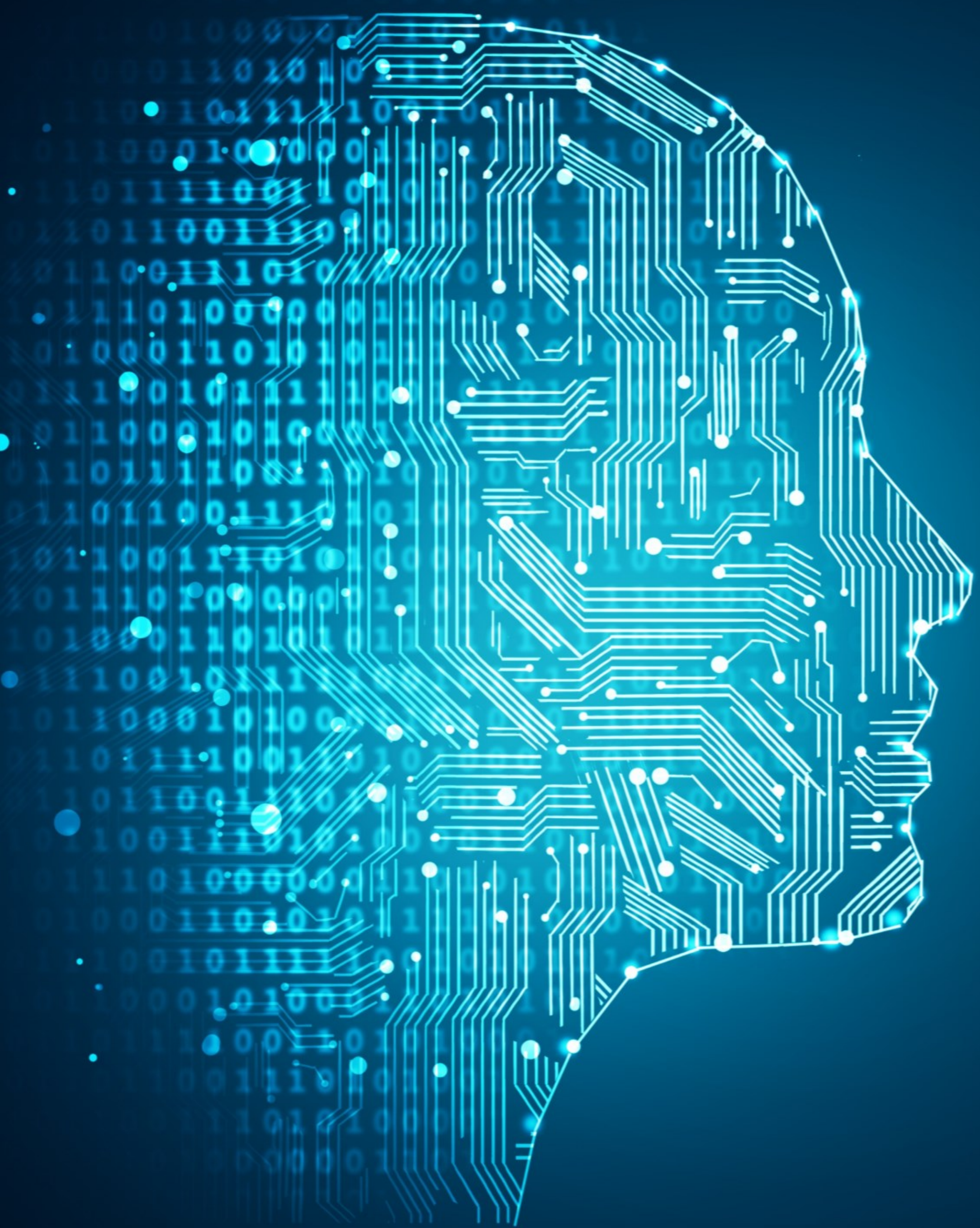

AI6103 Optimization (Part 2)

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Outline

- Bias-variance Tradeoff
- Optimization with Deterministic Gradient Descent
- Stochastic Gradient Descent
- Batch Size and Learning Rate
- Implicit Regularization of SGD

Underfitting vs. Overfitting

The Art of Balancing

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Deep Learning Intuition

- Underfitting: Not learning enough from the observed data.
  - Even if the model is large, the optimization could be poor.
- Overfitting: The observed data contain some random errors, some idiosyncrasies that do not apply to the general population. Overfitting is to learn from such noise.
  - Example: Learning from a weird horse image and thinking that it describes many real-world horses.
- DL deals with more complex semantics than traditional ML.
  - What is noise using one set of features is signal under another set of features.
  - Quality of feature representation matters a lot.
  - Sometimes increasing capacity could reduce generalization error!

Bias-variance Tradeoff

- We want to estimate random variables (e.g, neural network weights) from data
  - Low bias = the estimate fits data well but may overfit
  - Low variance = the estimate is not overly influenced by noise in data, but may underfit
- Adding L2 regularization to linear regression lowers the variance in the estimate of model parameter $\boldsymbol{\beta}$
- http://cs229.stanford.edu/summer2019/BiasVarianceAnalysis.pdf

Bias-variance Tradeoff

- Dataset $D = \{(\boldsymbol{x}^{(1)}, y^{(1)}), \ldots, (\boldsymbol{x}^{(n)}, y^{(n)})\}$ drawn i.i.d from a distribution $P(X, Y)$
- i.i.d = independently and identically distributed
- **Expected label**

$$\bar{y}(\mathbf{x}) = E_{y|\mathbf{x}}[Y] = \int_y y \Pr(y|\mathbf{x}) \partial y.$$

- The label y depends on x but the relationship is not 100% deterministic. So we compute its expectation from distribution $\Pr(y|\boldsymbol{x})$
- This noise in y could reflect annotation error, or simply the semantics in $\boldsymbol{x}$ that the model cannot understand. Recall: coin toss is deterministic.

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Bias-variance Tradeoff

- The machine learning algorithm A learns a model (or hypothesis) h_D from the dataset D. $h_D = A(D)$.
- Expected model

$$\bar{h} = E_{D \sim P^n}\left[h_D\right] = \int_D h_D \Pr(D) \partial D$$

- Expected test error

$$E_{(\mathbf{x},y)\sim P}\left[\left(h_D(\mathbf{x}) - y\right)^2\right] = \int_x \int_y \left(h_D(\mathbf{x}) - y\right)^2 \Pr(\mathbf{x}, y) \partial y \partial \mathbf{x}.$$

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Bias-variance Tradeoff

- Combining everything we have

$$E_{\substack{(\mathbf{x},y)\sim P \\ D\sim P^n}}\left[\left(h_D(\mathbf{x})-y\right)^2\right]=\int_D\int_{\mathbf{x}}\int_y \left(h_D(\mathbf{x})-y\right)^2 \mathrm{P}(\mathbf{x},y)\mathrm{P}(D)\partial\mathbf{x}\partial y\partial D$$

- That is, the expectation is over the observed dataset D and all possible data $(\boldsymbol{x}, y)$

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Bias-variance Tradeoff

$$E_{\substack{(\mathbf{x},y)\sim P\\ D\sim P^n}}\left[(h_D(\mathbf{x})-y)^2\right]=\int_D\int_{\mathbf{x}}\int_y (h_D(\mathbf{x})-y)^2\mathrm{P}(\mathbf{x},y)\mathrm{P}(D)\partial\mathbf{x}\partial y\partial D$$

$$\begin{aligned}E_{\mathbf{x},y,D}\left[[h_D(\mathbf{x})-y]^2\right] &= E_{\mathbf{x},y,D}\left[\left[\left(h_D(\mathbf{x})-\bar{h}(\mathbf{x})\right)+\left(\bar{h}(\mathbf{x})-y\right)\right]^2\right]\\ &= E_{\mathbf{x},D}\left[(\bar{h}_D(\mathbf{x})-\bar{h}(\mathbf{x}))^2\right]+\underbrace{\boxed{2\,E_{\mathbf{x},y,D}\left[\left(h_D(\mathbf{x})-\bar{h}(\mathbf{x})\right)\left(\bar{h}(\mathbf{x})-y\right)\right]}}_{=0}+E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-y\right)^2\right]\end{aligned}$$

$$\begin{aligned}E_{\mathbf{x},y,D}\left[\left(h_D(\mathbf{x})-\bar{h}(\mathbf{x})\right)\left(\bar{h}(\mathbf{x})-y\right)\right] &= E_{\mathbf{x},y}\left[E_D\left[h_D(\mathbf{x})-\bar{h}(\mathbf{x})\right]\left(\bar{h}(\mathbf{x})-y\right)\right]\\ &= E_{\mathbf{x},y}\left[\left(E_D\left[h_D(\mathbf{x})\right]-\bar{h}(\mathbf{x})\right)\left(\bar{h}(\mathbf{x})-y\right)\right]\\ &= E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-\bar{h}(\mathbf{x})\right)\left(\bar{h}(\mathbf{x})-y\right)\right]\\ &= E_{\mathbf{x},y}[0]\\ &= 0\end{aligned}$$

Content credit: https://www.cs.cornell.edu/courses/cs4780/2018fa/lectures/lecturenote12.html

Bias-variance Tradeoff

$$
\begin{aligned}
E_{\mathbf{x},y,D}\left[\left(h_D(\mathbf{x}) - \bar{h}(\mathbf{x})\right)\left(\bar{h}(\mathbf{x}) - y\right)\right] &= E_{\mathbf{x},y}\left[E_D\left[h_D(\mathbf{x}) - \bar{h}(\mathbf{x})\right]\left(\bar{h}(\mathbf{x}) - y\right)\right] \\
&= E_{\mathbf{x},y}\left[\left(E_D\left[h_D(\mathbf{x})\right] - \bar{h}(\mathbf{x})\right)\left(\bar{h}(\mathbf{x}) - y\right)\right] \\
&= E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x}) - \bar{h}(\mathbf{x})\right)\left(\bar{h}(\mathbf{x}) - y\right)\right] \\
&= E_{\mathbf{x},y}\left[0\right] \\
&= 0
\end{aligned}
$$

Recall: The expectation operation is linear

$$
E_a[f(a)b] = \int f(a)b\,P(a)\,da = b\int f(a)\,P(a)\,da = bE_a[f(a)]
$$

$$
E_a[f(a) + g(a)] = \int \big(f(a) + g(a)\big)\,P(a)\,da = \int f(a)P(a)\,da + \int g(a)P(a)\,da
$$

$$
= E_a[f(a)] + E_a[g(a)]
$$

Bias-variance Tradeoff

$$E_{\mathbf{x},y,D}\left[\left(h_D(\mathbf{x})-y\right)^2\right] = \underbrace{E_{\mathbf{x},D}\left[\left(h_D(\mathbf{x})-\bar{h}(\mathbf{x})\right)^2\right]}_{\text{Variance}} + E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-y\right)^2\right]$$

- Variance of $h_D(\boldsymbol{x})$ shows how much h_D changes when the observed dataset D changes.
- If we happen to observe a few outliers in the data, is the learned function heavily affected by them?

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Bias-variance Tradeoff

$$
\begin{aligned}
E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-y\right)^2\right] &= E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)+\left(\bar{y}(\mathbf{x})-y\right)^2\right] \\
&= \underbrace{E_{\mathbf{x},y}\left[\left(\bar{y}(\mathbf{x})-y\right)^2\right]}_{\text{Noise}} + \underbrace{E_{\mathbf{x}}\left[\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)^2\right]}_{\text{Bias}^2} + \underbrace{\boxed{2\ E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\left(\bar{y}(\mathbf{x})-y\right)\right]}}_{=0}
\end{aligned}
$$

$\underbrace{E_{\mathbf{x},y}\left[\left(\bar{y}(\mathbf{x})-y\right)^2\right]}_{\text{Noise}}$ is the variance in y

$\underbrace{E_{\mathbf{x}}\left[\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)^2\right]}_{\text{Bias}^2}$ Bias measures how much $h(\boldsymbol{x})$ deviate from the expected label $\bar{y}$
Note that $\bar{h}$ is the average over all possible dataset D, so D has no influence here.

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Bias-variance Tradeoff

$$
\begin{aligned}
E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-y\right)^2\right] &= E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)+\left(\bar{y}(\mathbf{x})-y\right)^2\right] \\
&= \underbrace{E_{\mathbf{x},y}\left[\left(\bar{y}(\mathbf{x})-y\right)^2\right]}_{\text{Noise}} + \underbrace{E_{\mathbf{x}}\left[\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)^2\right]}_{\text{Bias}^2} + \underbrace{\boxed{2\ E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\left(\bar{y}(\mathbf{x})-y\right)\right]}}_{=0}
\end{aligned}
$$

$$
\begin{aligned}
E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\left(\bar{y}(\mathbf{x})-y\right)\right] &= E_{\mathbf{x}}\left[E_{y|\mathbf{x}}\left[\bar{y}(\mathbf{x})-y\right]\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\right] \\
&= E_{\mathbf{x}}\left[E_{y|\mathbf{x}}\left[\bar{y}(\mathbf{x})-y\right]\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\right] \\
&= E_{\mathbf{x}}\left[\left(\bar{y}(\mathbf{x})-E_{y|\mathbf{x}}\left[y\right]\right)\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\right] \\
&= E_{\mathbf{x}}\left[\left(\bar{y}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\right] \\
&= E_{\mathbf{x}}\left[0\right] \\
&= 0
\end{aligned}
$$

Content credit: https://www.cs.cornell.edu/courses/cs4780/2018fa/lectures/lecturenote12.html

Bias-variance Tradeoff

- Combining everything,

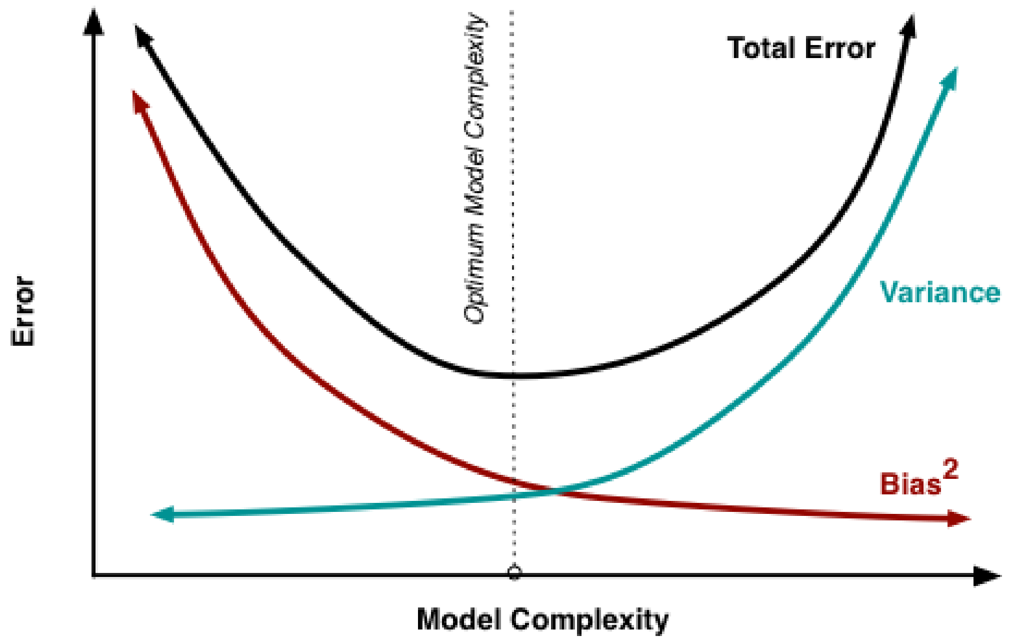
$$\underbrace{E_{\mathbf{x},y,D}\left[\left(h_D(\mathbf{x}) - y\right)^2\right]}_{\text{Expected Test Error}} = \underbrace{E_{\mathbf{x},D}\left[\left(h_D(\mathbf{x}) - \bar{h}(\mathbf{x})\right)^2\right]}_{\text{Variance}} + \underbrace{E_{\mathbf{x},y}\left[\left(\bar{y}(\mathbf{x}) - y\right)^2\right]}_{\text{Noise}} + \underbrace{E_{\mathbf{x}}\left[\left(\bar{h}(\mathbf{x}) - \bar{y}(\mathbf{x})\right)^2\right]}_{\text{Bias}^2}$$

Variance: Captures how much your classifier changes if you train on a different training set. How "over-specialized" is your classifier to a particular training set (overfitting)? If we have the best possible model for our training data, how far off are we from the average classifier?

