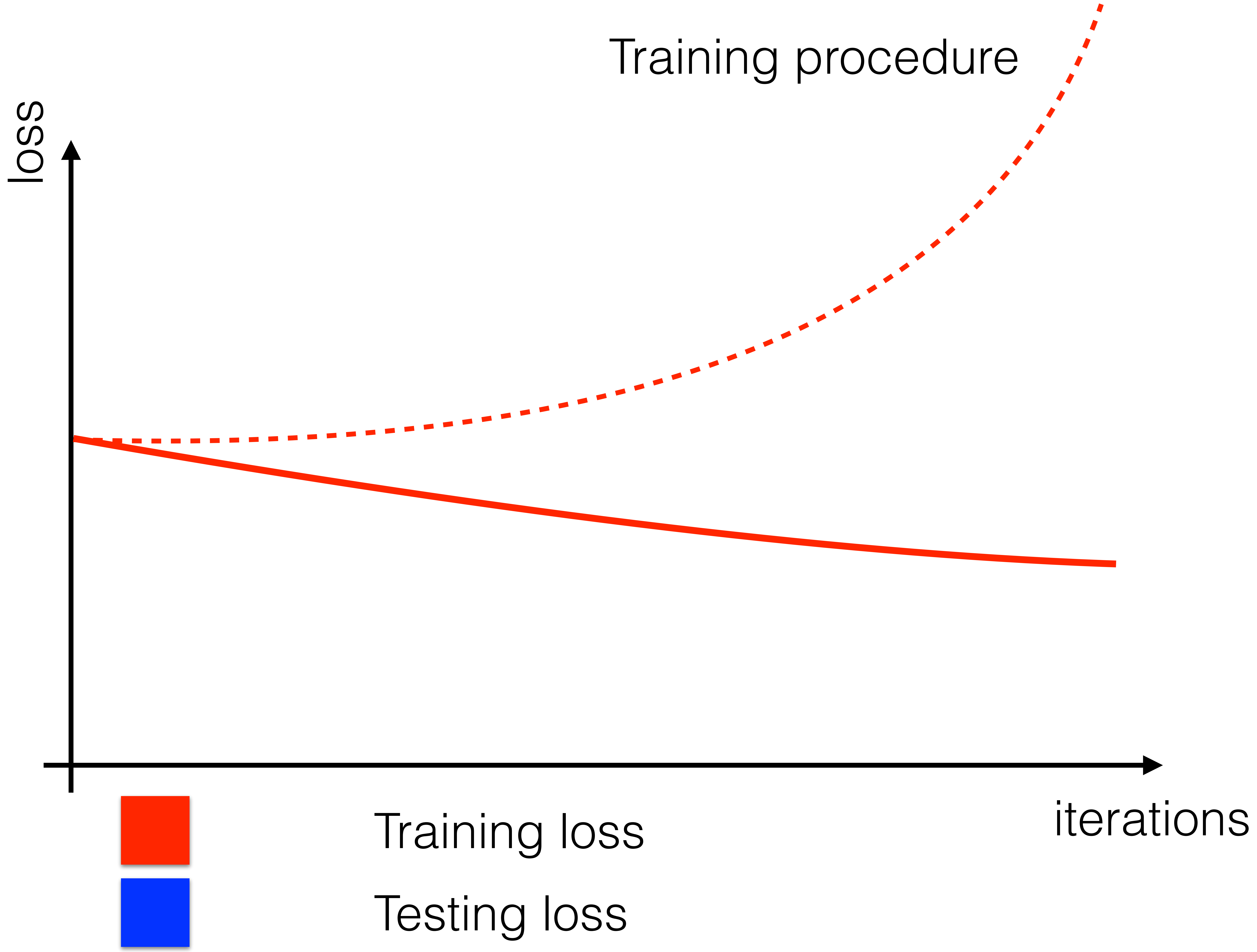






Training loss

Testing loss


Training procedure
loss
