Optimization Techniques for ML (1)

Piyush Rai

Introduction to Machine Learning (CS771A)

August 23, 2018

Recap: Generative Classification

Class-Marginal
or
Class Prior

Class-Conditional

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naïve Bayes assumption: $p(\boldsymbol{x}|y=k) = \prod_{d=1}^{D} p(x_d|y=k)$

(reduces the number of parameters to be estimated for $p(\boldsymbol{x}|y=k)$)

E.g.: Gaussian with
Diagonal or Spherical
Covariance Matrix

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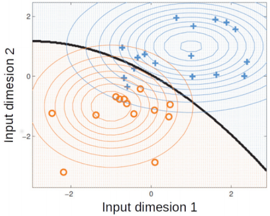
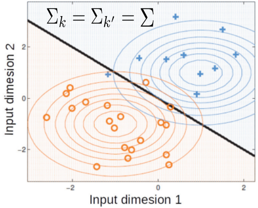
- Quadratic decision boundary if covariances unequal, linear if covariances equal





$$(\mathbf{x}-\boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\mathbf{x}-\boldsymbol{\mu}_k) - (\mathbf{x}-\boldsymbol{\mu}_{k'})^\top \boldsymbol{\Sigma}_{k'}^{-1}(\mathbf{x}-\boldsymbol{\mu}_{k'}) = 0$$

(a quadratic function of $\boldsymbol{x}$)

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(reduces to the form $\boldsymbol{w}^\top \boldsymbol{x} + b = 0$)

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$$p(y = k|\boldsymbol{x}, \theta) \propto \pi_k \exp\left[-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}_k)\right]$$

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- Interestingly, this has exactly the same form as the softmax classification model

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- If we further assume $\Sigma = \mathbf{I}$, we get the exact same model as prototype based clasification

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- Generative and discriminative models can be combined as well

Optimization Techniques for ML

Optimization Problems in ML

- The generic form of most optimization problems in ML

$$\hat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}) = \arg\min_{\boldsymbol{w}} \sum_{n=1}^{N} \ell_n(\boldsymbol{w}) + R(\boldsymbol{w})$$

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- Some common examples

$$\hat{w} = \arg\min_{\boldsymbol{w}} \sum_{n=1}^{N} (y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2 + \lambda ||w||_2^2$$

$$\hat{w} = \arg\min_{\boldsymbol{w}} \sum_{n=1}^{N} (y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2 + \lambda ||\boldsymbol{w}||_1$$

ℓ_1 regularizer

$$\hat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} - \left[\sum_{n=1}^{N} (y_n \boldsymbol{w}^\top \boldsymbol{x}_n - \log(1 + \exp(\boldsymbol{w}^\top \boldsymbol{x}_n))) \right] + \lambda ||\boldsymbol{w}||^2$$

ℓ_2 regularized logistic regression assuming $y_n \in \{0, 1\}$

$$\hat{w} = \arg\min_{\boldsymbol{w}} \sum_{n=1}^{N} \log(1 + \exp(-y_n \boldsymbol{w}^\top \boldsymbol{x}_n) + \lambda ||\boldsymbol{w}||^2$$

ℓ_2 regularized logistic regression assuming $y_n \in \{-1, 1\}$

$$\hat{\mathbf{W}} = \arg\min_{\mathbf{W}} - \sum_{n=1}^{N} \sum_{k=1}^{K} \mathbb{I}[y_n = k] \log \left[\frac{\exp(\boldsymbol{w}_k^\top \boldsymbol{x}_n)}{\sum_{k=1}^{K} \exp(\boldsymbol{w}_k^\top \boldsymbol{x}_n)} \right]$$

Softmax Regression with K classes (assuming no regularization)

$$\hat{\theta}_{MAP} = \arg\min_{\theta} - \left[\sum_{n=1}^{N} \log p(y_n|\theta) + \log p(\theta) \right]$$

A general MAP estimation problem

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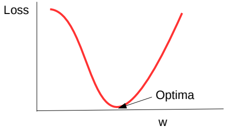

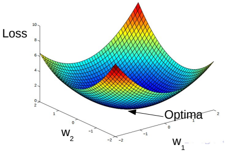

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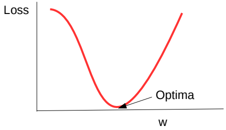