Bias: What is the inherent error that you obtain from your classifier even with infinite training data? This is due to your classifier being "biased" to a particular kind of solution (e.g. linear classifier). In other words, bias is inherent to your model.

Noise: How big is the data-intrinsic noise? This error measures ambiguity due to your data distribution and feature representation. You can never beat this, it is an aspect of the data.

Bias-variance Tradeoff



As model complexity increases, overfitting increases.

Conventional ML wisdom says that you need to have fewer parameters than training data points.

In deep learning, models are heavily overparameterized and achieve zero training loss, but still generalize well.

Still, you can have too many parameters even in deep learning. Overfitting is a severe problem and researchers developed many techniques to mitigate it .

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Optimization: Gradient Descent

Gradient Descent

- We seek $\boldsymbol{w}$ that minimizes a differentiable function $L(x, \boldsymbol{w})$
- Input: loss function $L(\boldsymbol{w})$, initial position $\boldsymbol{w}_0$, learning rates η_t
- Algorithm: Repeat until termination criterion
  - Move in the direction of negative gradient
  - $\boldsymbol{w}_t = \boldsymbol{w}_{t-1} - \eta_t \frac{\mathrm{d}L(\boldsymbol{w})}{\mathrm{d}\boldsymbol{w}}\Big|_{\boldsymbol{w}_{t-1}}$

Taylor Series for Function Approximation

- We can approximate an infinitely differentiable function $f(x): \mathbb{R} \rightarrow \mathbb{R}$ with the following sum

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2 + \frac{1}{3!} f'''(x_0)(x - x_0)^3 + \cdots$$

- Alternatively

$$f(x) = \sum_{n=0}^{\infty} a_n (x - x_0)^n, a_n = \boxed{\frac{f^{(n)}(x_0)}{n!}}$$

n^{th} derivative

Taylor Series for Function Approximation

- We can approximate an infinitely differentiable function $f(x): \mathbb{R} \to \mathbb{R}$ with the following sum

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2 + \frac{1}{3!} f'''(x_0)(x - x_0)^3 + \cdots$$

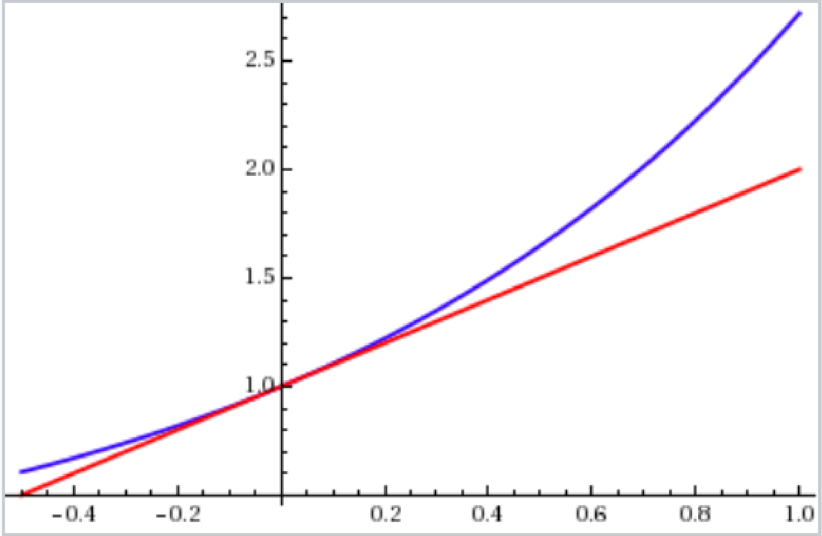
- When $|x - x_0| = \epsilon$ is small ($\epsilon \ll 1$), $(x - x_0)^2$ is $\epsilon^2 \ll \epsilon$
- Every term after that is even smaller.
- Thus, for approximation around x_0, we may take only the first two terms.

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + O(\epsilon^2)$$

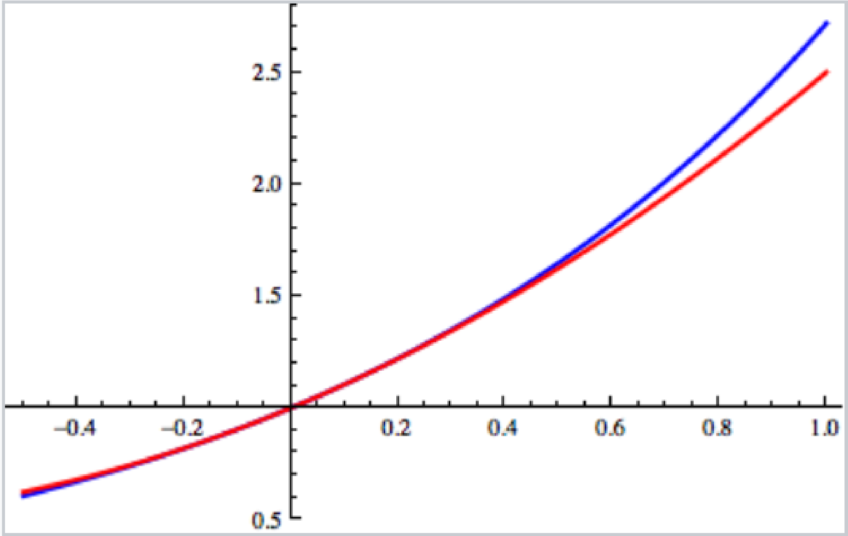
- For slightly larger ϵ, three terms allow us to be more precise

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2 + O(\epsilon^3)$$

Taylor Series for Function Approximation



Graph of $f(x) = e^x$ (blue) with its linear approximation $P_1(x) = 1 + x$ (red) at $a = 0$.



Graph of $f(x) = e^x$ (blue) with its quadratic approximation $P_2(x) = 1 + x + x^2/2$ (red) at $a = 0$. Note the improvement in the approximation.

Multivariate Taylor Polynomial

- For small Δ

$$f(\boldsymbol{x}+\Delta) = \underbrace{f(\boldsymbol{x})}_{\text{Constant term}} + \underbrace{\left(\frac{df}{d\boldsymbol{x}}\right)^{\mathsf{T}} \Delta}_{\text{Linear Term (in } \Delta)} + \underbrace{\frac{1}{2}\Delta^{\mathsf{T}} \left(\frac{d^2 f}{d\boldsymbol{x}^2}\right) \Delta}_{\text{Quadratic term with Hessian.}} + \underbrace{\cdots}_{\text{Additional terms are increasingly less important.}}$$

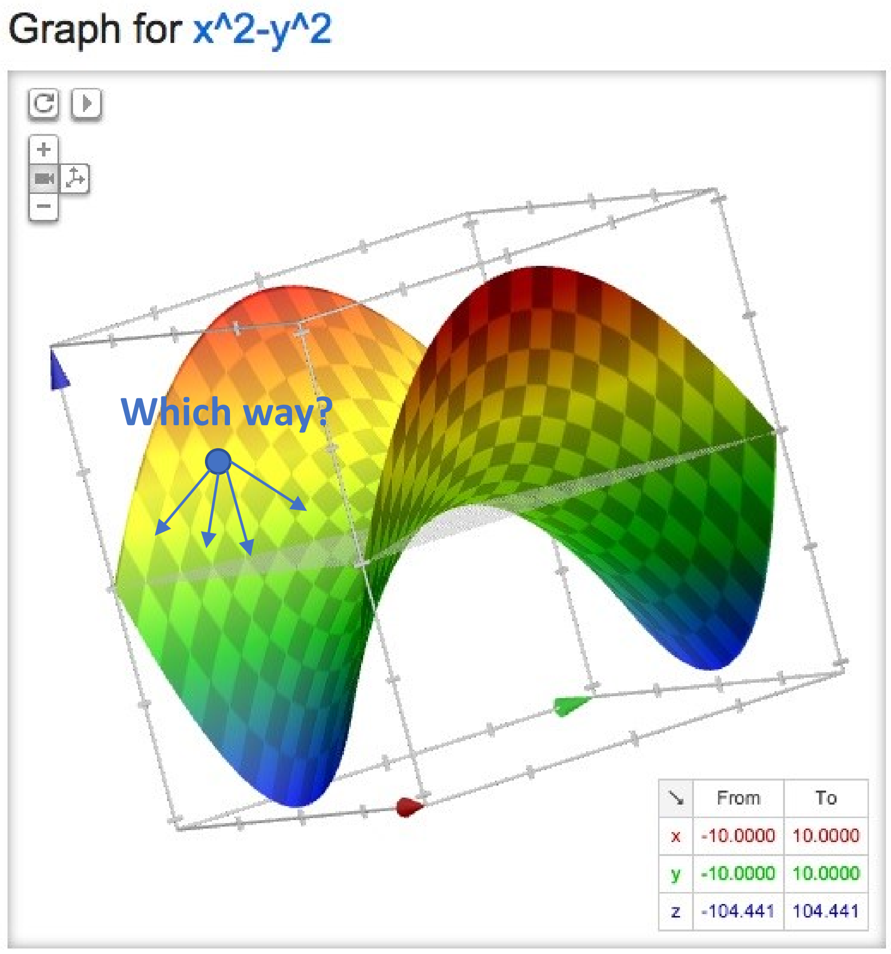
Gradient Descent is Steepest Descent

- We want to find a direction $\boldsymbol{v} \in \mathbb{R}^n$ that leads to the fastest decrease in $f(\boldsymbol{x})$.
- If we can find $\boldsymbol{v}$, we will move a little bit in that direction.

$$\boldsymbol{x}_t = \boldsymbol{x}_{t-1} + \eta \boldsymbol{v}$$

- We look for $v_{sd} = \underset{\boldsymbol{v}}{\operatorname{argmin}} \frac{f(\boldsymbol{x}+\boldsymbol{v})}{\|\boldsymbol{v}\|}$
- As we plan to take a small step, we can use a first-order approximation.

$$f(\boldsymbol{x}+\boldsymbol{v}) = f(\boldsymbol{x}) + \left(\frac{df}{d\boldsymbol{x}}\right)^{\top} \boldsymbol{v}$$



Steepest Descent under Euclidean Norm

- We want to find a direction $\boldsymbol{v} \in \mathbb{R}^n$ that leads to the fastest decrease in $f(\boldsymbol{x})$.
- If we can find $\boldsymbol{v}$, we will move a little bit in that direction.

$$\boldsymbol{x}_t = \boldsymbol{x}_{t-1} + \eta \boldsymbol{v}$$

- We look for $v_{sd} = \underset{\boldsymbol{v}}{\operatorname{argmin}} \frac{f(\boldsymbol{x}+\boldsymbol{v})}{\|\boldsymbol{v}\|}$
- As we plan to take a small step, we can use a first-order approximation.

$$f(\boldsymbol{x}+\boldsymbol{v}) = f(\boldsymbol{x}) + \left(\frac{df}{d\boldsymbol{x}}\right)^{\top} \boldsymbol{v}$$

- Fact: $\frac{\boldsymbol{v}^{\top}\boldsymbol{g}}{\|\boldsymbol{v}\|} = \|\boldsymbol{g}\| \cos\theta$
- All it matters is $\cos\theta$
- To minimize $\frac{\boldsymbol{v}^{\top}\boldsymbol{g}}{\|\boldsymbol{v}\|}$, we can choose $\boldsymbol{v} = -\boldsymbol{g}$
- That is, $-\left(\frac{df}{d\boldsymbol{x}}\right)$ is the direction for steepest descent.
- Note: we may choose a different norm and get different results.