iterations
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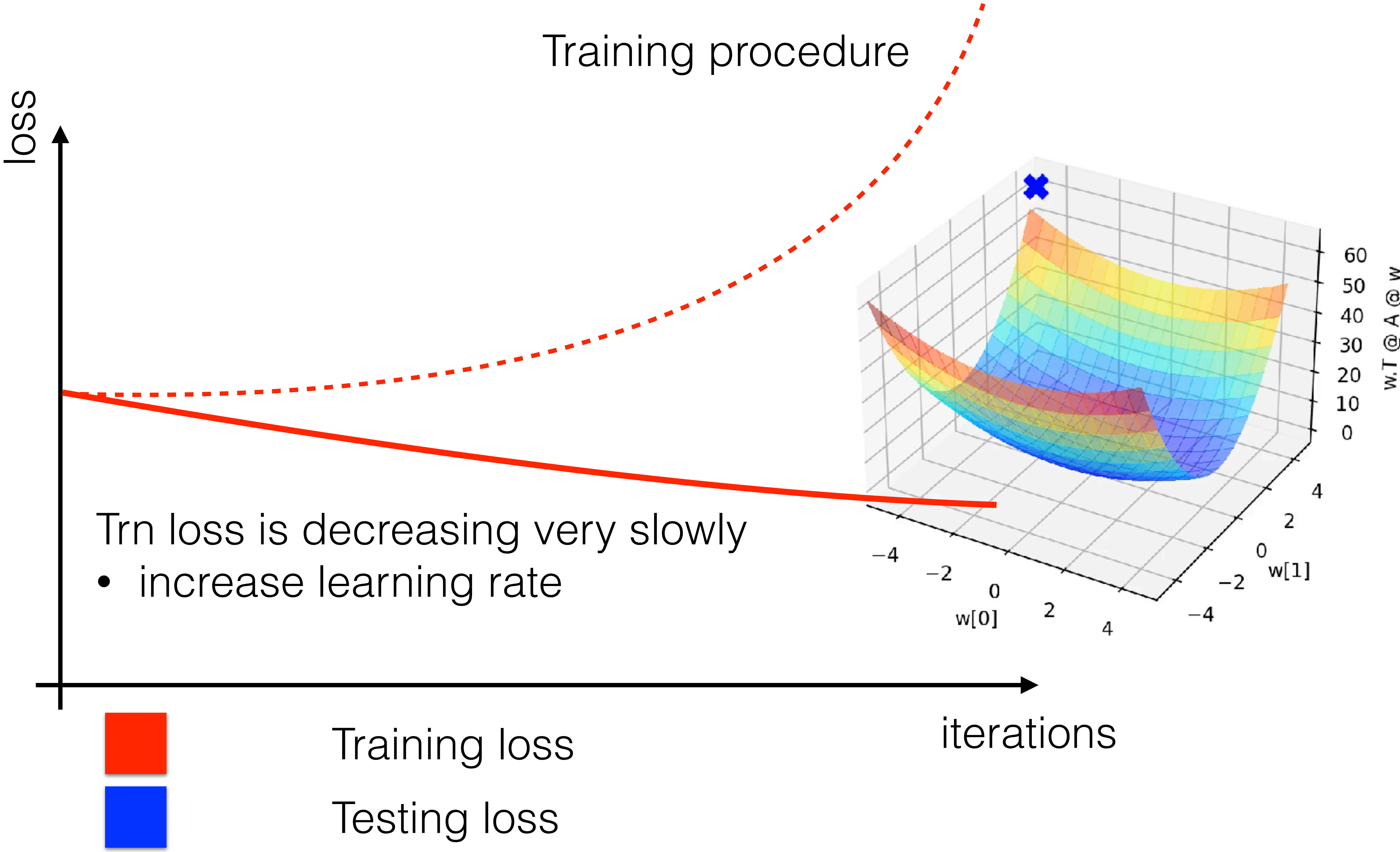
