COS234:

Introduction To Machine Learning

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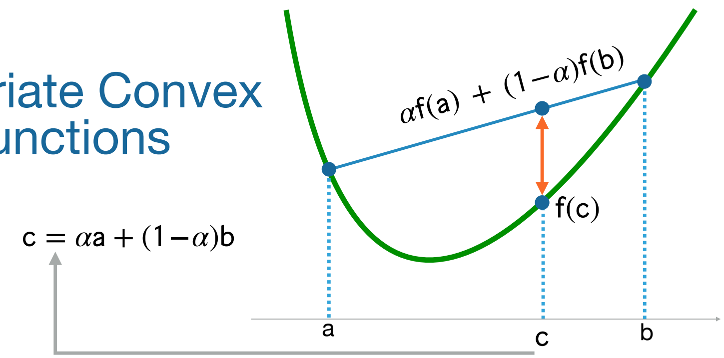
Topic: Gradient-Based Learning - Part II

$$\alpha \in [0,1]: \ f\big(\alpha a + (1-\alpha)b\big) \leq \alpha f(a) + (1-\alpha)f(b)$$

Univariate Convex Functions



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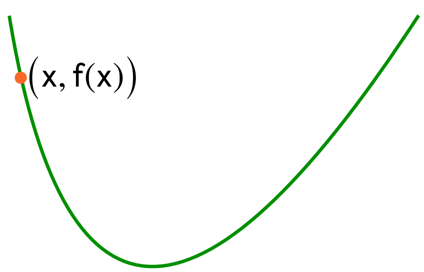

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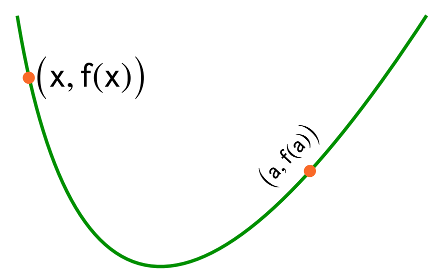

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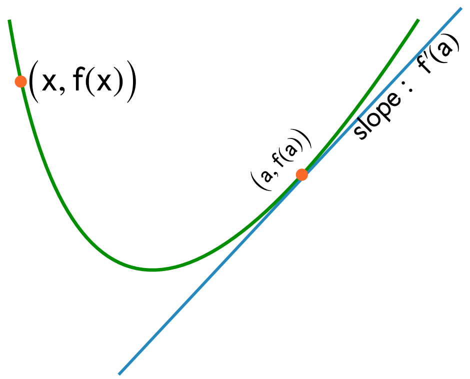

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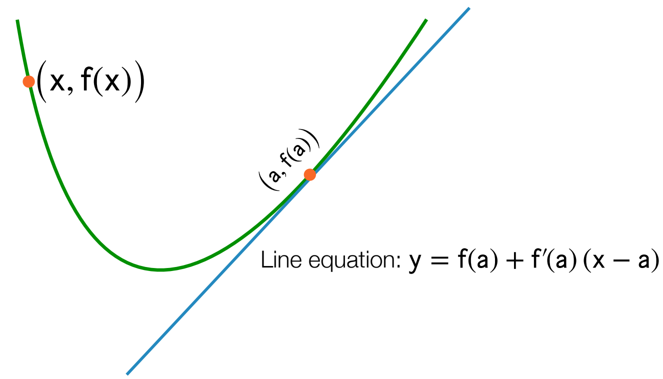

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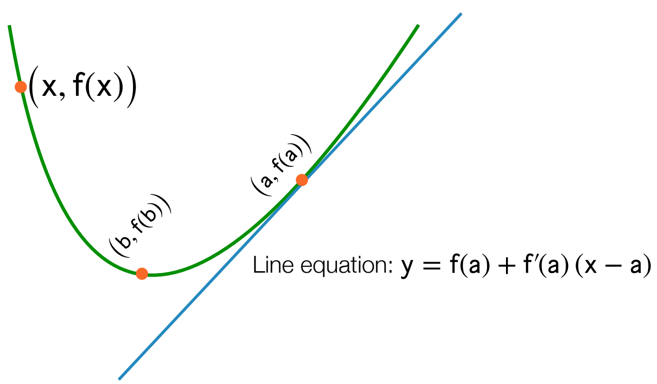

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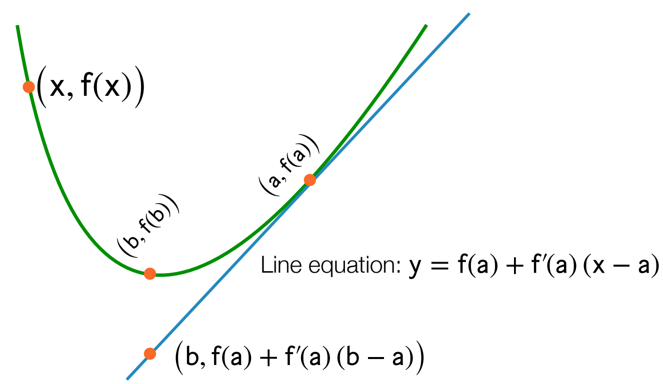