Further Analysis

- For the analysis of multiple GD iterations, we use a second-order approximation

$$f(\boldsymbol{x}+\Delta) = \underbrace{f(\boldsymbol{x})}_{\text{Constant term}} + \underbrace{\left(\frac{df}{d\boldsymbol{x}}\right)^{\mathsf{T}}\Delta}_{\text{Linear Term (in }\Delta)} + \underbrace{\frac{1}{2}\Delta^{\mathsf{T}}\left(\frac{d^2 f}{d\boldsymbol{x}^2}\right)\Delta}_{\text{Quadratic term with Hessian.}}$$

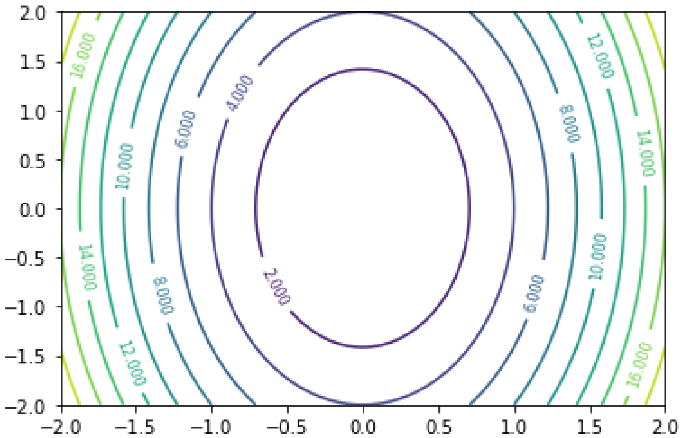
Hessian = Diagonal

Which contour diagram correctly depicts this function?

$$f(\boldsymbol{x}) = [x_1, x_2]\begin{bmatrix}4 & 0\\0 & 1\end{bmatrix}\begin{bmatrix}x_1\\x_2\end{bmatrix}$$

$$= 4x_1^2 + x_2^2$$

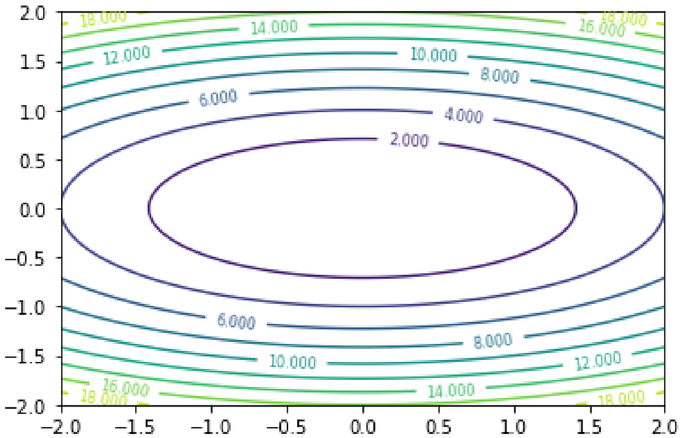
x_2



x_1

(A)

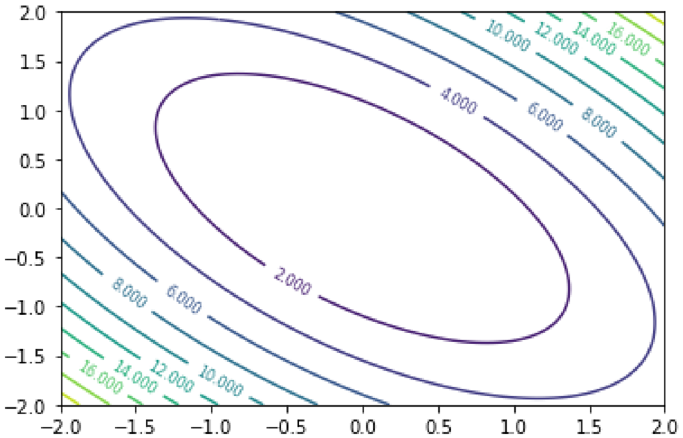
x_2



x_1

(B)

x_2



x_1

(C)

Hessian = Diagonal

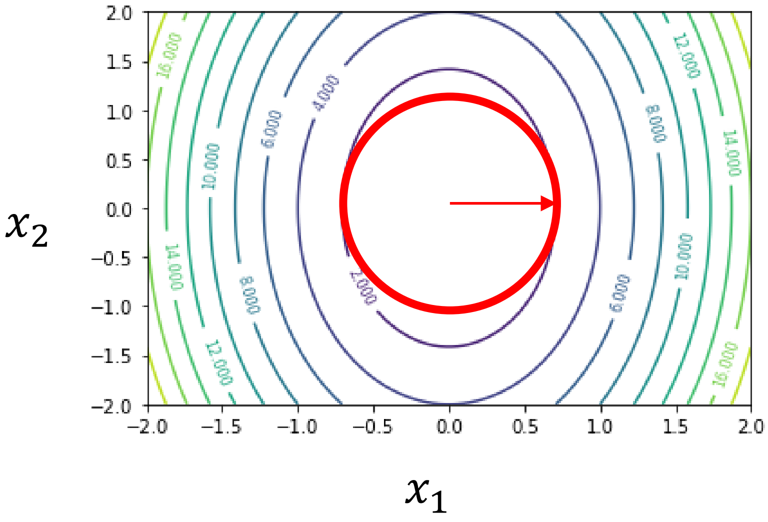
Which contour diagram correctly depicts this function?

Arrow: Moving by unit length in this direction increases the function value the most.

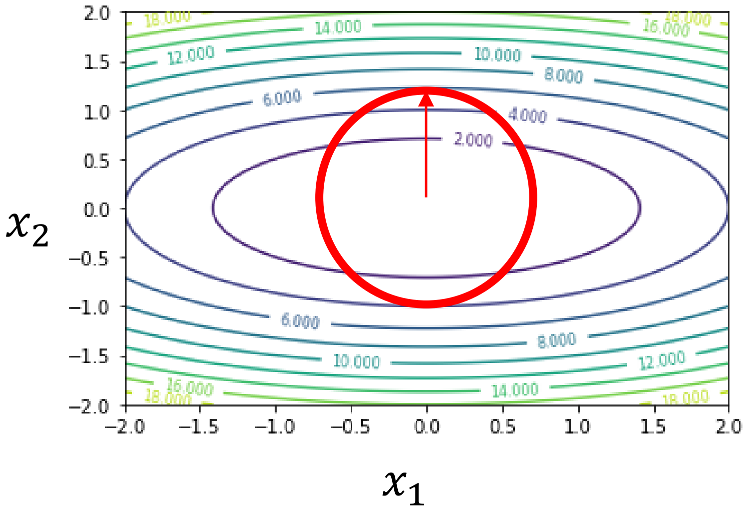
$$f(\boldsymbol{x}) = [x_1, x_2]\begin{bmatrix}4 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}x_1\\ x_2\end{bmatrix}$$

$$= 4x_1^2 + x_2^2$$

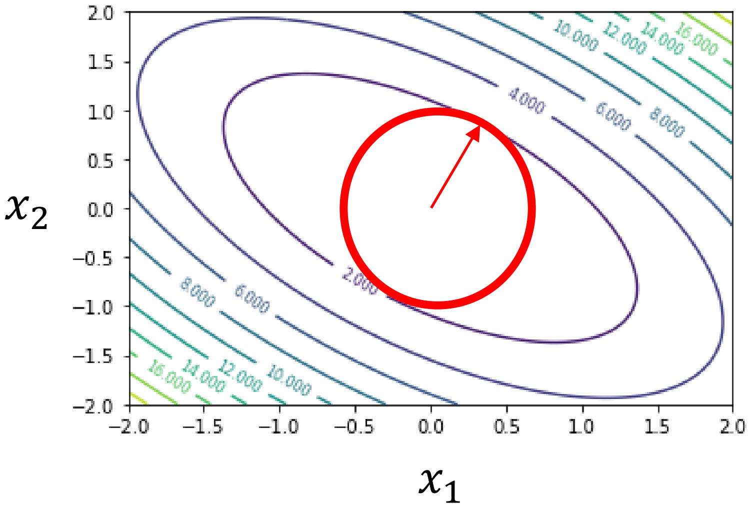
Plug in $\boldsymbol{x} = e_1 = \begin{bmatrix}1\\0\end{bmatrix}$, $e_2 = \begin{bmatrix}0\\1\end{bmatrix}$, or $\begin{bmatrix}\cos\theta\\ \sin\theta\end{bmatrix}$, which one has higher function value?



(A)



(B)



(C)

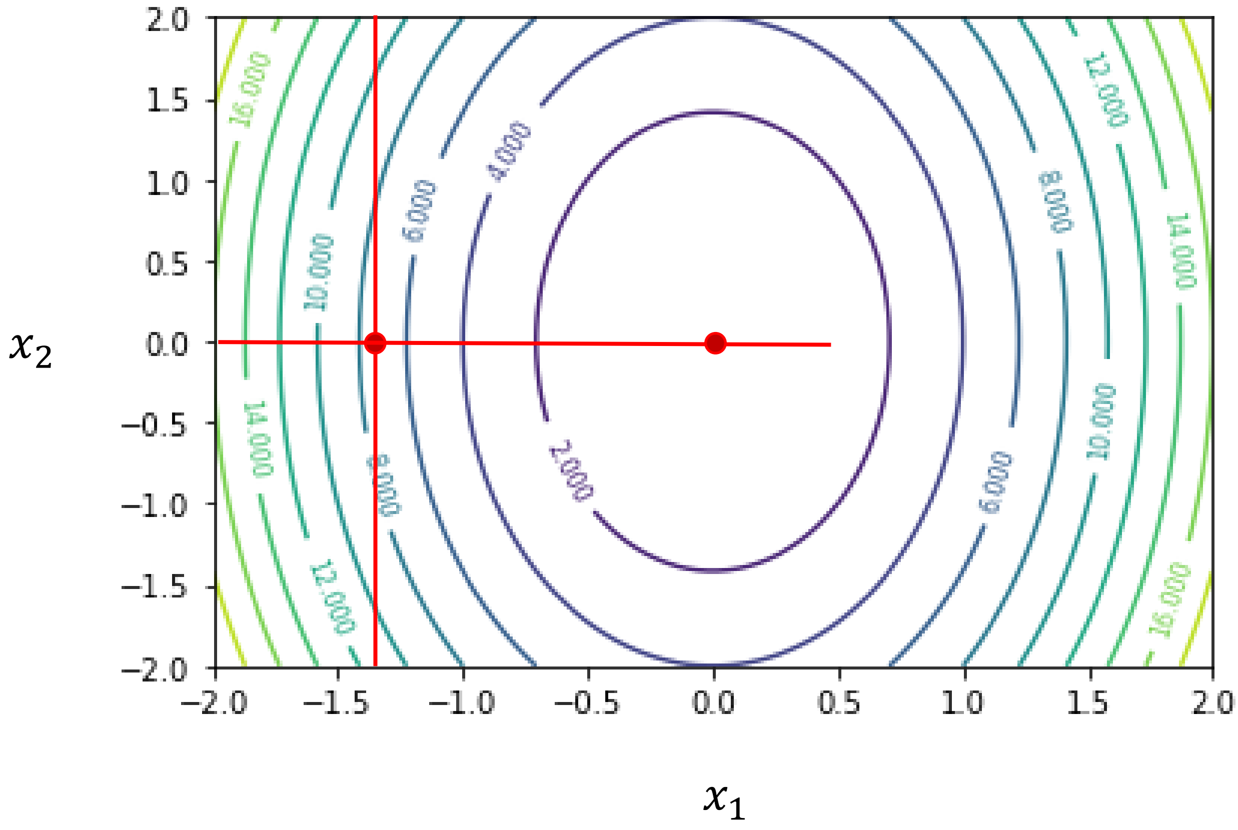
Diagonal Hessian

Easy to optimize. First find the best x_2 on any x_1, and find the best x_1 (coordinate descent).

$$f(\boldsymbol{x}) = [x_1, x_2] \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$= 4x_1^2 + x_2^2$$

All scaling happens along the coordinate axes.



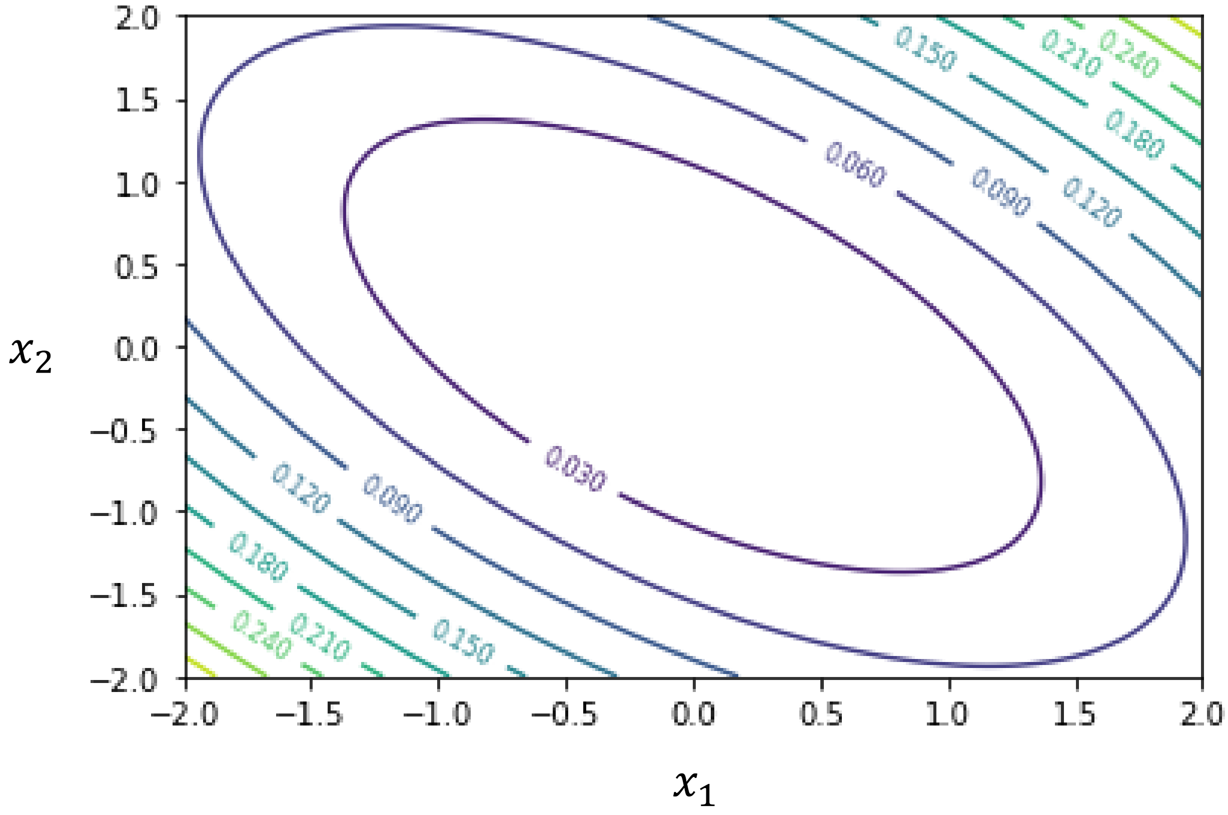
Hessian = Diagonal × Rotation

Clockwise 45° | Counter-clockwise 45°

$$f(\boldsymbol{x}) = [x_1, x_2]\begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix}\begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$f(\boldsymbol{x}) = \boldsymbol{x}^\top Q \Lambda Q^\top \boldsymbol{x}$$

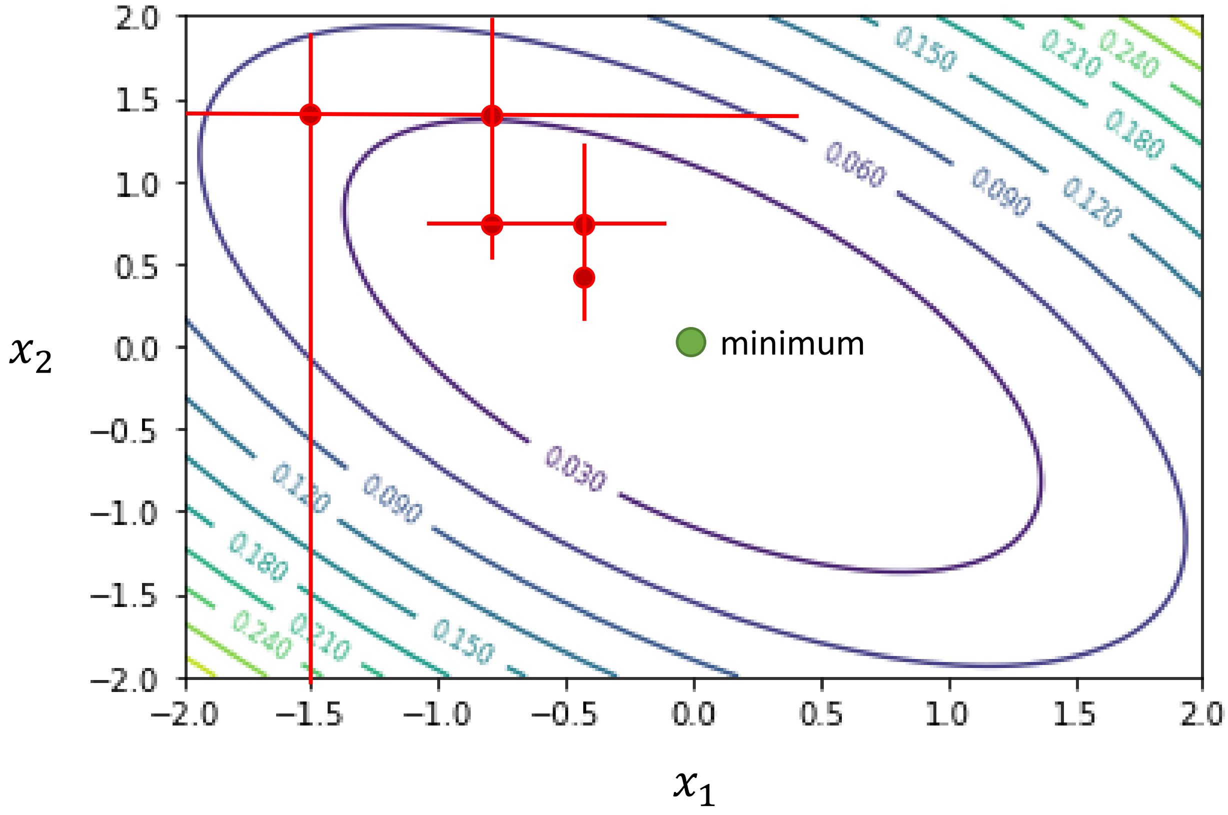
The eigenvalues of Hessian determine the ratio of the two axes of the ellipse.