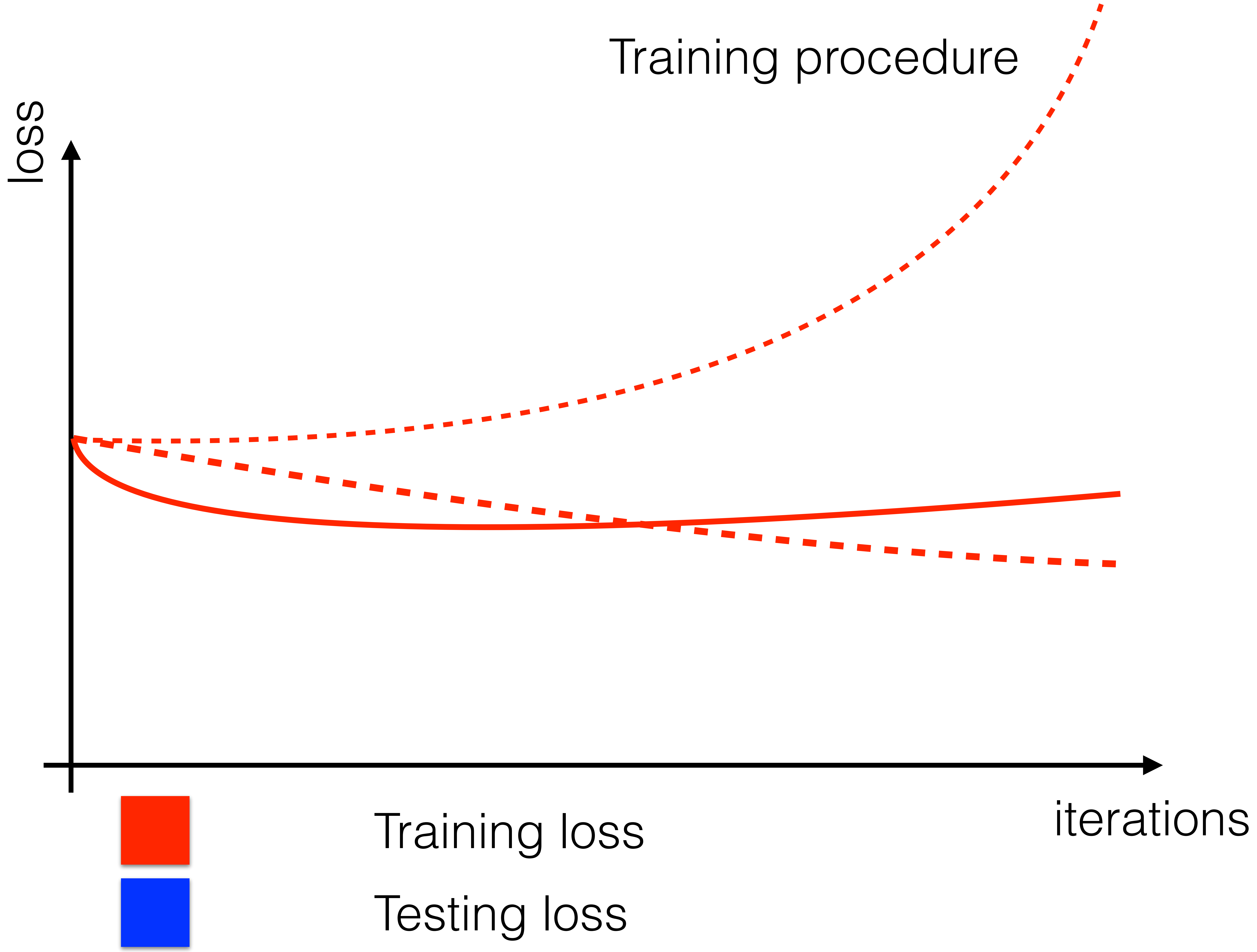
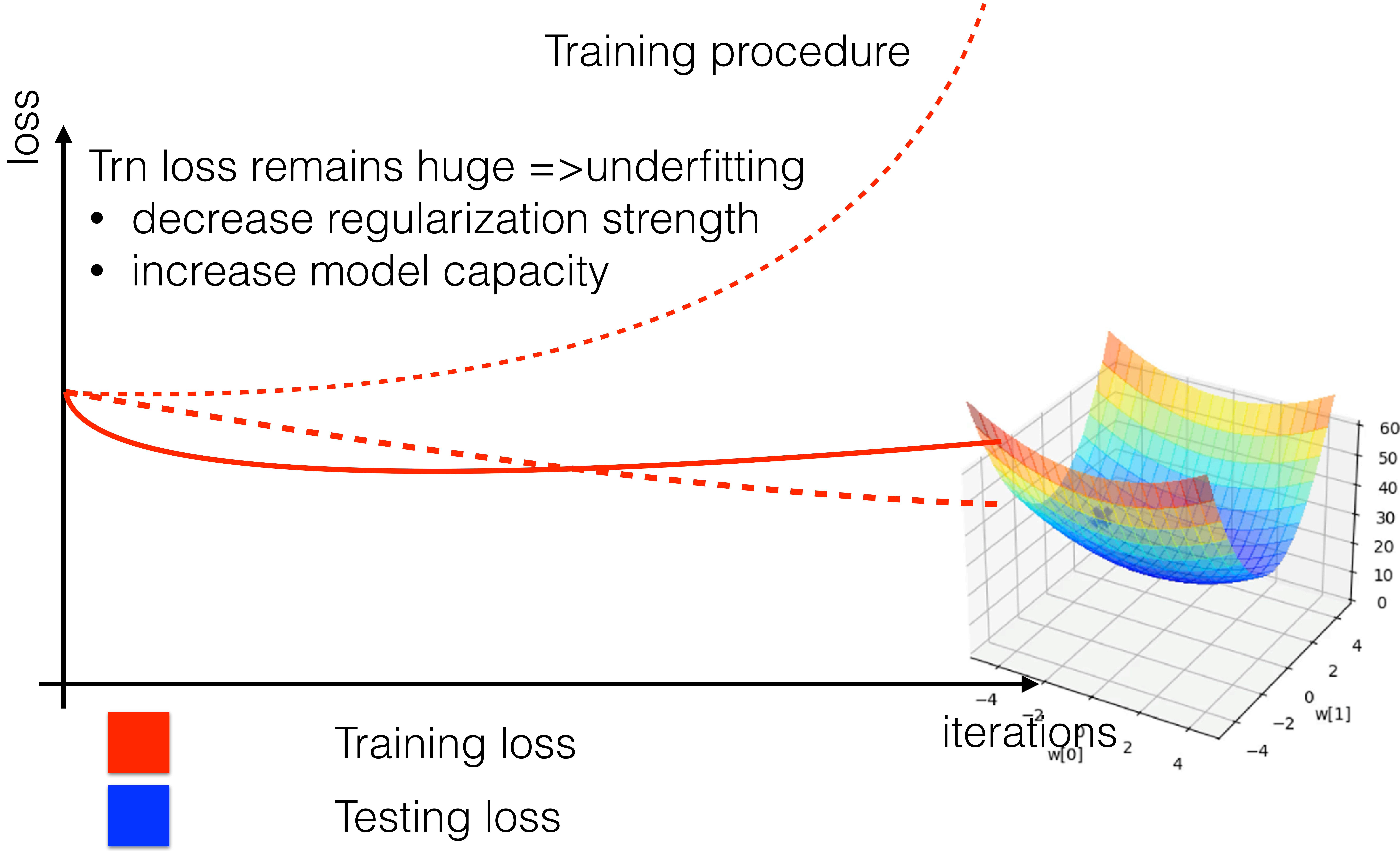
Training procedure