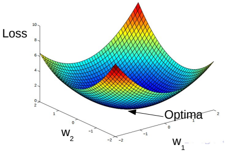

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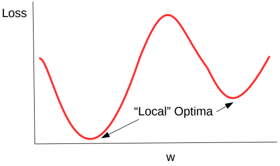

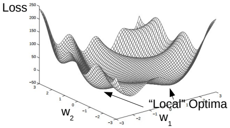

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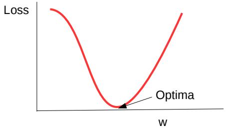

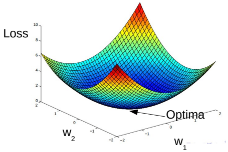

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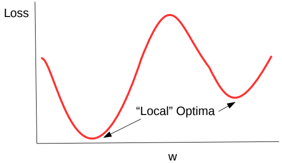
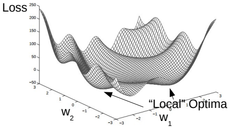




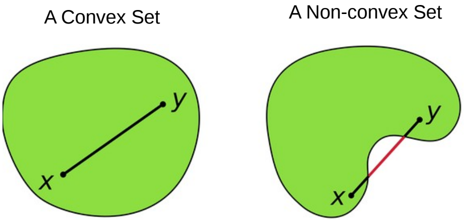
- Functions with unique minima: Convex; Functions with many local minima: Non-convex

Interlude: Convex Sets

- A set $\mathcal{S}$ of points is a convex set, if for any two points $x, y \in \mathcal{S}$, and $0 \leq \alpha \leq 1$

$$z = \alpha x + (1-\alpha) y \in \mathcal{S}$$

.. i.e., all points on the line-segment between x and y lie within the set



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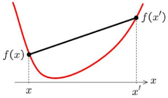

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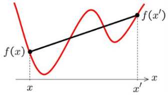

Note: "Chord lies above function" more formally means

If f is convex then given $\alpha_1, \ldots, \alpha_n$ s.t $\sum_{i=1}^{n} \alpha_i = 1$

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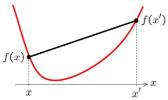

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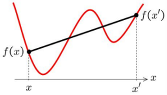

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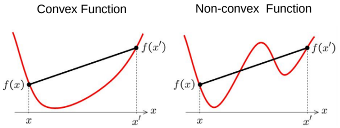

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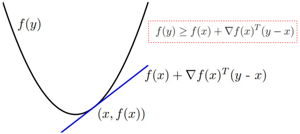

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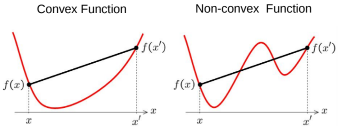

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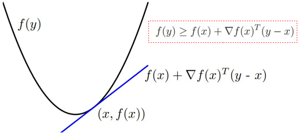

  - Second-order convexity: Second derivative a.k.a. Hessian (if exists) must be positive semi-definite

$$\nabla^2 f(x) \succeq 0$$

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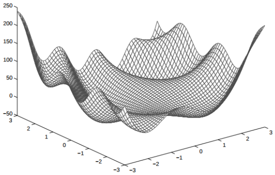
  - Most of these also apply when x is a vector (and many other rules)

Disclaimer:
It's OK to be non-convex :-)



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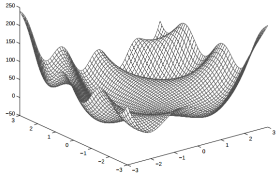
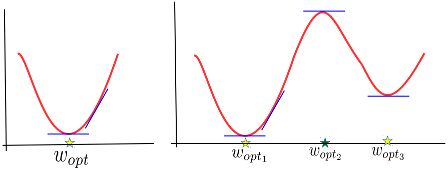


Many interesting ML problems are in fact non-convex and there are ways to optimize non-convex objectives (non-convex optimization is a research area in itself)

Solving Optimization Problems

- The most basic approach: Use first-order optimality condition



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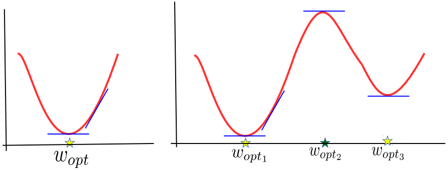