Hessian = Diagonal × Rotation

$$f(\boldsymbol{x}) = [x_1, x_2] \overbrace{\begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix}}^{\text{Clockwise } 45^\circ} \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix} \overbrace{\begin{bmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix}}^{\text{Counter-clockwise } 45^\circ} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

- Coordinate descent converges slowly in this scenario.
    - Not rotational invariant.
- Gradient descent is rotational invariant.



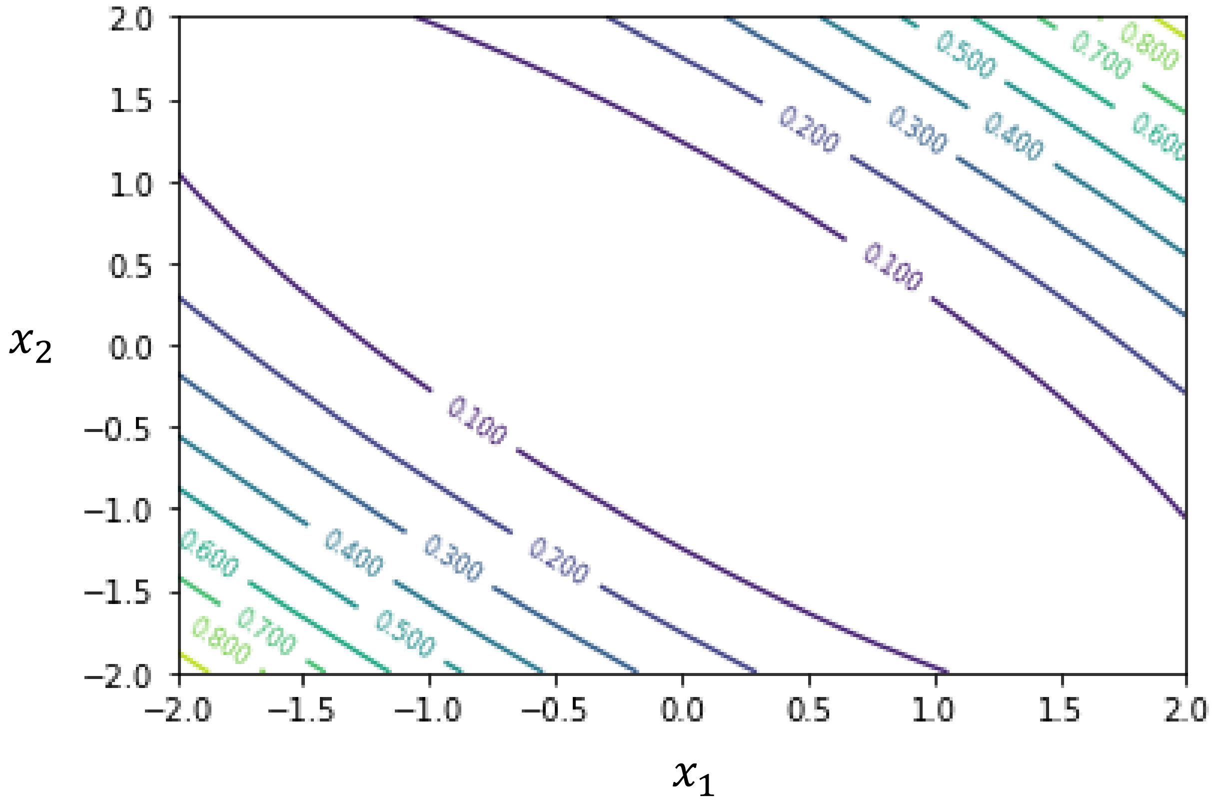
Hessian = Diagonal × Rotation

The eigenvalues of Hessian determine the ratio of the two axes of the ellipse.

Clockwise 45° / Counter-clockwise 45°

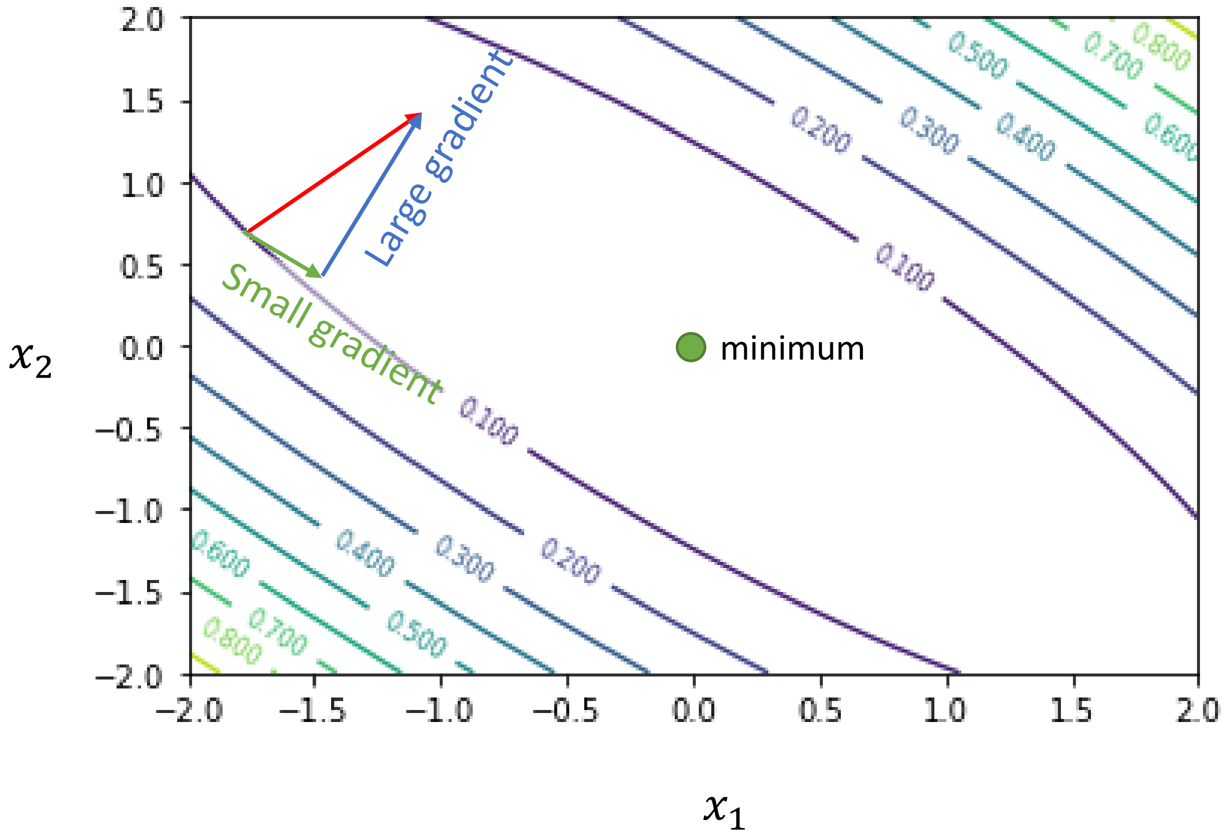
$$f(\boldsymbol{x}) = [x_1, x_2] \begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix} \begin{bmatrix} \color{red}{12} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$f(\boldsymbol{x}) = \boldsymbol{x}^\top Q \Lambda Q^\top \boldsymbol{x}$$



Hessian = Poorly Conditioned

- When the ellipse is really "squashed", the gradient on one direction is much greater than the other dimension.
- We need to set a learning rate λ such that we don't overshoot in one dimension.
- But it would be too small for fast convergence on the other dimension.
- A large condition number leads to slow convergence for GD.



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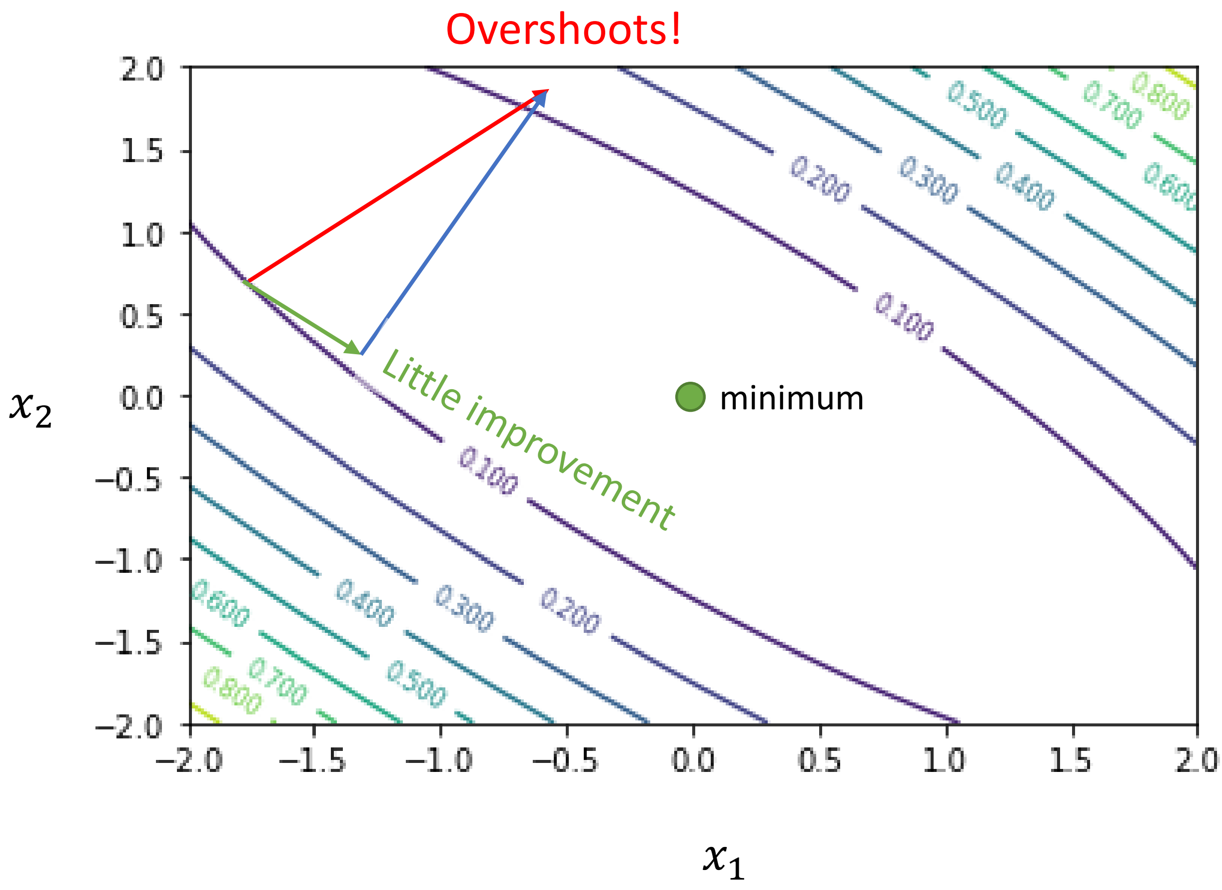
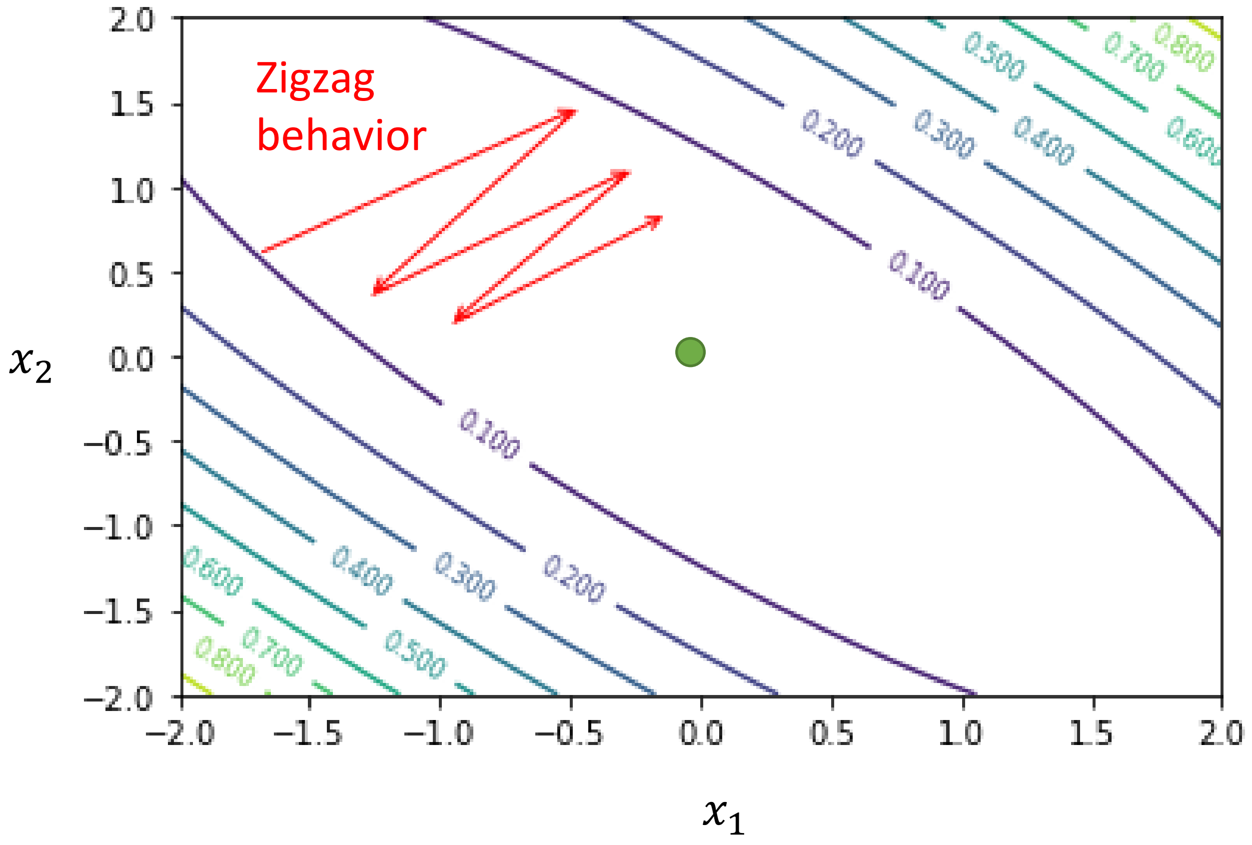
- But it would be too small for fast convergence on the other dimension.
- A large condition number leads to slow convergence for GD.