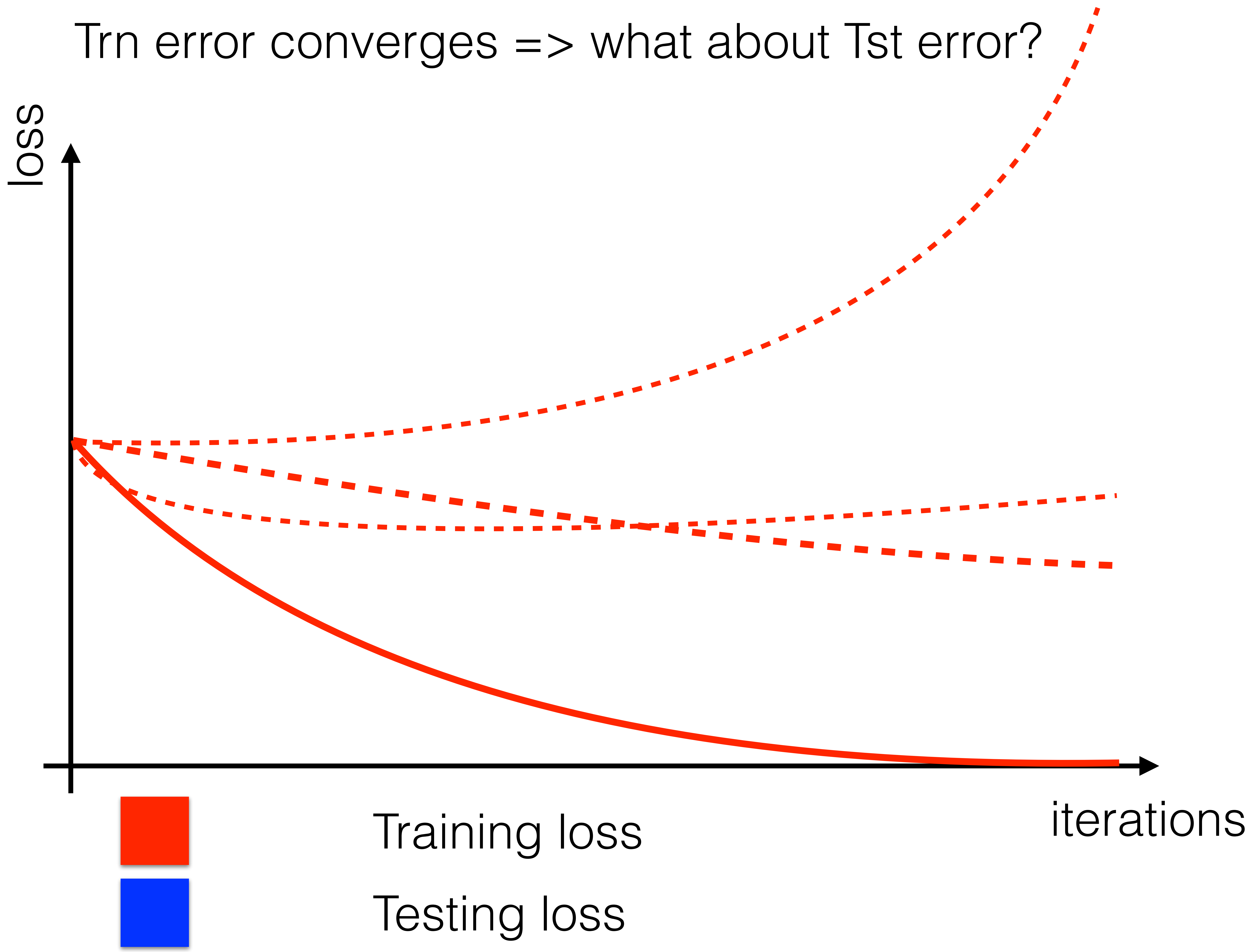

Training procedure
loss
iterations
Training loss
Testing loss

Training procedure

Trn loss remains huge =>underfitting
- decrease regularization strength
- increase model capacity

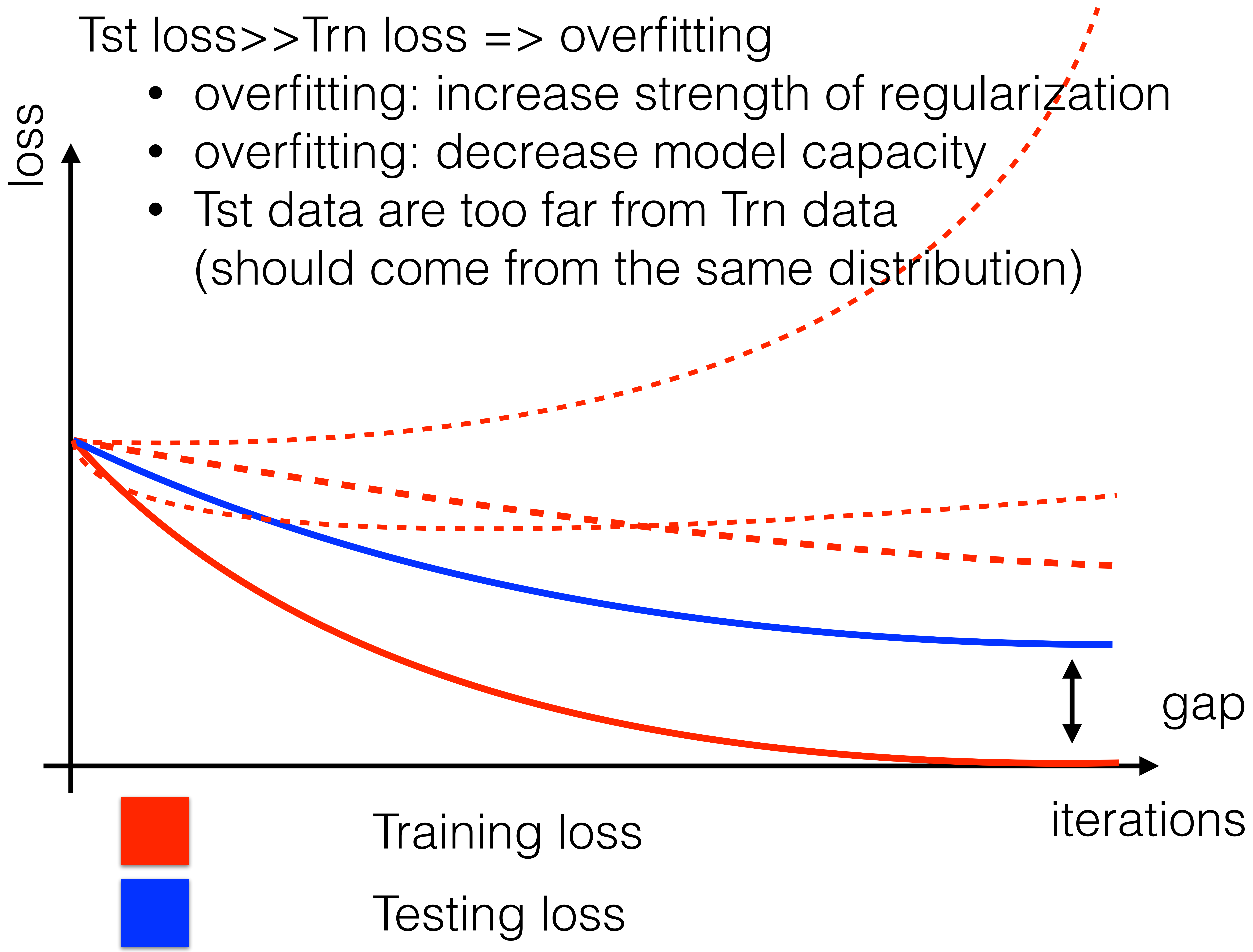


Trn error converges => what about Tst error?



