Machine Learning II

(Stochastic) Gradient descent

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How to minimize E_{in}

For logistic regression,

$$E_{\text{in}}(\mathbf{w}) \;=\; \frac{1}{N}\sum_{n=1}^{N} \ln\left(1 + e^{-y_n \mathbf{w}^{\mathsf{T}}\mathbf{x}_n}\right) \qquad \longleftarrow \textbf{iterative} \text{ solution}$$

Compare to linear regression:

$$E_{\text{in}}(\mathbf{w}) \;=\; \frac{1}{N}\sum_{n=1}^{N} (\mathbf{w}^{\mathsf{T}}\mathbf{x}_n - y_n)^2 \qquad \longleftarrow \text{closed-form solution}$$

Optimization for machine learning

Much of machine learning can be written as the following optimization problem:

$$\min_{\boldsymbol{w}} \frac{1}{N} \sum_{n=1}^{N} e_n(\boldsymbol{w}; (y_n, \boldsymbol{x}_n)) \equiv \ell(\boldsymbol{w})$$

where e_n is the error on the nth data point.

Types of optimization problems:

- **Convex optimization**
  - Many classes of convex optimization problems admit polynomial-time algorithms
  - Includes logistic regression, linear regression, etc.
- **Non-convex optimization**
  - NP-hard in general
  - Includes neural networks (deep learning)

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Optimization for machine learning

We want to minimize a convex and differentiable loss function $\ell(\boldsymbol{w})$ or $\mathrm{E}_{\mathrm{in}}(\boldsymbol{w})$. In some cases, it is possible to **analytically** compute $\boldsymbol{w}^*$ such that $\nabla \ell(\boldsymbol{w}^*) = 0$.

More commonly the condition that the gradient equal zero will not have an analytical solution. We will need **iterative methods**.

How can you minimize a function if you don't know much about it? The trick is to assume it is much simpler than it really is. This can be done by approximating the function using **Taylor's approximation** and **minimizing this approximation**.

Taylor's approximation

Let us approximate the function $\ell(\cdot)$ around $\boldsymbol{w}$, i.e. we want to approximate $\ell(\boldsymbol{w}+\boldsymbol{s})$ where $\|\boldsymbol{s}\|_2$ is small (i.e. $\boldsymbol{w}+\boldsymbol{s}$ is very close to $\boldsymbol{w}$). In that case, we can approximate the function $\ell(\boldsymbol{w}+\boldsymbol{s})$ by its first derivatives as

$$\ell(\boldsymbol{w}+\boldsymbol{s}) \approx \ell(\boldsymbol{w}) + g(\boldsymbol{w})^T\boldsymbol{s},$$

where $g(\boldsymbol{w}) = \nabla\ell(\boldsymbol{w})$ is the gradient.

Using its first and second derivatives, we can also write

$$\ell(\boldsymbol{w}+\boldsymbol{s}) \approx \ell(\boldsymbol{w}) + g(\boldsymbol{w})^T\boldsymbol{s} + \frac{1}{2}\boldsymbol{s}^T H(\boldsymbol{w})\boldsymbol{s},$$

where $H(\boldsymbol{w}) = \nabla^2\ell(\boldsymbol{w})$ is the Hessian of ℓ.

Both approximations are valid if $\|\boldsymbol{s}\|_2$ is small, but the second one assumes that ℓ is **twice differentiable** and is more expensive to compute but also more accurate than only using gradient.

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Gradient descent

In an iterative method, given $\boldsymbol{w}(t)$, we want to find $\boldsymbol{w}(t+1) = \boldsymbol{w}(t) + \boldsymbol{s}$ such that $\ell(\boldsymbol{w}(t+1)) - \ell(\boldsymbol{w}(t))$ is minimized.