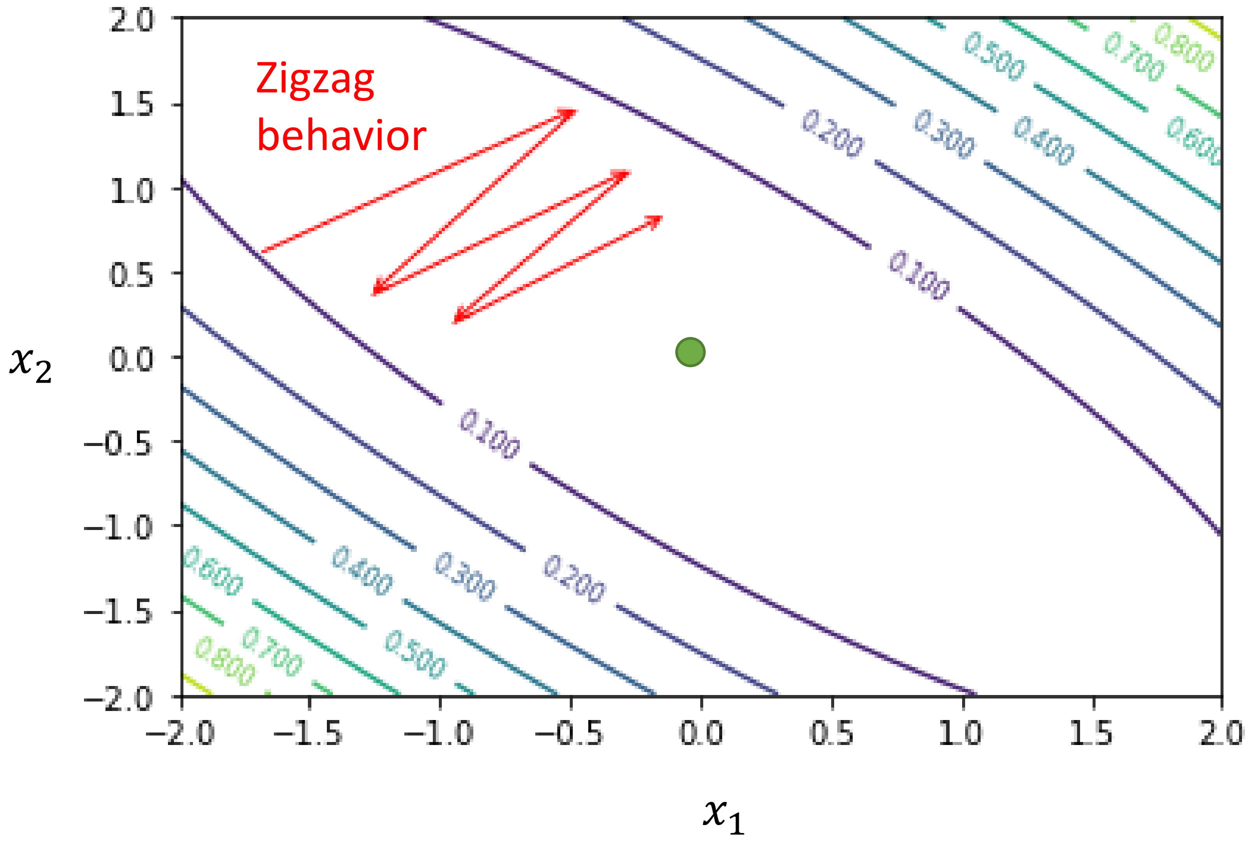
Hessian = Poorly Conditioned

- When the ellipse is really "squashed", the gradient on one direction is much greater than the other dimension.
- We need to set a learning rate λ such that we don't overshoot in one dimension.
- But it would be too small for fast convergence on the other dimension.
- A large condition number leads to slow convergence for GD.



Hessian = Poorly Conditioned

- This phenomenon is characterized by the ratio $\frac{\lambda_{\max}}{\lambda_{\min}}$ of the Hessian matrix, known as the condition number.
- A large condition number leads to slow convergence for GD.



Momentum

Initial condition:

$$\boldsymbol{v}_0 = \boldsymbol{0}$$

Velocity update:

$$\boldsymbol{v}_t = \alpha \boldsymbol{v}_{t-1} - \eta \frac{dL(\boldsymbol{w}_{t-1})}{d\boldsymbol{w}_{t-1}}, 0 < \alpha < 1$$

Parameter update:

$$\boldsymbol{w}_t = \boldsymbol{w}_{t-1} + \boldsymbol{v}_t$$

- Let $\boldsymbol{g}_t = \frac{dL(\boldsymbol{w}_{t-1})}{d\boldsymbol{w}_{t-1}}$
- $\boldsymbol{v}_0 = \boldsymbol{0}$
- $\boldsymbol{v}_1 = -\eta \boldsymbol{g}_1$
- $\boldsymbol{v}_2 = -\eta(\alpha \boldsymbol{g}_1 + \boldsymbol{g}_2)$
- $\boldsymbol{v}_t = -\eta\left(\sum_{i=1}^{t-1} \alpha^{t-k} \boldsymbol{g}_k + \boldsymbol{g}_t\right)$
- The contribution of $\boldsymbol{g}_k$ decreases exponentially.
- This is known as exponential moving average (EMA).

Momentum

Initial condition:

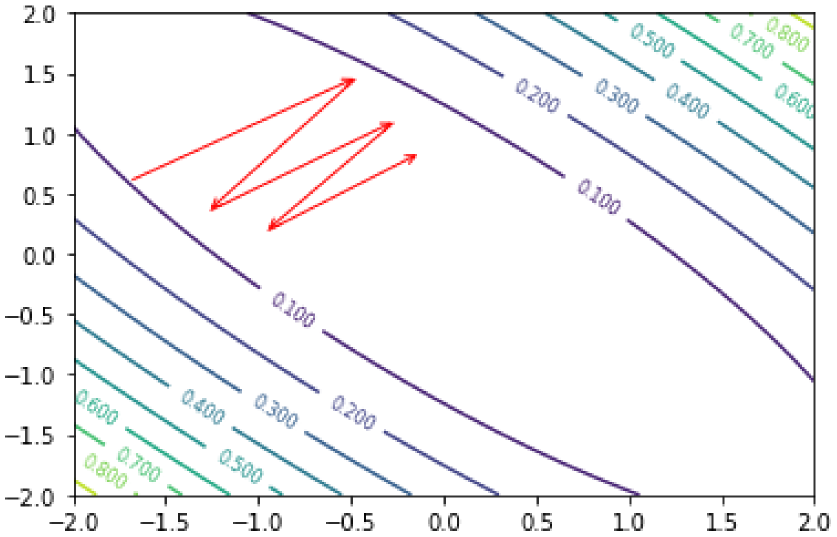
$$\boldsymbol{v}_0 = \boldsymbol{0}$$

Velocity update:

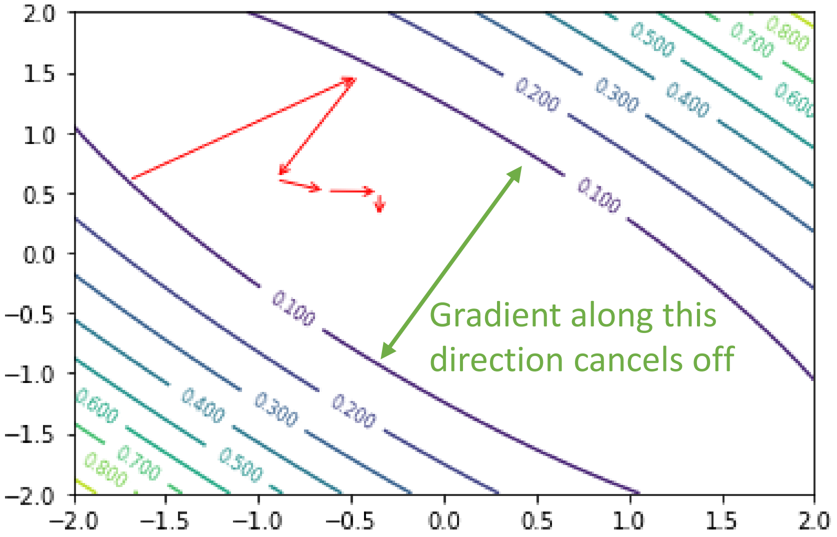
$$\boldsymbol{v}_t = \alpha \boldsymbol{v}_{t-1} - \eta \frac{dL(\boldsymbol{w}_{t-1})}{d\boldsymbol{w}_{t-1}}, 0 < \alpha < 1$$

Parameter update:

$$\boldsymbol{w}_t = \boldsymbol{w}_{t-1} + \boldsymbol{v}_t$$



$\alpha = 0$
(No momentum)



$\alpha = 0.3$

Momentum

Initial condition:

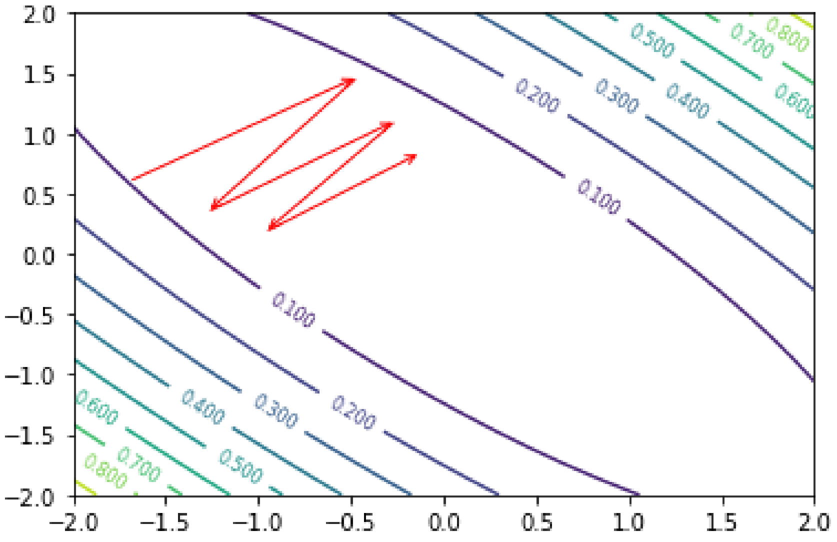
$$\boldsymbol{v}_0 = \boldsymbol{0}$$

Velocity update:

$$\boldsymbol{v}_t = \alpha \boldsymbol{v}_{t-1} - \eta \frac{dL(\boldsymbol{w}_{t-1})}{d\boldsymbol{w}_{t-1}}, 0 < \alpha < 1$$

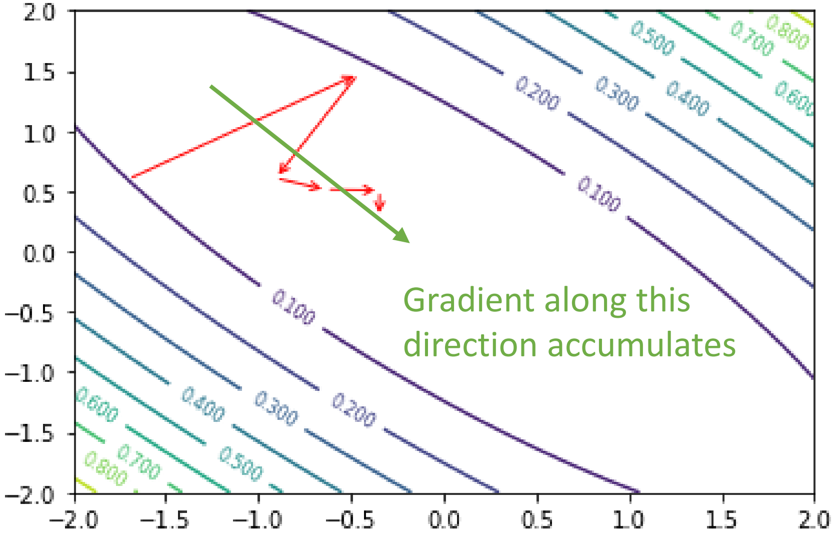
Parameter update:

$$\boldsymbol{w}_t = \boldsymbol{w}_{t-1} + \boldsymbol{v}_t$$



$\alpha = 0$

(No momentum)



$\alpha = 0.3$

Momentum

Initial condition:

$$\boldsymbol{v}_0 = \boldsymbol{0}$$

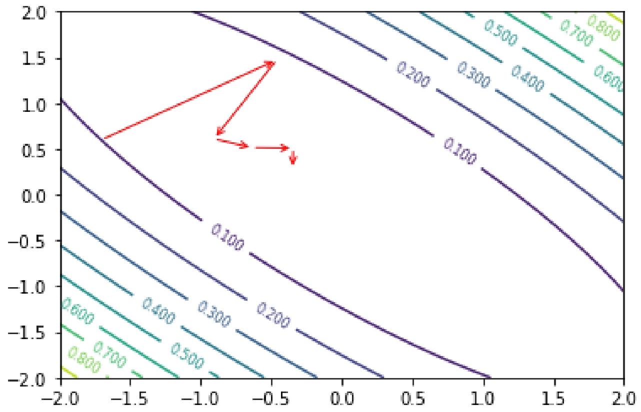
Velocity update:

$$\boldsymbol{v}_t = \alpha \boldsymbol{v}_{t-1} - \eta \frac{dL(\boldsymbol{w}_{t-1})}{d\boldsymbol{w}_{t-1}}, 0 < \alpha < 1$$

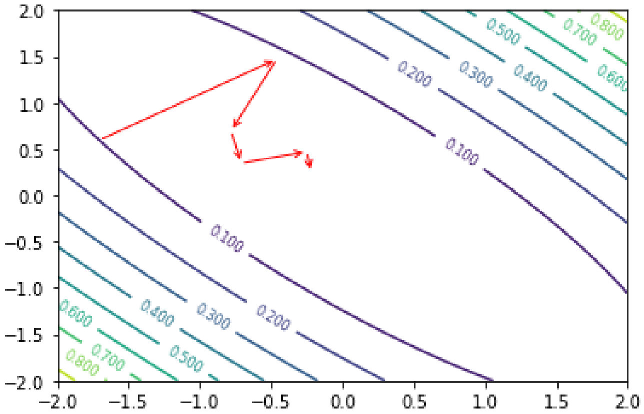
Parameter update:

$$\boldsymbol{w}_t = \boldsymbol{w}_{t-1} + \boldsymbol{v}_t$$

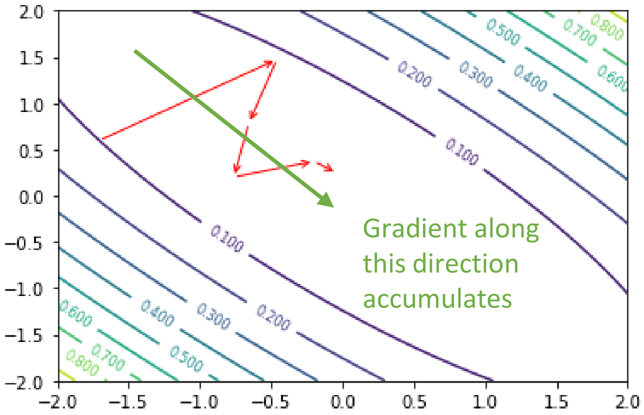
$\alpha = 0.3$



$\alpha = 0.4$



$\alpha = 0.5$



Effects of Data Whitening

- Whitening data = setting per-feature mean to 0 and variance to 1
- For each feature, we subtract its mean and divide by its standard deviation. These two values are computed from the entire training set.
- It is very commonly used in machine learning and has modern variants in deep learning.
- Why does it work?