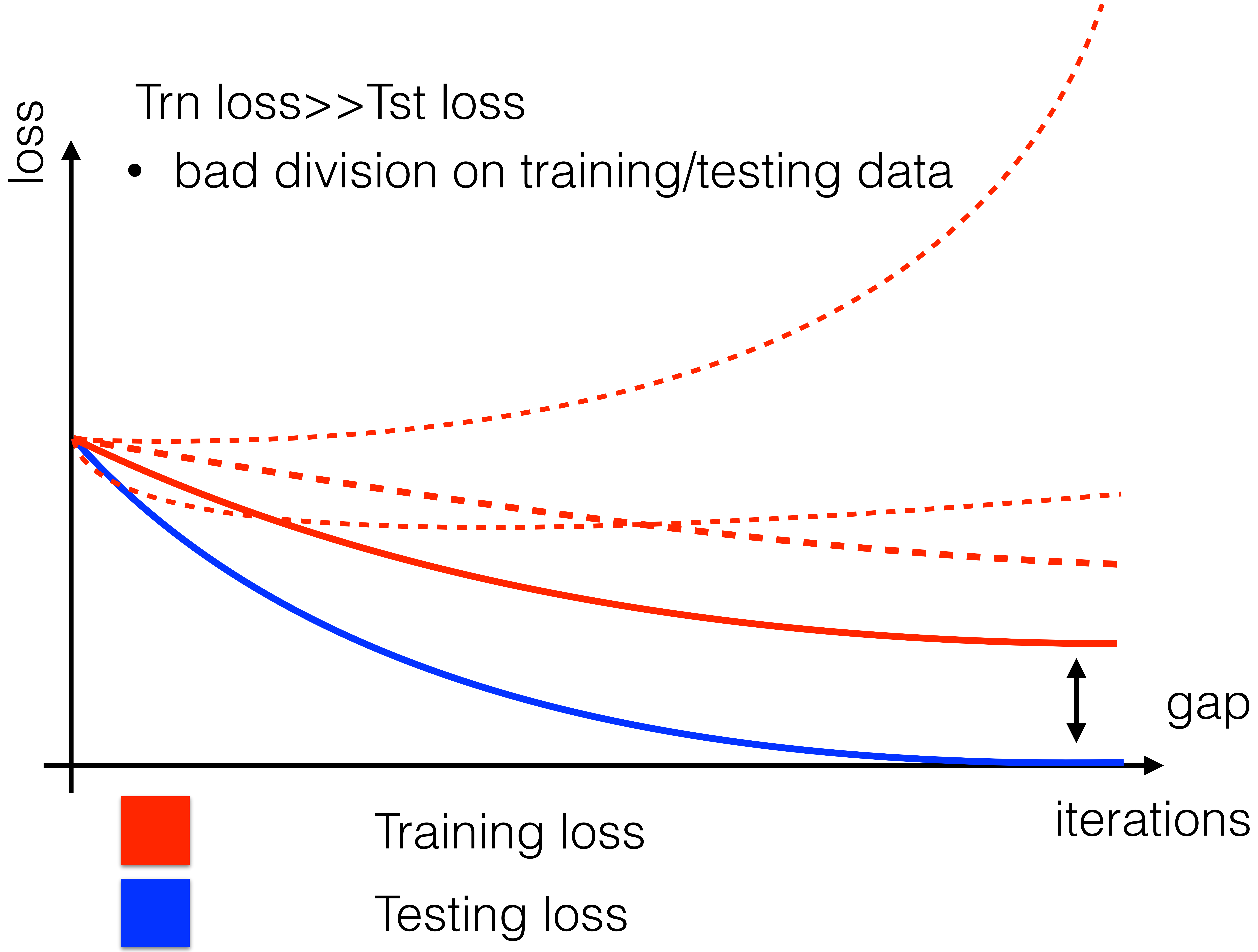
Tst loss>>Trn loss => overfitting

- overfitting: increase strength of regularization
- overfitting: decrease model capacity
- Tst data are too far from Trn data
(should come from the same distribution)