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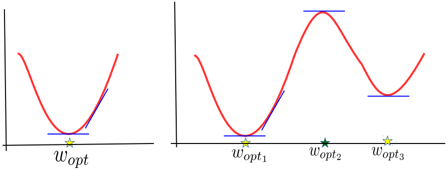

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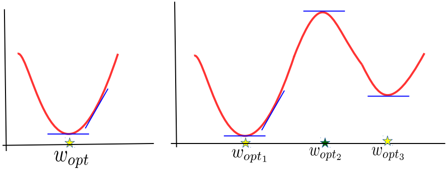

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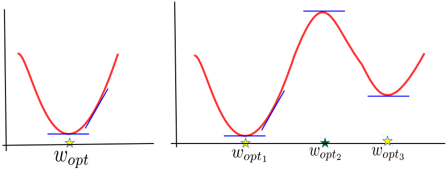

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- Sometimes, setting $\boldsymbol{g} = 0$ and solving for $\boldsymbol{w}$ gives a closed form solution (recall linear regression)
- .. and often it does NOT (recall logistic regression)
- The gradient $\boldsymbol{g}$ can still be helpful since we can use it in iterative optimization methods

Iterative Optimization via Gradient Descent

Gradient Descent

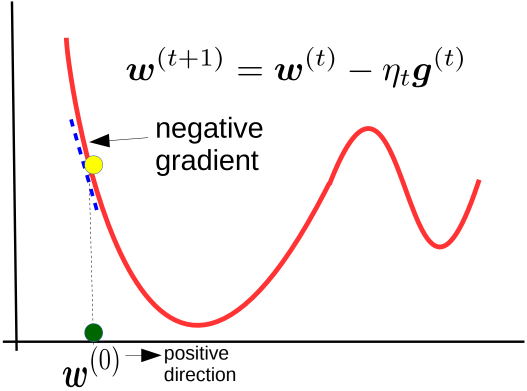
1. Initialize $\boldsymbol{w}$ as $\boldsymbol{w}^{(0)}$
2. Update $\boldsymbol{w}$ as follows

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \eta_t \boldsymbol{g}^{(t)}$$

3. Repeat until convergence

Gradient Descent

- A very simple, first-order method (uses only the gradient $\boldsymbol{g}$ of the objective)
- Basic idea: Start at some location $\boldsymbol{w}^{(0)}$ and move in the opposite direction of the gradient



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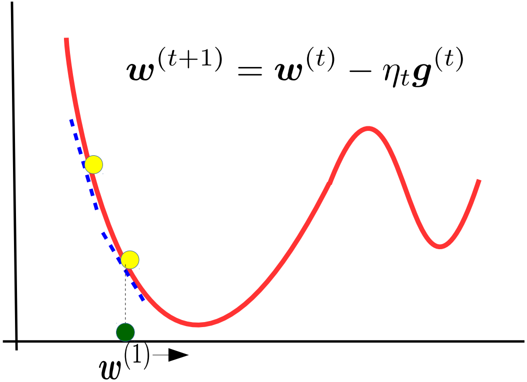

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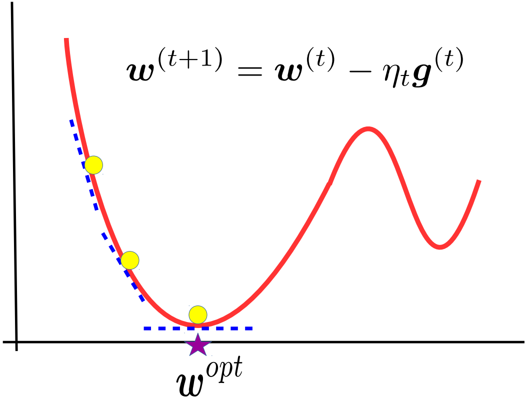

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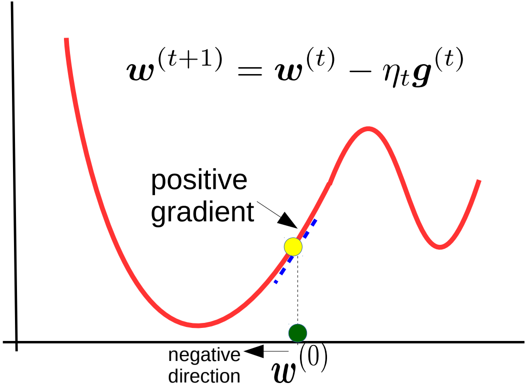