Let us write $\boldsymbol{s} = \eta \boldsymbol{v}$ where $\eta > 0$ is the step-size in the direction $\boldsymbol{v}$ with $\|\boldsymbol{v}\|_2 = 1$. We want to find the direction $\boldsymbol{v}$ which minimizes $\ell(\boldsymbol{w}(t) + \eta \boldsymbol{v}) - \ell(\boldsymbol{w}(t))$, i.e.

$$\begin{aligned}\min_{\boldsymbol{v}, \|\boldsymbol{v}\|_2 = 1} \ell(\boldsymbol{w}(t) + \eta \boldsymbol{v}) - \ell(\boldsymbol{w}(t)) &\equiv \min_{\boldsymbol{v}, \|\boldsymbol{v}\|_2 = 1} g(\boldsymbol{w}(t))^T \boldsymbol{v} \\ &\equiv \min_{\boldsymbol{v}, \|\boldsymbol{v}\|_2 = 1} \|g(\boldsymbol{w}(t))\| \, \|\boldsymbol{v}\| \cos(\theta) \\ &\equiv \min_{\boldsymbol{v}, \|\boldsymbol{v}\|_2 = 1} \cos(\theta),\end{aligned}$$

where θ is the angle between the vectors $g(\boldsymbol{w}(t))$ and $\boldsymbol{v}$.

Gradient descent

This quantity is minimized when $\cos(\theta) = -1$, i.e. $\theta = 180°$, where $\boldsymbol{v}$ is pointing in the opposite direction of the gradient, i.e. $-g(\boldsymbol{w}(t)$, and since $\boldsymbol{v}$ is a unit vector, we can write

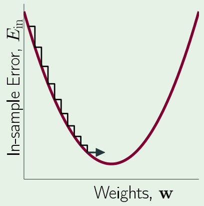
$$\boldsymbol{v} = \frac{-g(\boldsymbol{w}(t))}{\|g(\boldsymbol{w}(t))\|}.$$

In other words, we have

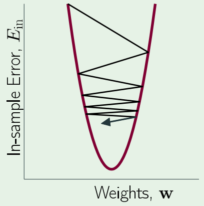
$$\boldsymbol{w}(t+1) = \boldsymbol{w}(t) - \eta \frac{g(\boldsymbol{w}(t))}{\|g(\boldsymbol{w}(t))\|}$$

Fixed-size step?

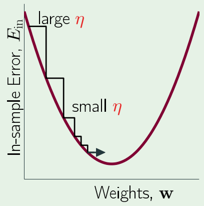
How η affects the algorithm:



η too small



η too large



variable η – just right

η should increase with the slope

Gradient descent - from step size to learning rate

Instead of

$$\boldsymbol{w}(t+1) = \boldsymbol{w}(t) - \eta \frac{g(\boldsymbol{w}(t))}{\|g(\boldsymbol{w}(t))\|},$$

we use

$$\boldsymbol{w}(t+1) = \boldsymbol{w}(t) - \eta_t \frac{g(\boldsymbol{w}(t))}{\|g(\boldsymbol{w}(t))\|},$$

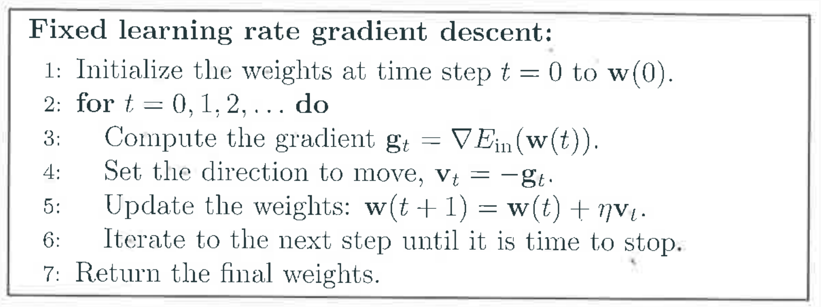
where $\eta_t = \eta \, \|g(\boldsymbol{w}(t))\|$, i.e. the step size is proportional to the length of the gradient.

We obtain

$$\boldsymbol{w}(t+1) = \boldsymbol{w}(t) - \eta g(\boldsymbol{w}(t)),$$

where η is now a (redefined) fixed **learning rate**.