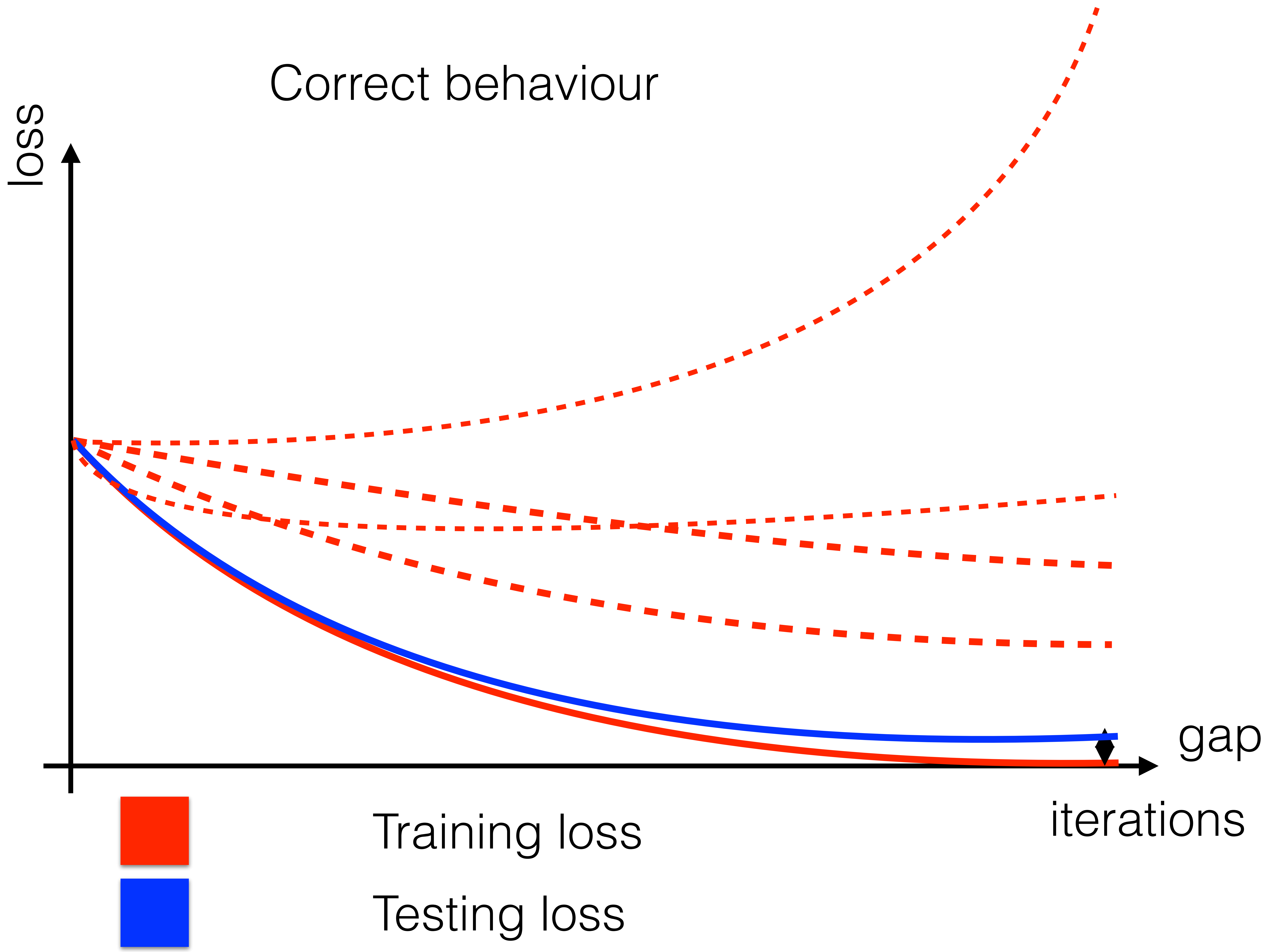


Trn loss>>Tst loss

- bad division on training/testing data



Correct behaviour



Hyper parameters tuning

- Weight initialization (Xavier)
- Trn loss is huge =>underfitting
  - decrease regularization strength
  - increase model capacity
- Trn loss explodes to infinity=> huge learning rate
  - decrease the learning rate
- Trn loss is decreasing very slowly => small learning rate
  - increase learning rate
- Tst loss>>Trn loss => overfitting
  - increase strength of regularization
  - decrease model capacity
  - Tst data are too far from Trn data
    (should come from the same distribution)
- Trn loss>>Tst loss =>bad division on training/testing data

Epilog

- Structural vs optimization issues
- Newton : $f(\mathbf{x}) \approx \frac{1}{2}\mathbf{x}^\top H\mathbf{x} + \mathbf{g}\mathbf{x} + c \quad \Rightarrow H\mathbf{x} + \mathbf{g} = 0 \quad \Rightarrow \mathbf{x} = H^{-1}\mathbf{g}$
- Adam : $\hat{H} = \begin{bmatrix} \bar{g}_1 & 0 & \dots & 0 \\ 0 & \bar{g}_2 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & \bar{g}_n \end{bmatrix} \quad \Rightarrow \mathbf{x} = \hat{H}^{-1}\mathbf{g}$

- Optimization vs Learning

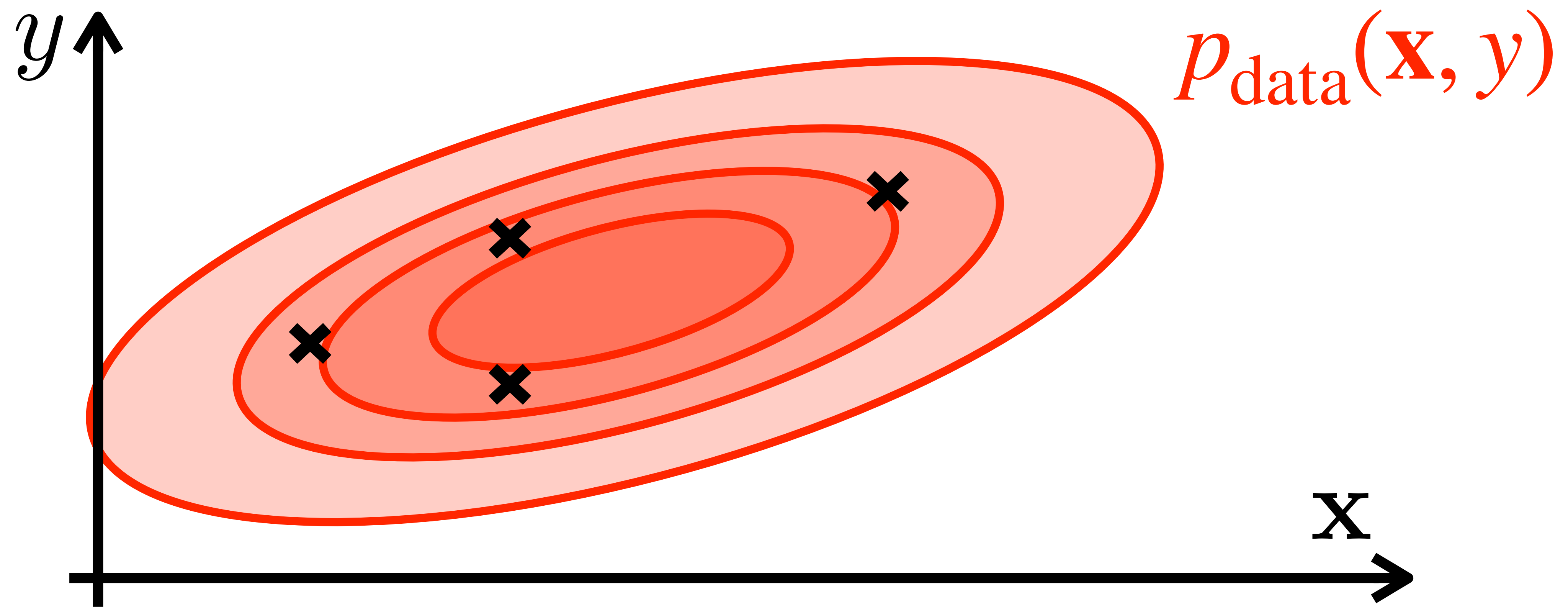
$$J(\mathbf{w}) = \mathbb{E}_{(\mathbf{x},y)\sim p_{\text{data}}}\left[\log p(\mathbf{x}, y \mid \mathbf{w})\right]$$