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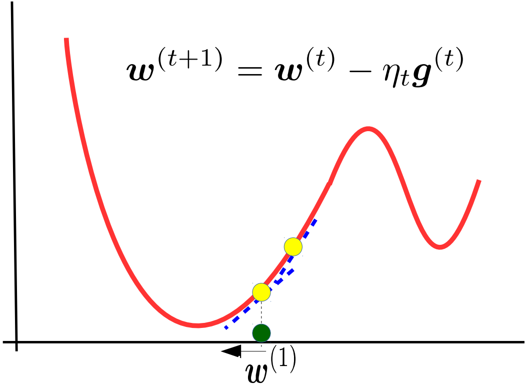

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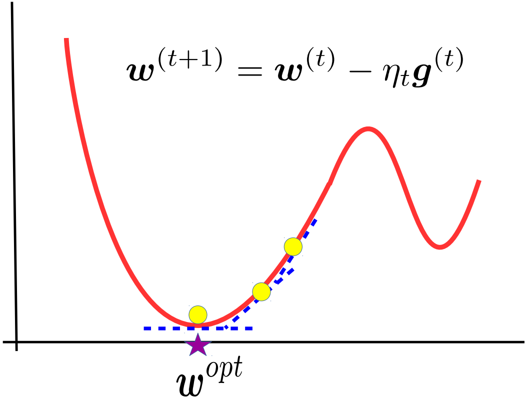

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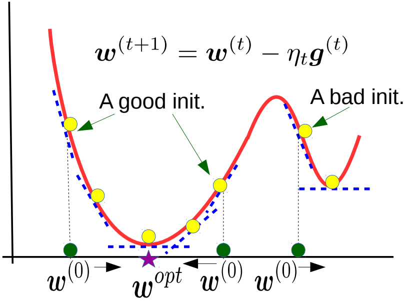

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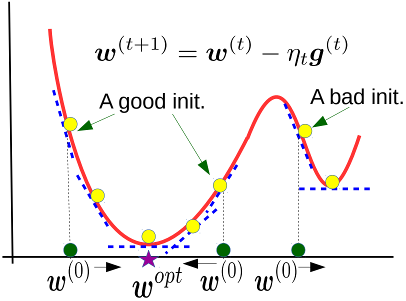

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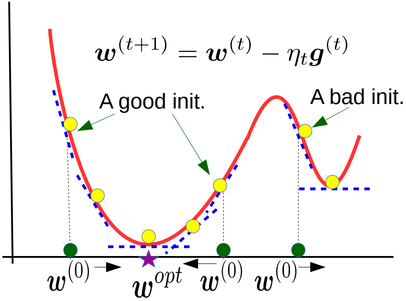

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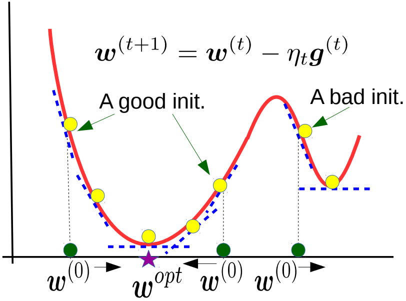

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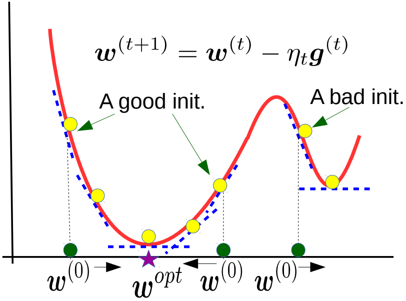

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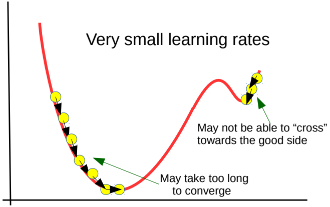
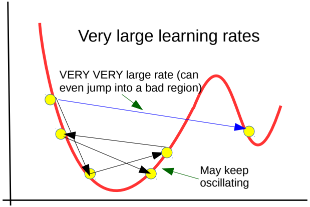
- **When to stop:** Many criteria, e.g., gradients become too small, or validation error starts increasing

Gradient Descent

- The learning rate η_t is important
- Very small learning rates may result in very slow convergence
- Very large learning rates may lead to oscillatory behavior or result in a bad local optima