Effects of Data Whitening

- Consider the loss function of linear regression with data matrix $X \in \mathbb{R}^{n\times(p+1)}$, label vector $\boldsymbol{y} \in \mathbb{R}^{n\times 1}$, and model parameter $\boldsymbol{\beta}$

$$\mathrm{L} = \frac{1}{n}(X\boldsymbol{\beta} - \boldsymbol{y})^\top (X\boldsymbol{\beta} - \boldsymbol{y})$$

$$\mathrm{L} = \frac{1}{n}\boldsymbol{\beta}^\top X^\top X\boldsymbol{\beta} - 2\boldsymbol{y}^\top X\beta + \boldsymbol{y}^\top\boldsymbol{y}$$

$$\frac{d^2L}{d\boldsymbol{\beta}^2} = \frac{1}{n}X^\top X \in \mathbb{R}^{(p+1)\times(p+1)}$$

The uncentered feature covariance matrix

- The condition number of the feature covariance matrix affects the speed of convergence.

Real covariance matrix: $\frac{1}{n}(X - \mathbf{1}\mu^\top)^\top (X - \mathbf{1}\mu^\top)^\top$

Effects of Data Whitening

- Whitening data has the effect of lowering the condition number and improving optimization.
- Modern deep neural networks utilize a variety of normalization operations (e.g., BatchNorm, LayerNorm, GroupNorm, etc)
  - We will see them later on.
- [Optional] See detailed discussion at https://www.cs.toronto.edu/~rgrosse/courses/csc2541_2021/readings/L01_intro.pdf

Adam

- Sometimes the gradient is too large and overshoots.
- Sometimes the gradient is too small, and optimization stagnates.
- <u>What if we adjust the gradient so it's neither too large nor too small?</u>
- Adam often works well for recurrent networks (introduced later).

- Input: loss function $L(\boldsymbol{w})$ and initial position $\boldsymbol{w}_0$
- Initialize: $\boldsymbol{s}_0 = \boldsymbol{0}, \boldsymbol{r}_0 = \boldsymbol{0}, t = 0$
- Hyperparameters: $\beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 10^{-8}$
- Repeat until termination condition
  - $t = t + 1$
  - $\boldsymbol{g}_t = \frac{\mathrm{d}L(\boldsymbol{w})}{\mathrm{d}\boldsymbol{w}}\Big|_{\boldsymbol{w}_{t-1}}$
  - $\boldsymbol{s}_t = \beta_1 \boldsymbol{s}_{t-1} + (1 - \beta_1)\boldsymbol{g}_t$ // EMA for $\boldsymbol{g}_t$
  - $\boldsymbol{r}_t = \beta_2 \boldsymbol{r}_{t-1} + (1 - \beta_2)\|\boldsymbol{g}_t\|^2$ // EMA for $\|\boldsymbol{g}_t\|^2$
  - $\hat{\boldsymbol{s}}_t = \boldsymbol{s}_t / (1 - \beta_1^t)$ // bias correction for $\boldsymbol{s}_t$
  - $\hat{\boldsymbol{r}}_t = \boldsymbol{r}_t / (1 - \beta_2^t)$ // bias correction for $\boldsymbol{r}_t$
  - $\Delta \boldsymbol{w} = -\frac{\eta \hat{\boldsymbol{s}}_t}{\sqrt{\hat{\boldsymbol{r}}_t + \epsilon}}$ // component-wise division
  - $\boldsymbol{w}_\mathrm{t} = \boldsymbol{w}_{\mathrm{t}-1} + \Delta \boldsymbol{w}$

Adam: Bias Correction

- Let $\boldsymbol{g}_t = \frac{dL(\boldsymbol{w}_{t-1})}{d\boldsymbol{w}_{t-1}}$
- $\boldsymbol{s}_0 = \boldsymbol{0}$
- $\boldsymbol{s}_1 = (1 - \beta_1)\boldsymbol{g}_1$
- $\boldsymbol{s}_2 = (1 - \beta_1)(\beta_1 \boldsymbol{g}_1 + \boldsymbol{g}_2)$
- $\boldsymbol{s}_t = (1 - \beta_1)\left(\sum_{i=1}^{t-1} {\beta_1}^{t-k} \boldsymbol{g}_k + \boldsymbol{g}_t\right)$

The first few $\boldsymbol{s}$ are too small

- Thus, we introduce bias correction.
- $\hat{\boldsymbol{s}}_t = \boldsymbol{s}_t / (1 - \beta_1^t)$
- Since $0 < 1 - \beta_1^t < 1$, $\|\hat{\boldsymbol{s}}_t\| > \|\boldsymbol{s}_t\|$
- When $t \longrightarrow \infty$, $\hat{\boldsymbol{s}}_t \longrightarrow \boldsymbol{s}_t$

Adam

- Adam may not converge well near the minimum.
- Near the minimum, the gradients have small magnitudes. So Adam scales the gradients up, which may lead to overshooting.
- Can be handled by decaying the learning rate or switching to SGD with momentum near the end.

- Input: loss function $L(\boldsymbol{w})$ and initial position $\boldsymbol{w}_0$
- Initialize: $\boldsymbol{s}_0 = \boldsymbol{0}, \boldsymbol{r}_0 = \boldsymbol{0}, t = 0$
- Hyperparameters: $\beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 10^{-8}$
- Repeat until termination condition is met
  - $t = t + 1$
  - $\boldsymbol{g}_t = \left.\frac{\mathrm{d}L(\boldsymbol{w})}{\mathrm{d}\boldsymbol{w}}\right|_{\boldsymbol{w}_{t-1}}$
  - $\boldsymbol{s}_t = \beta_1 \boldsymbol{s}_{t-1} + (1-\beta_1)\boldsymbol{g}_t$ // EMA for $\boldsymbol{g}_t$
  - $\boldsymbol{r}_t = \beta_2 \boldsymbol{r}_{t-1} + (1-\beta_2)\|\boldsymbol{g}_t\|^2$ // EMA for $\|\boldsymbol{g}_t\|^2$
  - $\hat{\boldsymbol{s}}_t = \boldsymbol{s}_t / (1-\beta_1^t)$ // bias correction for $\boldsymbol{s}_t$
  - $\hat{\boldsymbol{r}}_t = \boldsymbol{r}_t / (1-\beta_2^t)$ // bias correction for $\boldsymbol{r}_t$
  - $\Delta\boldsymbol{w} = -\eta \frac{\hat{\boldsymbol{s}}_t}{\sqrt{\hat{\boldsymbol{r}}_t} + \epsilon}$ // component-wise division
  - $\boldsymbol{w}_t = \boldsymbol{w}_{t-1} + \Delta\boldsymbol{w}$

Newton's Method

- Newton's method is a second-order optimization technique that models the objective function as quadratic.
- Starting from $\boldsymbol{w}_0$, we seek Δ that minimizes

$$f(\boldsymbol{w}_0 + \Delta) = f(\boldsymbol{w}_0) + \left(\frac{df}{d\boldsymbol{w}}\right)^{\top} \Delta + \frac{1}{2}\Delta^{\top}\left(\frac{d^2 f}{d\boldsymbol{w}^2}\right)\Delta$$

- Setting the derivative to zero, we get

$$\frac{\mathrm{d}f(\boldsymbol{w}_0 + \Delta)}{d\Delta} = \left(\frac{df}{d\boldsymbol{w}}\right) + \left(\frac{d^2 f}{d\boldsymbol{w}^2}\right)\Delta = 0 \;\Rightarrow\; \Delta = -\left(\frac{d^2 f}{d\boldsymbol{w}^2}\right)^{-1}\left(\frac{df}{d\boldsymbol{w}}\right) = -H^{-1}g$$

Newton's Method

- Newton's step

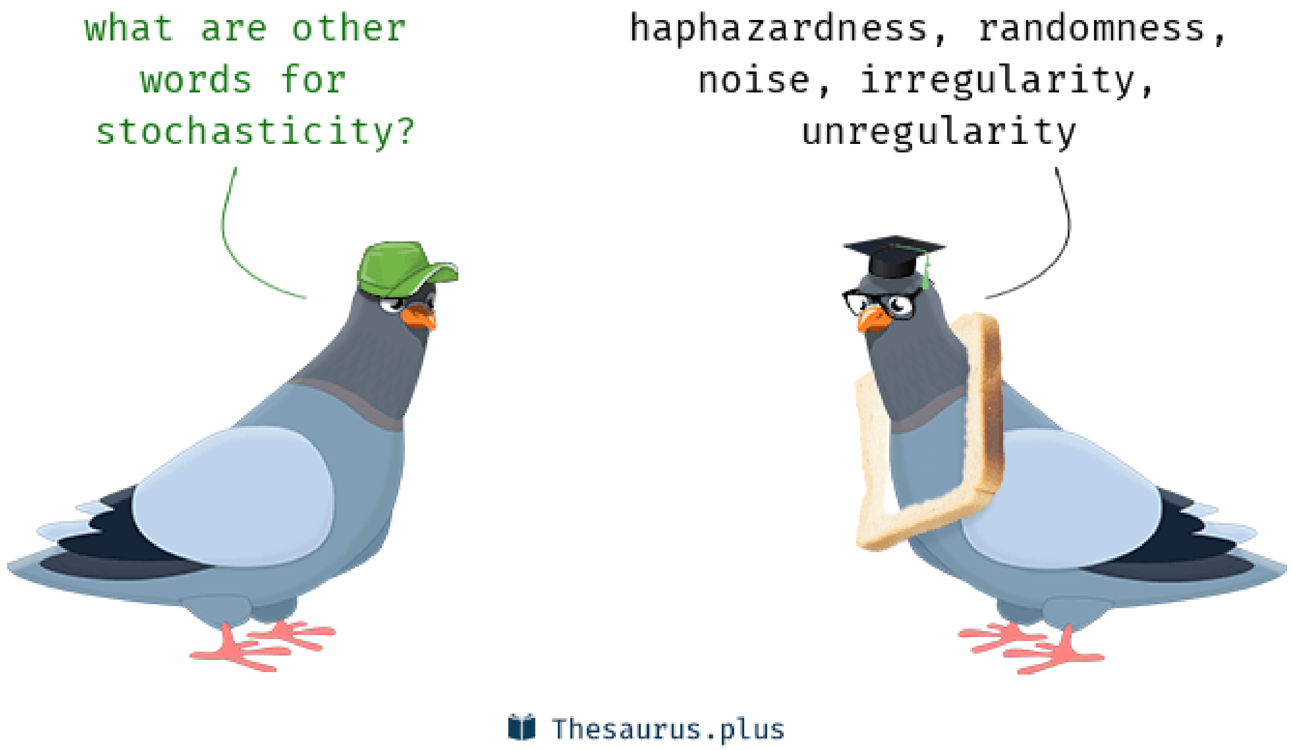
$$\Delta = -\left(\frac{d^2 f}{d\boldsymbol{w}^2}\right)^{-1}\left(\frac{df}{d\boldsymbol{w}}\right) = -H^{-1}g$$

- If the function is indeed quadratic, Newton's method converges in a single step.
- Superior convergence speed compared to first-order gradient descent.

Newton's Method

- The Newton's method has many advantages, but it does not work well for deep neural networks
  - H is $n \times n$. Storage is hard for large n. For a network with 1M parameters, H takes a few TB to store
  - Finding H^{-1} naively take $O(n^3)$ operations, which very expensive for large n. (though can be simplified).
  - Estimating $H^{-1}g$ with sufficient accuracy may need a lot of data.