Gradient descent algorithm



Fixed learning rate gradient descent:

```
1: Initialize the weights at time step $t = 0$ to $\mathbf{w}(0)$.
2: for $t = 0, 1, 2, \ldots$ do
3:     Compute the gradient $\mathbf{g}_t = \nabla E_{\text{in}}(\mathbf{w}(t))$.
4:     Set the direction to move, $\mathbf{v}_t = -\mathbf{g}_t$.
5:     Update the weights: $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta \mathbf{v}_t$.
6:     Iterate to the next step until it is time to stop.
7: Return the final weights.
```

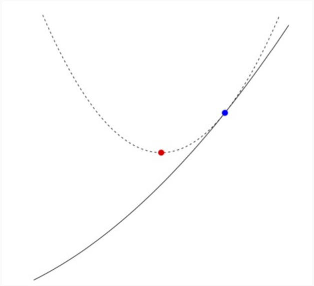
$\boldsymbol{v}_t$ is a direction that is no longer restricted to unit length.

Logistic regression algorithm

```
1: Initialize the weights at $t = 0$ to $\mathbf{w}(0)$
2: for $t = 0, 1, 2, \ldots$ do
3:     Compute the gradient
           $$\nabla E_{\text{in}} = -\frac{1}{N}\sum_{n=1}^{N}\frac{y_n\mathbf{x}_n}{1+e^{\,y_n\mathbf{w}^{\mathsf{T}}(t)\mathbf{x}_n}}$$
4:     Update the weights: $\mathbf{w}(t+1) = \mathbf{w}(t) - \eta\nabla E_{\text{in}}$
5:     Iterate to the next step until it is time to stop
6: Return the final weights $\mathbf{w}$
```

Gradient descent (another interpretation)

Another way to retrieve the gradient descent algorithm consists in minimizing a specific quadratic approximation of the function[1].



[1]Note that trying to directly minimize a linear approximation to our function wouldn't be very useful since the solution is infinity.

Gradient descent (another interpretation)

The second-order Taylor expansion of ℓ is given by

$$\begin{aligned}\ell(\boldsymbol{w}(t+1)) \approx \ell(\boldsymbol{w}(t)) &+ g(\boldsymbol{w}(t))^T(\boldsymbol{w}(t+1)-\boldsymbol{w}(t)) \\ &+ \frac{1}{2}(\boldsymbol{w}(t+1)-\boldsymbol{w}(t))^T H(\boldsymbol{w}(t))(\boldsymbol{w}(t+1)-\boldsymbol{w}(t)).\end{aligned}$$

Consider the quadratic approximation of ℓ, replacing $H(\boldsymbol{w}(t))$ by $\frac{1}{\eta}\boldsymbol{I}$ (replacing the curvature given by the Hessian with a much simpler notion of curvature). We can write

$$\begin{aligned}\ell(\boldsymbol{w}(t+1)) \approx \ell(\boldsymbol{w}(t)) &+ g(\boldsymbol{w}(t))^T(\boldsymbol{w}(t+1)-\boldsymbol{w}(t)) \\ &+ \frac{1}{2\eta}\left\|(\boldsymbol{w}(t+1)-\boldsymbol{w}(t))\right\|^2.\end{aligned}$$

Gradient descent (another interpretation)

$\ell(\boldsymbol{w}(t+1))$ is approximated by a convex quadratic, so we know we can minimize it just by setting its gradient to 0.

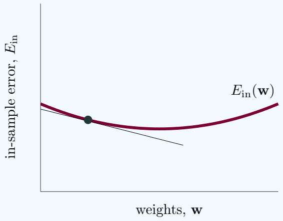
We have

$$\nabla \ell(\boldsymbol{w}(t+1)) \approx g(\boldsymbol{w}(t)) + \frac{1}{\eta}(\boldsymbol{w}(t+1) - \boldsymbol{w}(t)) = 0.$$

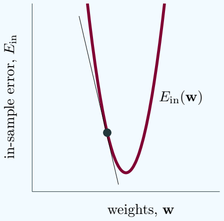
$$\implies \boldsymbol{w}(t+1) = \boldsymbol{w}(t) - \eta g(\boldsymbol{w}(t))$$

Choosing the learning rate

In gradient descent, the learning rate η multiplies the negative gradient to give the move $-\eta \nabla E_{\text{in}}$. The size of the step taken is proportional to η . The optimal step size (and hence learning rate η) depends on how **wide** or **narrow** the error surface is near the minimum.



wide: use large η.