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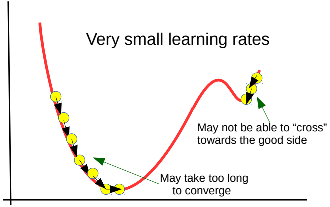

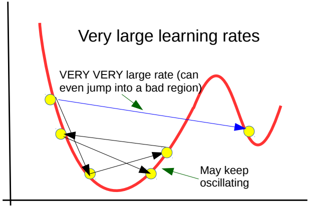

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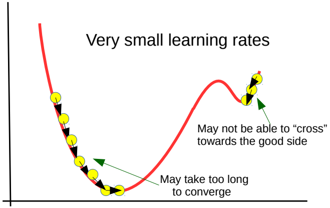

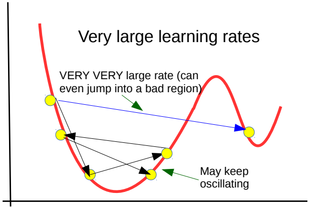

- Many ways to set the learning rate, e.g.,
  - Constant (if properly set, can still show good convergence behavior)
  - Decreasing with t (e.g. $1/t$, $1/\sqrt{t}$, etc.)
  - Use adaptive learning rates (e.g., using methods such as Adagrad, Adam)

Gradient Descent: Gradient Computations may be Expensive

- Gradient computation in GD may be very expensive
- Reason: Need to evaluate N terms. Assuming no regularization term, something like

$$\boldsymbol{g} = \nabla_{\boldsymbol{w}} \left[\sum_{n=1}^{N} \ell_n(\boldsymbol{w}) \right] = \sum_{n=1}^{N} \boldsymbol{g}_n$$

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- SGD updates use this approximation of the actual gradient

Stochastic Gradient Descent

1. Initialize $\boldsymbol{w}$ as $\boldsymbol{w}^{(0)}$
2. Pick a random $i \in \{1, \ldots, N\}$. Update $\boldsymbol{w}$ as follows

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \eta_t \boldsymbol{g}_i^{(t)}$$

3. Repeat until convergence

(Stochastic) Gradient Descent

- SGD uses a single example to compute the gradient
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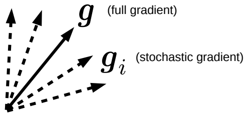

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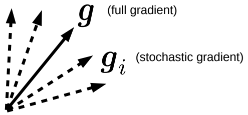

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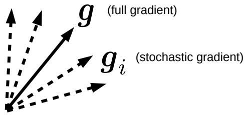

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- This is known as mini-batch SGD

Gradient Descent: Some Simple Examples

- Ignoring the regularizer, consider the loss functions for linear and logistic regression

$$\text{Linear Regression:} \quad \mathcal{L}(\boldsymbol{w}) = \sum_{n=1}^{N}(y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2$$

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- Note that highly mispredicted inputs $\boldsymbol{x}_n$ contribute more to $\boldsymbol{g}$ and thus to the weight updates!
- SGD is also straightforward (same as GD but with one or few inputs for each gradient computation)

GD and SGD: Some Comments

- Note that we could solve linear regression in closed form

$$\mathbf{w} = (\sum_{n=1}^{N} \mathbf{x}_n \mathbf{x}_n^\top)^{-1} \sum_{n=1}^{N} y_n \mathbf{x}_n = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

.. this has $O(D^3 + ND^2)$ cost

- GD for linear regression avoided the matrix inversion
- In general, cost of batch GD with N examples having D features: $O(ND)$
- SGD cost will be $O(D)$ or $O(BD)$ with mini-batch of size B
- There exist theoretical results on convergence rates of GD/SGD (beyond the scope)
  - GD will take $O\left(\frac{1}{\epsilon^2}\right)$ iterations reach ϵ-close solution, which is defined as

$$\mathcal{L}(\mathbf{w}^{(t)}) \leq \mathcal{L}(\mathbf{w}^{(opt)}) + \epsilon \qquad \text{(up to } \epsilon \text{ worse than optimal)}$$

Gradient Descent: Updates are "Corrective"

- The GD updates for the linear and logistic regression case look like

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- Try the same for the logistic regression case (reason about it in terms of probabilities)

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- Will look at these in the next class..