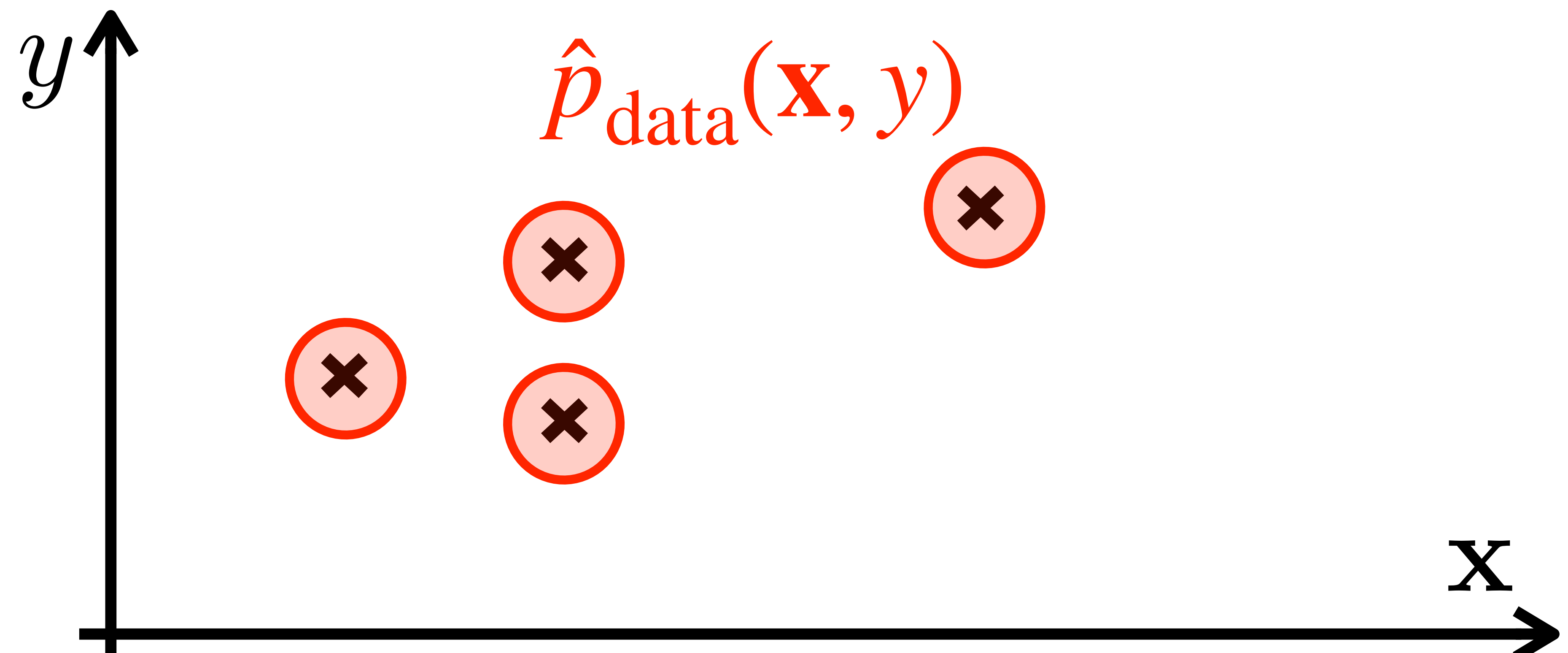
$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \mathbb{E}_{(\mathbf{x},y)\sim p_{\text{data}}}\left[\nabla_{\mathbf{w}} \log\left(p(\mathbf{x}, y \mid \mathbf{w})\right)\right]$$

vs.

$$\hat{J}(\mathbf{w}) = \mathbb{E}_{(\mathbf{x},y)\sim \hat{p}_{\text{data}}}\left[\log p(\mathbf{x}, y \mid \mathbf{w})\right]$$

$$\nabla_{\mathbf{w}} \hat{J}(\mathbf{w}) = \mathbb{E}_{(\mathbf{x},y)\sim p_{\text{data}}}\left[\nabla_{\mathbf{w}} \log\left(p(\mathbf{x}, y \mid \mathbf{w})\right)\right]$$