Adding Stochasticity …



Stochastic Gradient Descent

- GD computes the gradient on the loss function

$$\mathcal{L} = \frac{1}{N}\sum_{i} \ell(x^{(i)}, y^{(i)}, w)$$

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}} = \frac{1}{N}\sum_{i} \frac{\partial \ell(x^{(i)}, y^{(i)}, \boldsymbol{w})}{\partial \boldsymbol{w}}$$

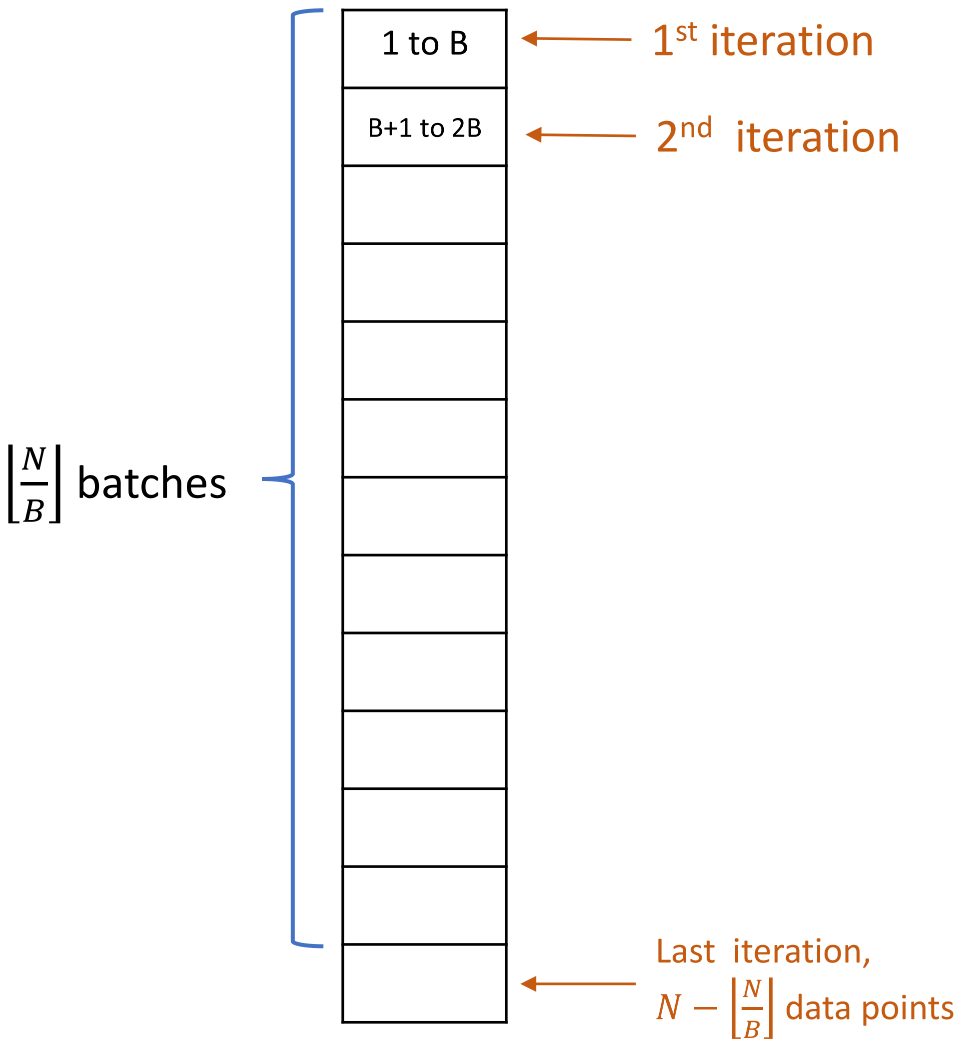
Summation over all training data

- When there are too many training data, the above average is too expensive to compute.
- We use only a small subset randomly sampled from the training dataset to compute the gradient.

Implementation

1. Shuffle all training data into a random permutation.
2. Start from the beginning of the shuffled sequence.
3. In every iteration, take the next B data points, which form a mini-batch, and perform training on the mini-batch.
4. When the sequence is exhausted, go back to Step 1. This is one epoch of training.

Random shuffling is necessary for unbiased gradient estimates.



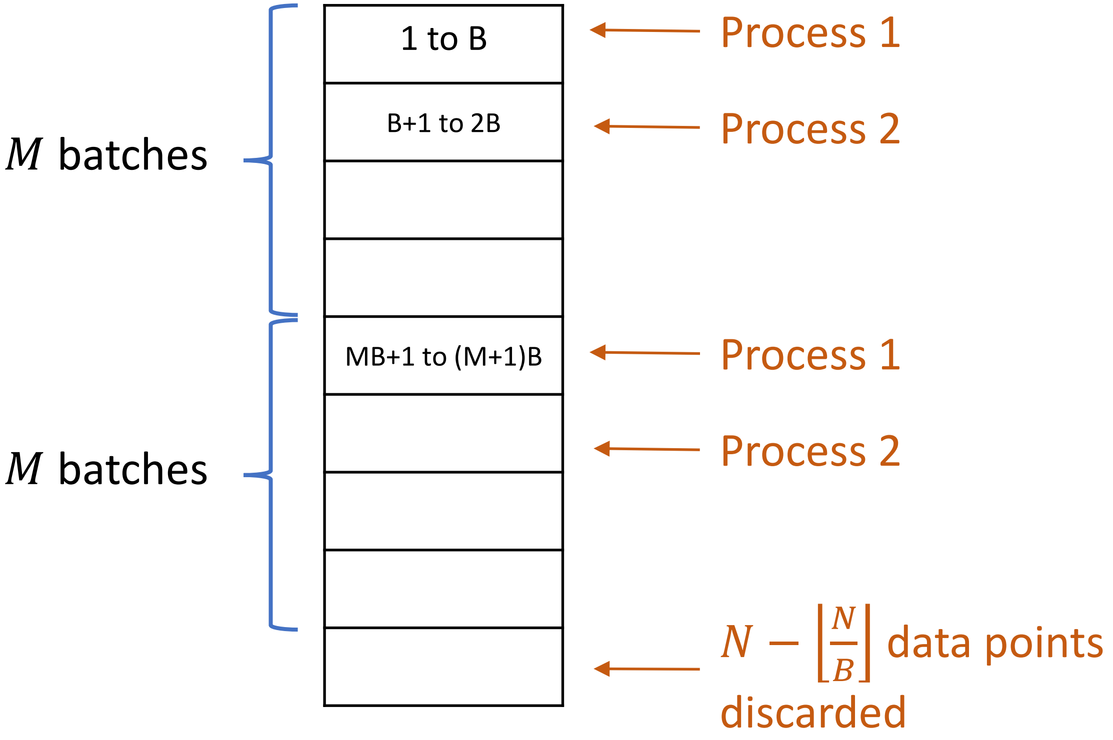
The last batch with less than B data points may be discarded if small batches cause problems (e.g., for BatchNorm)

Pseudo-random Number Generator (PNG)

- Pseudo-random number generators are not really “random”.
  - What is really random? A philosophical discussion that we will not get into.
- It is a completely deterministic function of the random seed.
  - Always generates the same sequence if the seed is the same.
  - A.k.a deterministic random bit generator
- However, the sequence of numbers satisfy certain statistical properties that they can be considered random if the seed is not known.
  - Do not change seeds if you want good randomness. Use the sequence.
- If we give the same seed to two generators w/ the same algorithm, they will create the same sequence.
  - We can align multiple processes or multiple training sessions.

Synchronous Training on Multiple GPUs / Nodes

- Multiple processes (total number = M) use PNGs sharing the same seed when shuffling the dataset.
- Based on its process id, a process uses one batch of size B every M batches.
- The gradients from M processes are averaged and the model is updated once (synchronization).
- Equivalent to a global batch size of MB



Stochastic Gradient Descent

- From a probabilistic perspective, $\left(x^{(i)}, y^{(i)}\right)$ is drawn from the data distribution $\mathcal{D}$. $\bar{g}$ is the expected value of the gradient.

$$\bar{g} = E_{\left(x^{(i)}, y^{(i)}\right) \sim \mathcal{D}} \left[\frac{\partial \ell\left(x^{(i)}, y^{(i)}, \boldsymbol{w}\right)}{\partial \boldsymbol{w}} \right]$$

Expected gradient

$$\hat{g}_{\text{all-data}} = \frac{1}{N} \sum_{i} \frac{\partial \ell\left(x^{(i)}, y^{(i)}, \boldsymbol{w}\right)}{\partial \boldsymbol{w}}$$

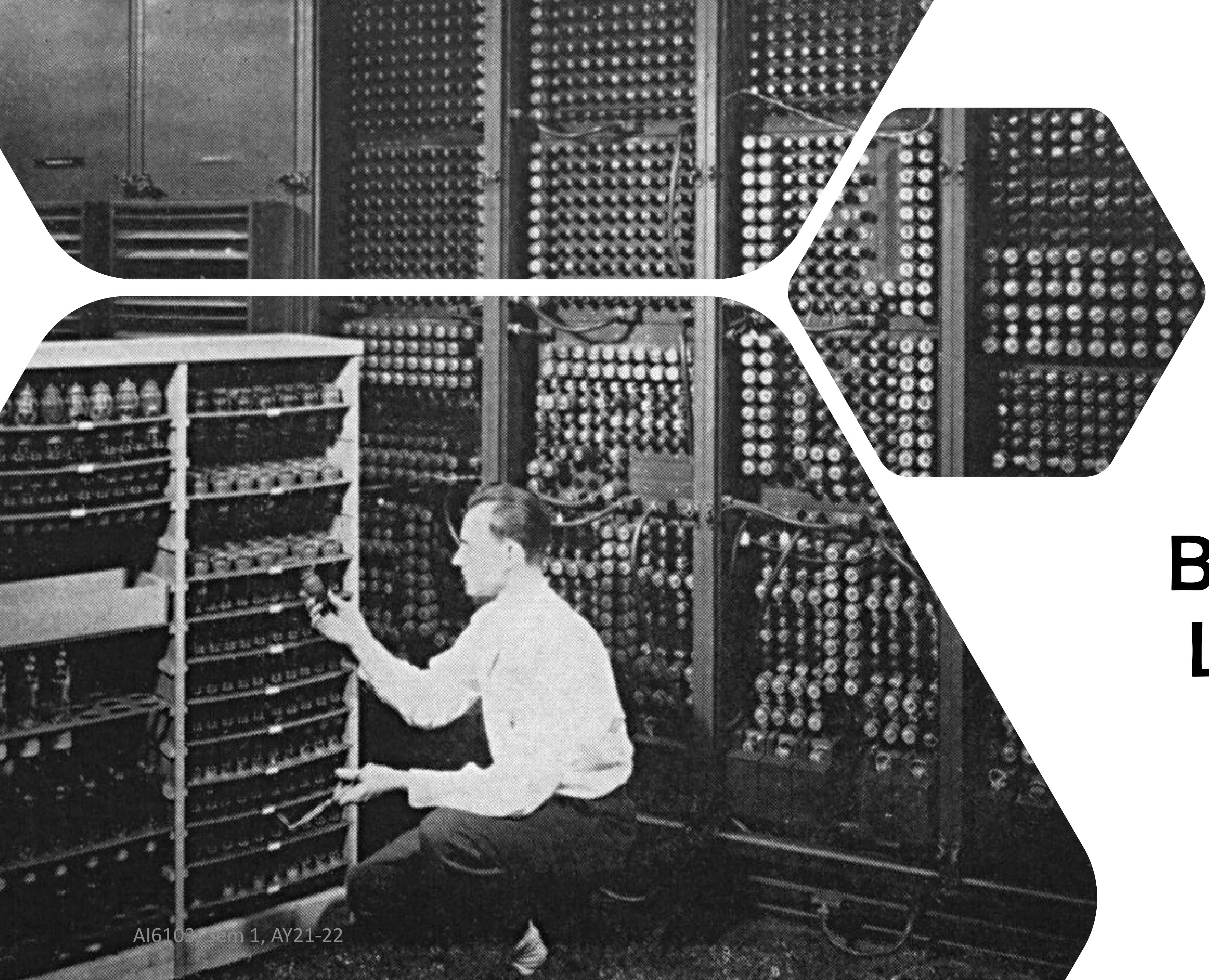
Estimated gradient using all available data

$$\hat{g}_{\text{mini-batch}} = \frac{1}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \frac{\partial \ell\left(x^{(i)}, y^{(i)}, \boldsymbol{w}\right)}{\partial \boldsymbol{w}}$$

Estimated gradient using all data from a mini-batch $\mathcal{B}$

The variance of the mean estimator is inversely proportional to sample size.

Li Boyang, Albert



Batch Size and Learning Rate

Stochastic Gradient Descent

$$\hat{g}_{\text{mini-batch}} = \frac{1}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \frac{\partial \ell\left(x^{(i)}, y^{(i)}, \boldsymbol{w}\right)}{\partial \boldsymbol{w}} = \bar{g} + \epsilon$$

- The mini-batch estimate of the gradient contains some random noise. Is that bad?
  - Bias is bad. We need to shuffle datasets to get unbiased estimates.
  - Variance may not be too bad. As long as the angle between the estimated gradient $\hat{g}$ and true gradient $\bar{g}$ is less than 90 degrees, we are still roughly in the right direction.
  - Getting more accurate gradient means a bigger batch, which can be more expensive

Effects of Batch Size

- The update $w_t = w_{t-1} - \eta \hat{g} = w_{t-1} - \frac{\eta}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} g_i(w_{t-1})$
- We can understand this as sequentially moving $\frac{\eta g_i(w_{t-1})}{|\mathcal{B}|}$
- The contribution of the i^{th} data point is $\frac{\eta}{|\mathcal{B}|}$
- We vary B while keeping $\alpha = \frac{\eta}{|\mathcal{B}|}$ fixed.

If $B = 1$

$$\begin{aligned} w_1 &= w_0 - \alpha g_1(w_0) \\ w_2 &= w_1 - \alpha g_2(w_1) \\ w_3 &= w_2 - \alpha g_3(w_2) \end{aligned}$$

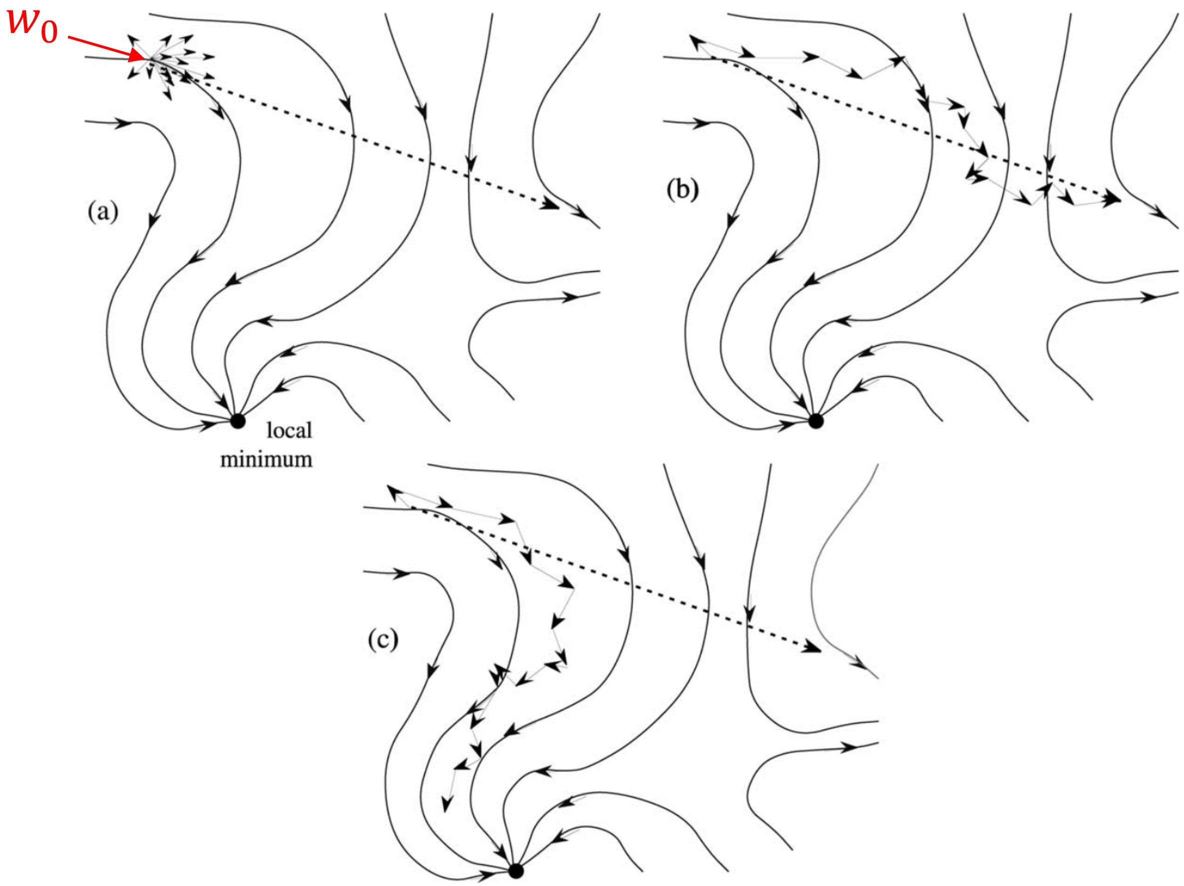
If $B = 3$

$$w_2 = w_0 - \alpha g_1(w_0) - \alpha g_2(w_0) - \alpha g_3(w_0)$$

$$\begin{aligned} w_{0,1} &= w_0 - \alpha g_1(w_0) \\ w_{0,2} &= w_{0,1} - \alpha g_2(w_0) \\ w_1 &= w_{0,2} - \alpha g_3(w_0) \end{aligned}$$

With a larger B, we use stale gradients computed at an old w.