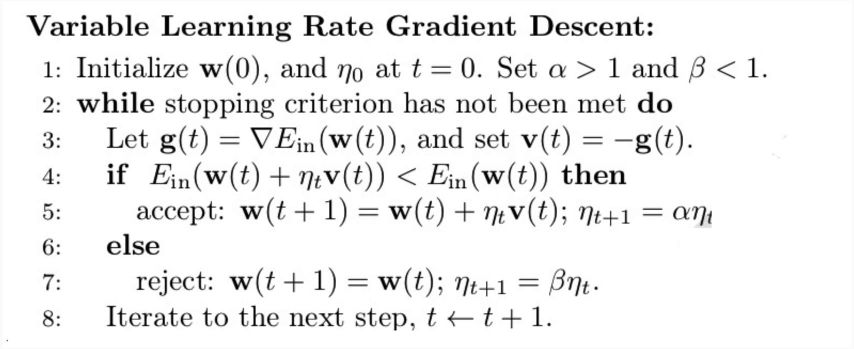


narrow: use small η.

When the surface is wider, we can take larger steps without overshooting; since $\|\nabla E_{\text{in}}\|$ is small, we need a large η. Since we do not know ahead of time how wide the surface is, it is easy to choose an inefficient value for η.

Variable learning rate gradient descent

A simple heuristic that adapts the learning rate to the error surface works well in practice. If the error drops, increase η; if not, the step was too large, so reject the update and decrease η.



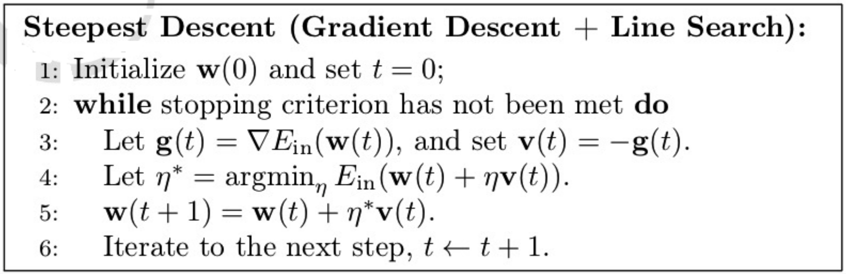
Variable Learning Rate Gradient Descent:

```
1: Initialize $\mathbf{w}(0)$, and $\eta_0$ at $t = 0$. Set $\alpha > 1$ and $\beta < 1$.
2: while stopping criterion has not been met do
3:     Let $\mathbf{g}(t) = \nabla E_{\text{in}}(\mathbf{w}(t))$, and set $\mathbf{v}(t) = -\mathbf{g}(t)$.
4:     if $E_{\text{in}}(\mathbf{w}(t) + \eta_t \mathbf{v}(t)) < E_{\text{in}}(\mathbf{w}(t))$ then
5:         accept: $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta_t \mathbf{v}(t)$; $\eta_{t+1} = \alpha\eta_t$
6:     else
7:         reject: $\mathbf{w}(t+1) = \mathbf{w}(t)$; $\eta_{t+1} = \beta\eta_t$.
8:     Iterate to the next step, $t \leftarrow t + 1$.
```

I is also called *Backtracking line search*.

Steepest descent – gradient descent with (exact) line search

Once the direction in which to move, $\boldsymbol{v}_t$, has been determined, why not simply continue along that direction until the error stops decreasing? This leads us to *steepest descent – gradient descent with (exact) line search*.