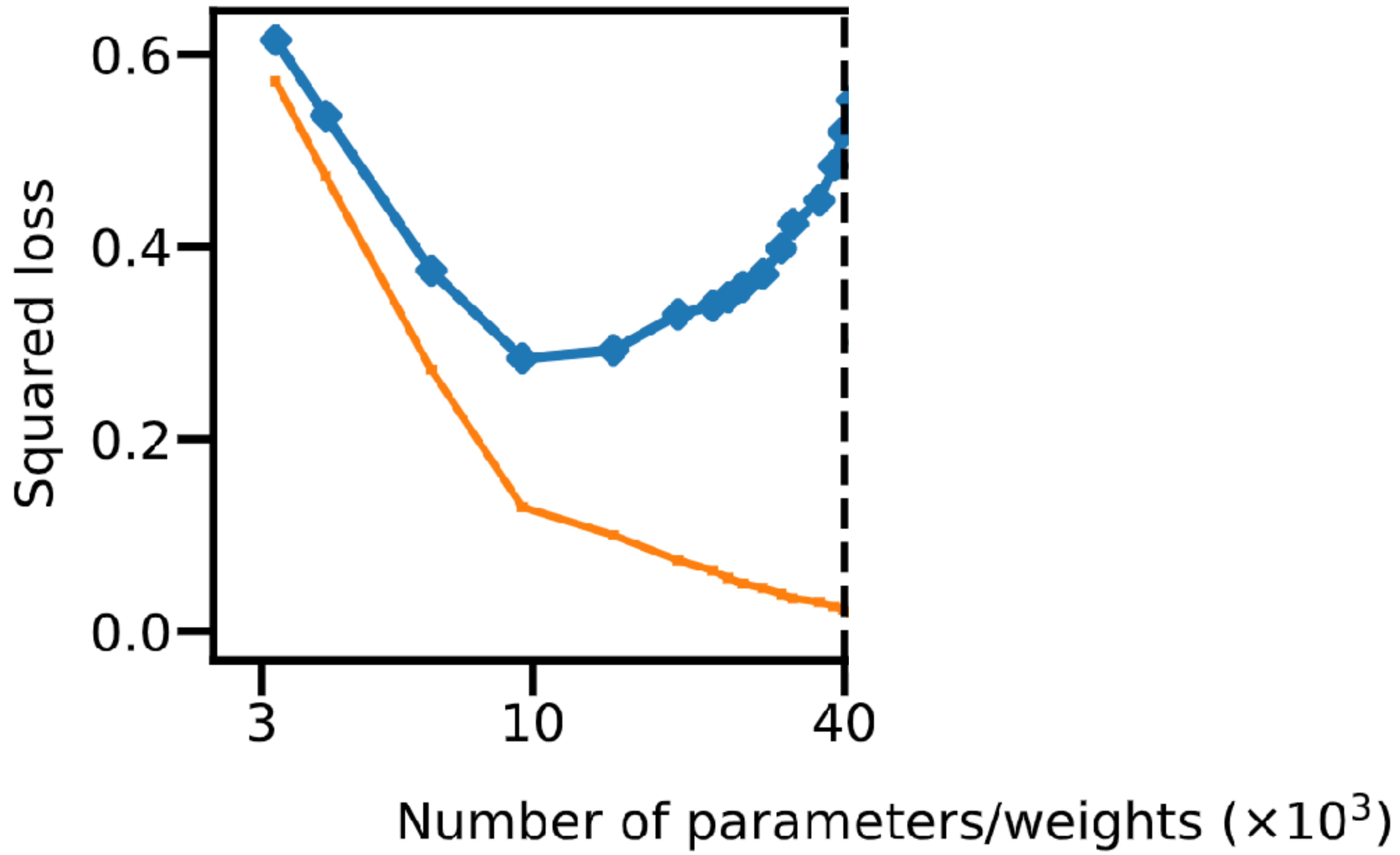




Epilog

- Stochasticity advantage:
  - reduces computational time and memory
  - works as an regularizer that helps in larger models (avoids wild hypothesis)
  - avoids getting stuck in saddle points
- Stochasticity drawback:
  - makes estimation of gradient and Hessian inaccurate (Standard deviation $\approx 1/\sqrt{N}$ => suffers from sub-linear returns)
  - smaller N +higher M avoids advanced Hessian approx methods (LBFGS) =>Adam is typically used
- Momentum advantage:
  - jumps over sharp minima
  - avoid getting stuck in flat regions
  - suppress oscillations

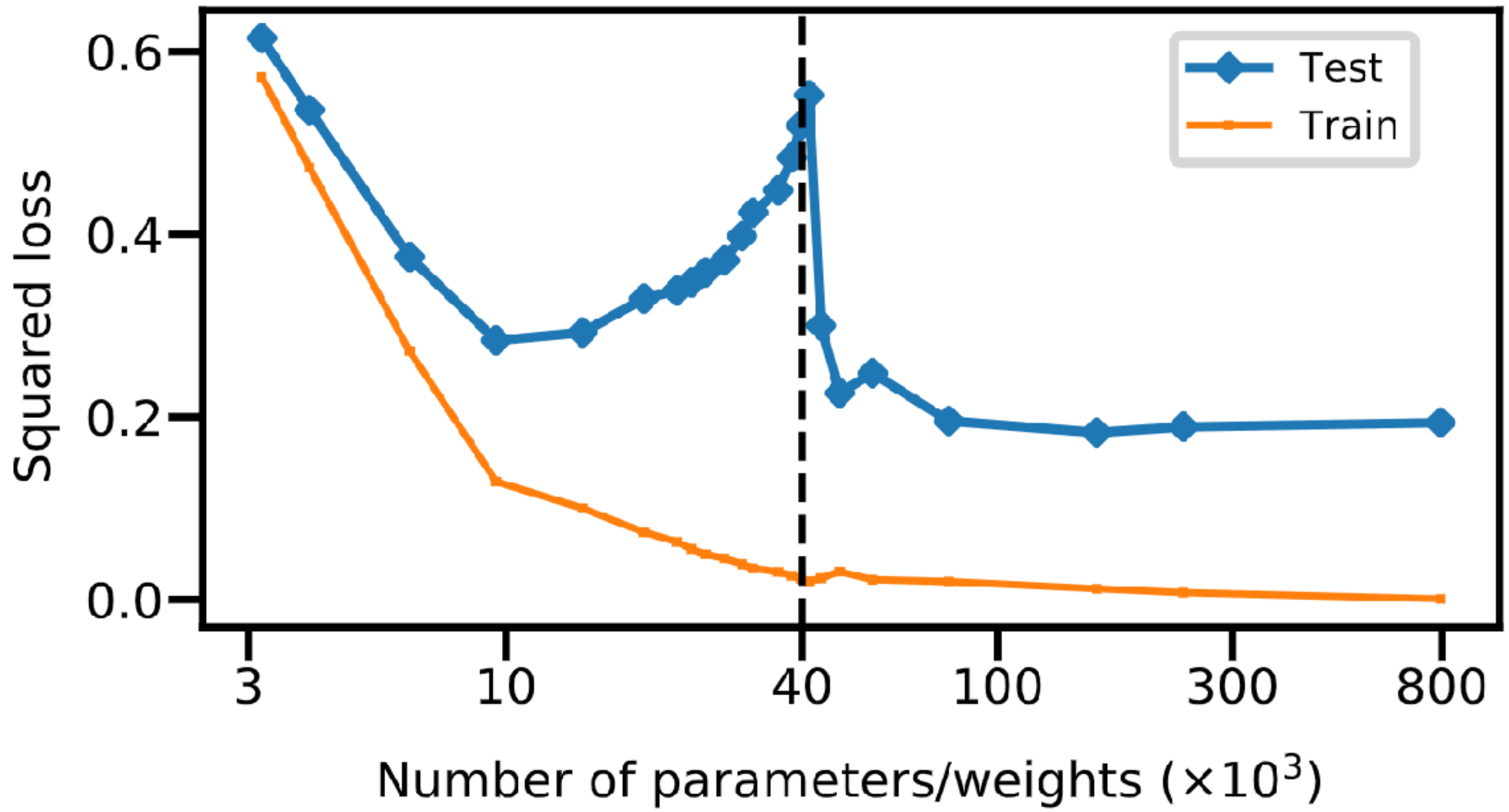
Double descent
[Belkin-DoubleDescent-2019]



Statistical wisdom: “Too large models are worse since they overfit.”

https://openai.com/blog/deep-double-descent/

Double descent
[Belkin-DoubleDescent-2019]



Statistical wisdom: “Too large models are worse since they overfit.”

Deep ML wisdom: “The larger the better”

https://openai.com/blog/deep-double-descent/

Double descent
[Belkin-DoubleDescent-2019]

https://openai.com/blog/deep-double-descent/