Effects of Batch Size



The directed curves indicate the underlying true gradient of the error surface.

(a) Batch training. Several weight change vectors and their sum.

(b) Batch training with weight change vectors placed end-to-end. As all vectors are computed at w_0, they do not reflect the landscape (i.e., "stale" gradients). We must use a smaller learning rate.

(c) On-line training ($B = 1$). The local gradient influences the direction of each weight change vector, allowing it to follow curves.

D. Randall Wilsona and Tony R. Martinezb. The general inefficiency of batch training for gradient descent learning. 2003

Effects of Batch Size

- In practice, setting $B = 1$ often leads to very effective optimization.
- The variance does not matter much as long as the angle between the estimated gradient $\hat{g}$ and true gradient g is less than 90 degrees.
- However, online learning ($B = 1$) fails to utilize modern GPU hardware, which is massively parallel.
- It is often desirable to use large batch sizes with the support of multiple GPU cards / nodes.

Large Batch Training

If $B = 1$

$$w_1 = w_0 - \alpha g_i(w_0)$$
$$w_2 = w_1 - \alpha g_{i+1}(w_1)$$
$$\vdots$$
$$w_K = w_{K-1} - \alpha g_{i+K}(w_{K-1})$$

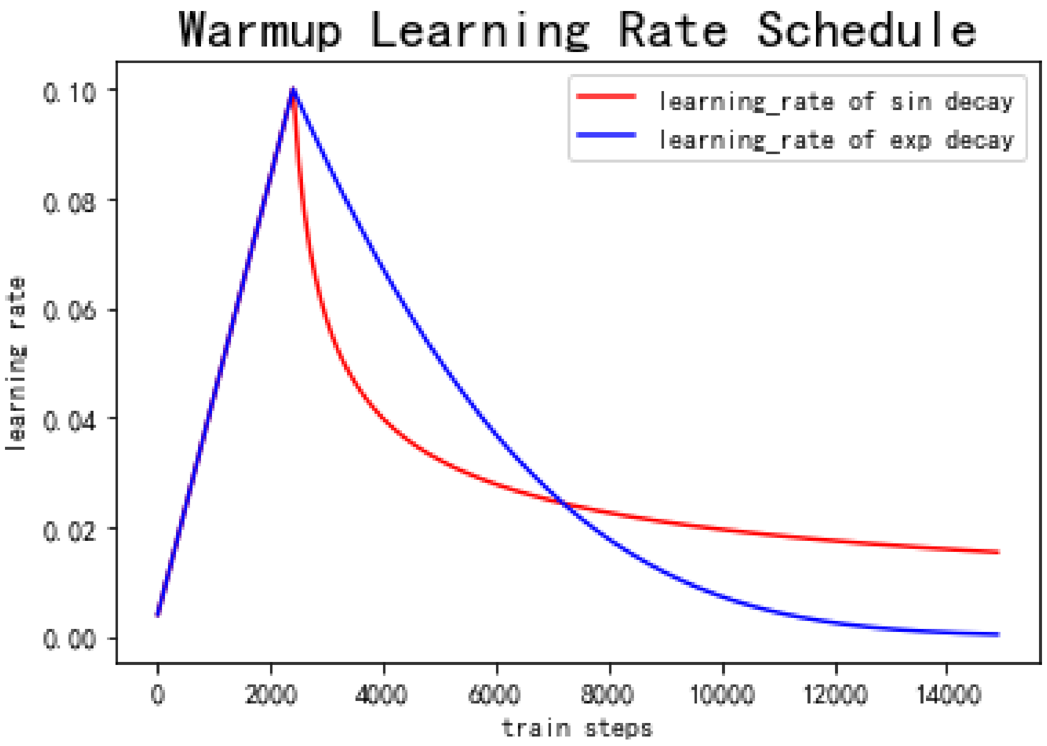
If $B = K$

$$w_{0,1} = w_0 - \alpha g_i(w_0)$$
$$w_{1,2} = w_{0,1} - \alpha g_{i+1}(w_0)$$
$$\vdots$$
$$w_1 = w_{0,K-1} - \alpha g_{i+K}(w_0)$$

- Under what conditions are the left side and the right side equivalent?
  - $\alpha = \frac{\eta}{|B|}$ is kept constant (Assumption 1)
  - The loss function is smooth enough, $g_i\left(w_{0,K-1}\right) \approx g_i(w_0)$ (Assumption 2)
- From Assumption 1, η and $|B|$ should increase proportionally (linear scaling).
- Assumption 2 usually does not hold at the beginning of the optimization. We must use small learning rates at the beginning.

Learning Rate Warm-up

- Linear growth of learning rate from 0 to $\eta_{\max}$ in the first few epochs.
- $\eta_{\max}$ grows proportionally with batch size.
- Proposed in
    - Goyal et al. Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour. 2017
- This technique allows batch size up to 8,000 for image recognition



LR Warm-up

LR decrease by factor of 10

- ResNet-50
- kn = batch size
- η = learning rate
- How to increase batch size even further?

Image from Goyal et al. Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour. 2017

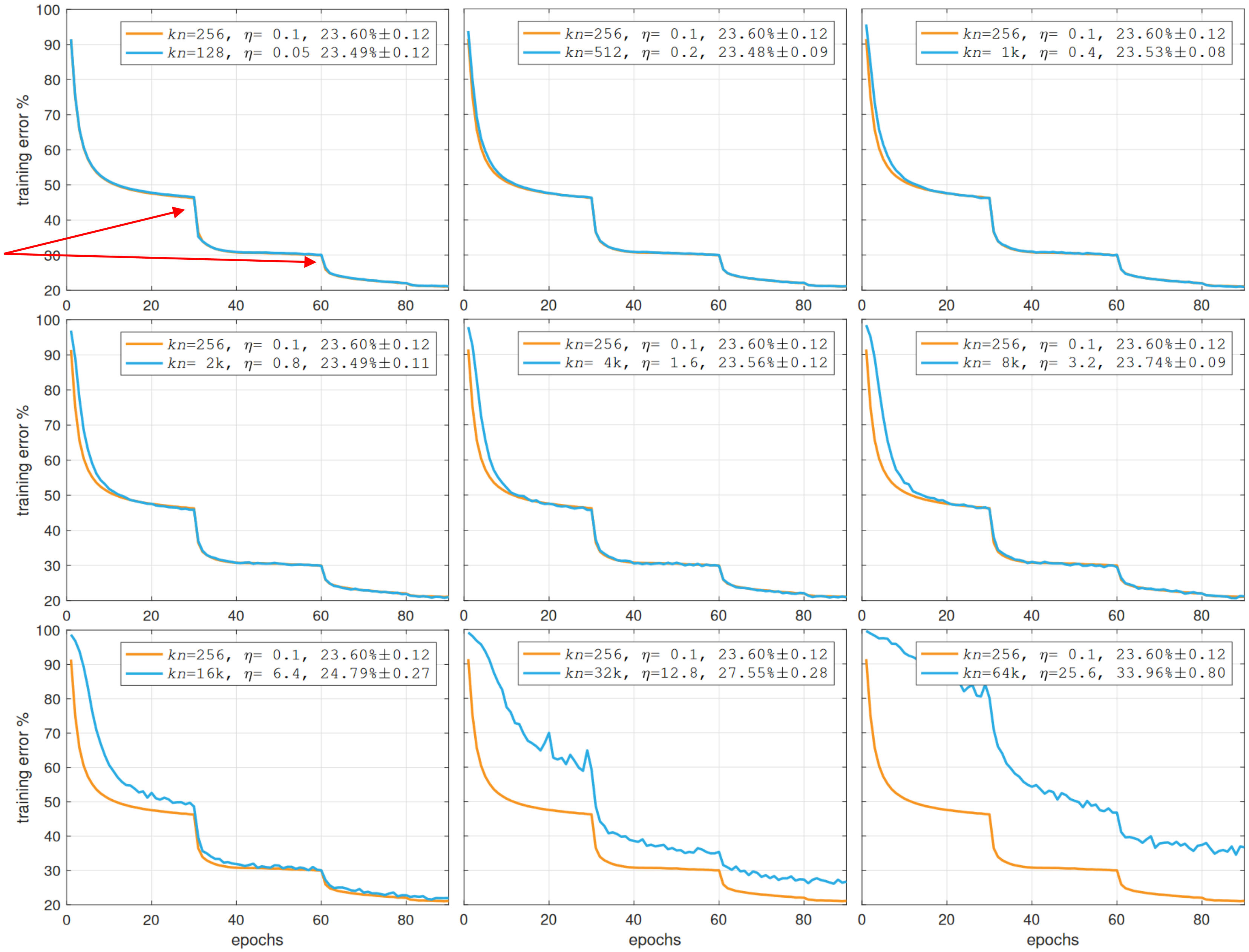


Figure 3. **Training error *vs.* minibatch size.** Training error curves for the 256 minibatch baseline and larger minibatches using gradual warmup and the linear scaling rule. Note how the training curves closely match the baseline (aside from the warmup period) up through 8k minibatches. *Validation* error (mean±std of 5 runs) is shown in the legend, along with minibatch size kn and reference learning rate η.

LR Warm-up

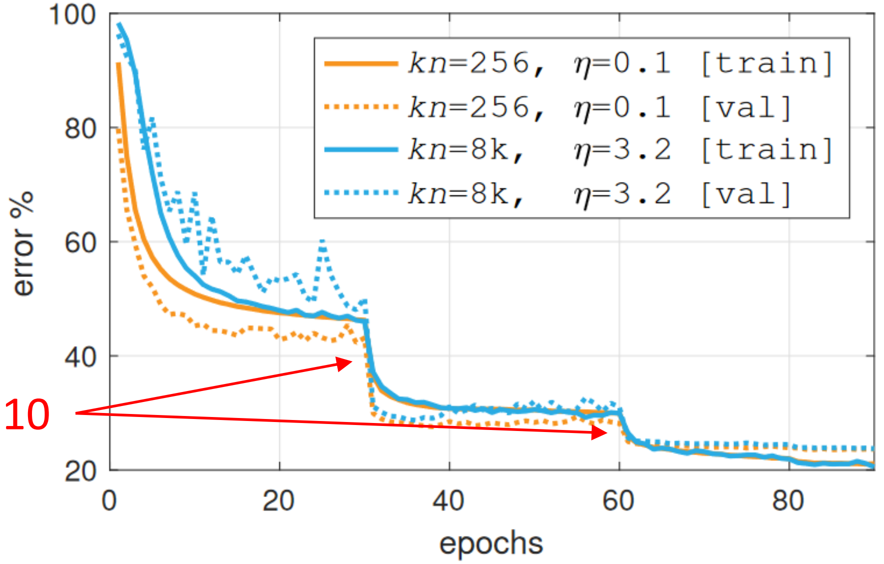


Figure 4. **Training and validation curves** for large minibatch SGD with gradual warmup *vs*. small minibatch SGD. Both sets of curves match closely after training for sufficient epochs. We note that the BN statistics (for inference only) are computed using *running* average, which is updated less frequently with a large minibatch and thus is noisier in early training (this explains the larger variation of the validation error in early epochs).

Image from Goyal et al. Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour. 2017

LARS

- Observation: gradient magnitudes differ at different network locations. Thus, optimization happens at different rates.
- Notation: $\nabla L(w) = \frac{\partial L}{\partial w}$

Table 2: AlexNet-BN: The norm of weights and gradients at 1st iteration.

Layer	conv1.b	conv1.w	conv2.b	conv2.w	conv3.b	conv3.w	conv4.b	conv4.w
$\|\|w\|\|$	1.86	0.098	5.546	0.16	9.40	0.196	8.15	0.196
$\|\|\nabla L(w)\|\|$	0.22	0.017	0.165	0.002	0.135	0.0015	0.109	0.0013
$\frac{\|\|w\|\|}{\|\|\nabla L(w)\|\|}$	8.48	**5.76**	33.6	83.5	69.9	127	74.6	148
Layer	conv5.b	conv5.w	fc6.b	fc6.w	fc7.b	fc7.w	fc8.b	fc8.w
$\|\|w\|\|$	6.65	0.16	30.7	6.4	20.5	6.4	20.2	0.316
$\|\|\nabla L(w)\|\|$	0.09	0.0002	0.26	0.005	0.30	0.013	0.22	0.016
$\frac{\|\|w\|\|}{\|\|\nabla L(w)\|\|}$	73.6	69	117	**1345**	68	489	93	19

Yang You, Igor Gitman, and Boris Ginsburg. *Large batch training of convolutional networks.* arXiv 1708.03888, 2017

LARS

- Proposal: Synchronize the learning speed of different layers and components.
- First, divide parameters into groups, $\mathbf{w}^1, \dots, \mathbf{w}^l, \dots, \mathbf{w}^L$
- For each group, apply updates with normalized gradients

$$w_{t+1}^l = w_t^l - \eta \frac{\nabla_{w_t} \mathcal{L}(\mathbf{w}_t^l) \, \|\mathbf{w}_t^l\|}{\|\nabla_{w_t} \mathcal{L}(\mathbf{w}_t^l)\|}$$

- Effect: $\frac{\|\Delta \mathbf{w}_t^l\|}{\|\mathbf{w}_t^l\|}$ is a constant η. At every iteration, fixed portion of $\mathbf{w}_t^l$ is being updated. This alleviates vanishing and exploding gradients.
- Scales batch size to 32K for ResNet-50.

Yang You, Igor Gitman, and Boris Ginsburg. *Large batch training of convolutional networks.* arXiv 1708.03888, 2017

Optimal Batch Size in Practice

- Too small a batch size
  - Fails to fully utilize parallel hardware (GPU).
  - Creates excessive noise for Batch Normalization, leading to unstable training
- Too large a batch size
  - Could create problems for optimization.
- Given enough GPUs, we usually use a large batch + Linear LR Scaling + LR warm-up in order to accelerate training