Steepest Descent (Gradient Descent + Line Search):

```
1: Initialize $\mathbf{w}(0)$ and set $t = 0$;
2: while stopping criterion has not been met do
3:     Let $\mathbf{g}(t) = \nabla E_{\text{in}}(\mathbf{w}(t))$, and set $\mathbf{v}(t) = -\mathbf{g}(t)$.
4:     Let $\eta^* = \text{argmin}_\eta \, E_{\text{in}}(\mathbf{w}(t) + \eta\mathbf{v}(t))$.
5:     $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta^*\mathbf{v}(t)$.
6:     Iterate to the next step, $t \leftarrow t + 1$.
```

Stopping criterion

Typically the initial point $\boldsymbol{w}(0)$ is picked randomly, or we use prior knowledge about the problem. But when to stop the algorithm?

Some common choices (ϵ is a small prescribed threshold):

- $\|\nabla E_{\text{in}}(\boldsymbol{w}(t))\| < \epsilon$
- $|E_{\text{in}}(\boldsymbol{w}(t+1)) - E_{\text{in}}(\boldsymbol{w}(t))| < \epsilon$
- $\|\boldsymbol{w}(t+1) - \boldsymbol{w}(t)\| < \epsilon$
- $\frac{|E_{\text{in}}(\boldsymbol{w}(t+1)) - E_{\text{in}}(\boldsymbol{w}(t))|}{\max\{1,\ |E_{\text{in}}(\boldsymbol{w}(t))|\}} < \epsilon$
- $t > T$

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About gradient descent

Many machine learning problems involve the following optimization problem The in-sample error is given by

$$\min_{\boldsymbol{w}} E_{\text{in}}(\boldsymbol{w}) = \frac{1}{N} \sum_{n=1}^{N} e(y_n, h(\boldsymbol{x}_n)), \tag{1}$$

e.g. for logistic regression, we have $e(y_n, h(\boldsymbol{x}_n)) = \ln(1 + e^{-y_n \boldsymbol{w}^T \boldsymbol{x}_n})$.

Minimizing (1) using **gradient descent** requires to compute

$$\nabla E_{\text{in}}(\boldsymbol{w}) = \frac{1}{N} \sum_{n=1}^{N} \nabla e(y_n, h(\boldsymbol{x}_n)),$$

In other words, $\nabla E_{\text{in}}(\boldsymbol{w})$ is based on <u>all</u> examples $(\boldsymbol{x}_n, y_n)$, also called **batch GD**.

- Computing the **full gradient** is slow for big data
- Stuck at stationary points (non-convex optimization)

Stochastic gradient descent

1. Pick <u>one</u> $(\boldsymbol{x}_n, y_n)$ at a time (uniformly at random)
2. Apply GD to $e(y_n, h(\boldsymbol{x}_n))$, i.e. compute

$$\boldsymbol{w}(t+1) = \boldsymbol{w}(t) - \nabla e(y_n, h(\boldsymbol{x}_n)).$$

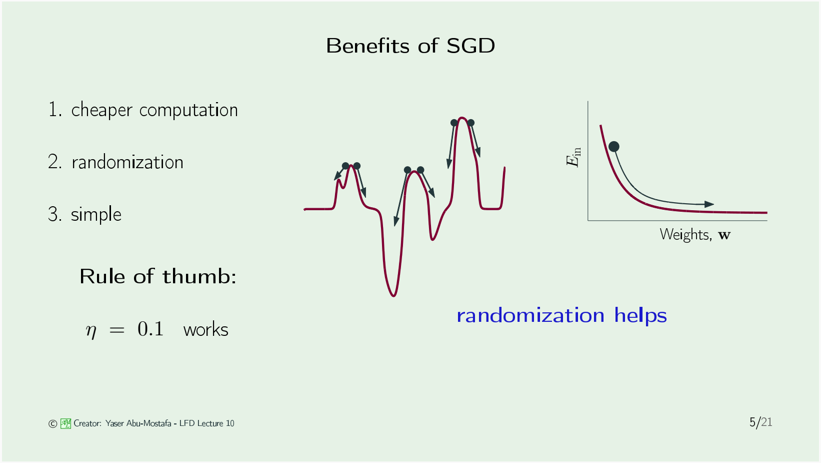
What is the average direction?

$$\begin{aligned}\mathbb{E}_n[-\nabla e(y_n, h(\boldsymbol{x}_n))] &= \sum_{n=1}^{N} \frac{1}{N}[-\nabla e(y_n, h(\boldsymbol{x}_n))] \\ &= -\frac{1}{N}\sum_{n=1}^{N} \nabla e(y_n, h(\boldsymbol{x}_n)) \\ &= -\nabla E_{\text{in}}(\boldsymbol{w})\end{aligned}$$

Stochastic gradient descent (SGD) is an unbiased estimate of GD with a **higher variance**.

Benefits of SGD

- Cheaper computation
- Randomization
- Simple

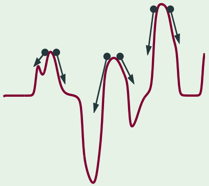


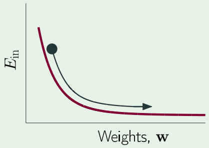
Benefits of SGD

1. cheaper computation
2. randomization
3. simple

Rule of thumb:

$\eta = 0.1$ works





randomization helps

Mini-batch gradient descent

Compute the gradient using $1 \leq b \leq N$ data points.

1. Pick b data points ($1 \leq b \leq N$)
2. Apply batch GD to these b points

- $b = N$ is GD and $b = 1$ is SGD
- Bias and variance tradeoff
- A single pass through the entire training data is called an *epoch*. With mini-batches of size b, we update the parameters N/b times per epoch.
- We often need multiple epochs to obtain a good training accuracy.

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Newton's method

Let us assume ℓ is twice differentiable, and minimize the second-order Taylor expansion of ℓ, given by

$$\begin{aligned}\ell(\boldsymbol{w}(t+1)) \approx \ell(\boldsymbol{w}(t)) &+ g(\boldsymbol{w}(t))^T(\boldsymbol{w}(t+1) - \boldsymbol{w}(t)) \\ &+ \frac{1}{2}(\boldsymbol{w}(t+1) - \boldsymbol{w}(t))^T H(\boldsymbol{w}(t))(\boldsymbol{w}(t+1) - \boldsymbol{w}(t)).\end{aligned}$$

We have

$$\begin{aligned}\nabla\ell(\boldsymbol{w}(t+1)) = g(\boldsymbol{w}(t)) + H(\boldsymbol{w}(t))(\boldsymbol{w}(t+1) - \boldsymbol{w}(t)) :& \\ \implies g(\boldsymbol{w}(t)) + H(\boldsymbol{w}(t))(\boldsymbol{w}(t+1) - \boldsymbol{w}(t)) = 0& \\ \implies \boldsymbol{w}(t+1) = \boldsymbol{w}(t) - H(\boldsymbol{w}(t))^{-1}g(\boldsymbol{w}(t))&\end{aligned}$$

The *damped* Newton's method with a small step size $0 < \eta < 1$:

$$\boldsymbol{w}(t+1) = \boldsymbol{w}(t) - \eta\ H(\boldsymbol{w}(t))^{-1}g(\boldsymbol{w}(t)).$$

See also Quasi-Newton methods which approximate the Hessian.

Other optimization methods

- Momentum and Acceleration
- Adaptive Gradient Algorithm (AdaGrad), Root Mean Square Propagation (RMSProp), Adam
- Stochastic Average Gradient (SAG), Stochastic Variance Reduced Gradient (SVRG)
- Conjugate gradient
- ...

An overview of gradient descent optimization algorithms: `https://ruder.io/optimizing-gradient-descent/`

Additional considerations

- **Gradient descent**
  - Simple idea, and each iteration is (usually) cheap
  - Fast for well-conditioned, strongly convex problems
  - Can often be slow, because many interesting problems aren't strongly convex or well-conditioned
  - Can't handle nondifferentiable functions
- **Stochastic Gradient Descent**
  - In many ML problems we don't care about optimizing to high accuracy, it doesn't pay off in terms of statistical performance
  - Can be super effective in terms of iteration cost, memory.
  - Can be slow to converge.
  - Popular in large-scale, continous, nonconvex optimization, but it is still not well-understood (e.g. implicit regularization)
- **Newton's method**
  - Requires more memory and computation per iteration
  - Not affected by a problem's conditioning,