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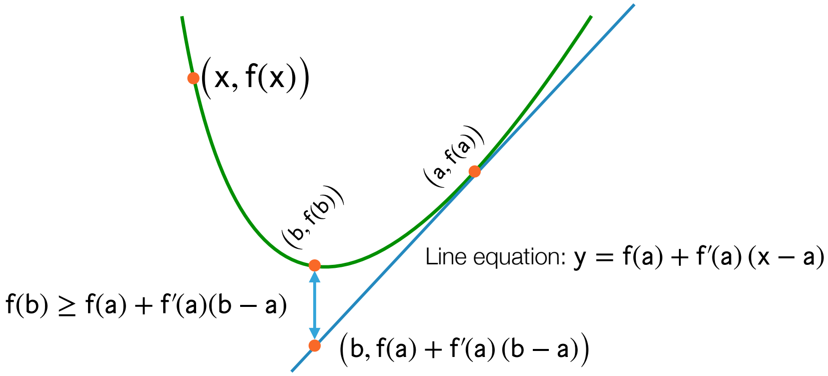
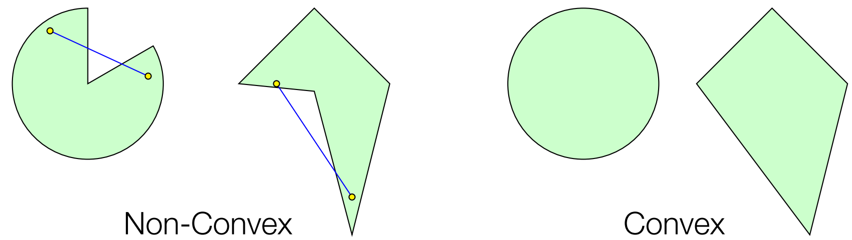


Convex Sets

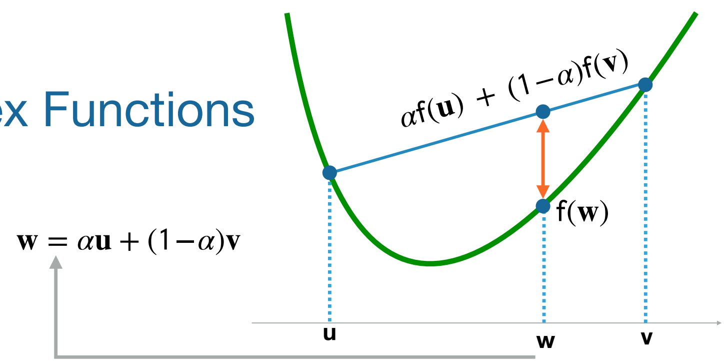
Set Ω is convex if for any $\mathbf{u}, \mathbf{v} \in \Omega$ line segment between $\mathbf{u}$ and $\mathbf{v}$ is in Ω:

$$\forall \alpha \in [0,1] : \alpha \mathbf{u} + (1 - \alpha)\mathbf{v} \in \Omega$$



$$\alpha \in [0, 1] : \; f\big(\alpha \mathbf{u} + (1 - \alpha)\mathbf{v}\big) \leq \alpha f(\mathbf{u}) + (1 - \alpha) f(\mathbf{v})$$

Convex Functions



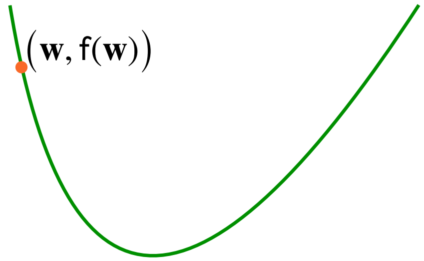
Gradients

$\mathscr{L}(\mathbf{w})$ is a function from $\mathbf{R}^{\mathbf{d}} \to \mathbf{R}_{+}$

We need switch from *derivatives* to *gradients:*

$$\nabla \mathscr{L}(\mathbf{w}) \equiv \frac{\partial \mathscr{L}(\mathbf{w})}{\partial \mathbf{w}} = \left(\frac{\partial \mathscr{L}}{\partial w_1}, \frac{\partial \mathscr{L}}{\partial w_2}, \quad \ldots, \frac{\partial \mathscr{L}}{\partial w_d} \right)$$

Multivariate Convex Functions



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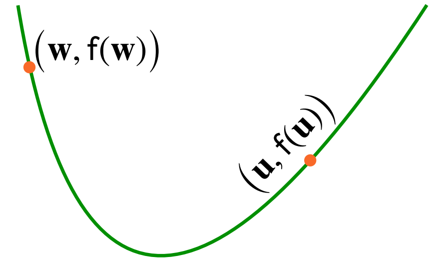

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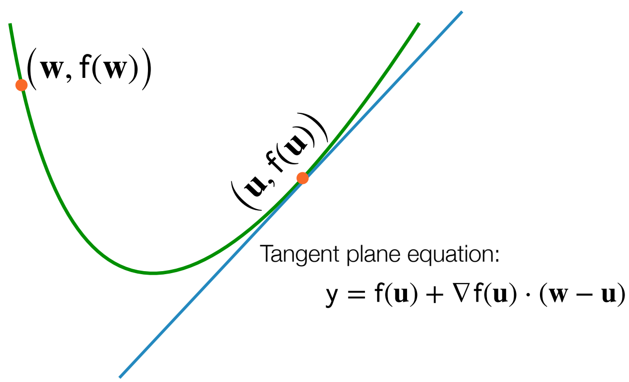

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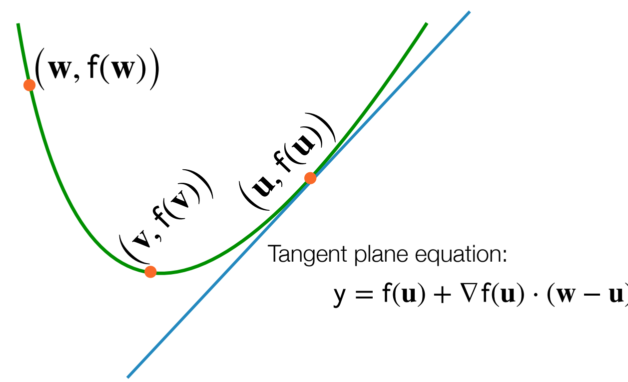

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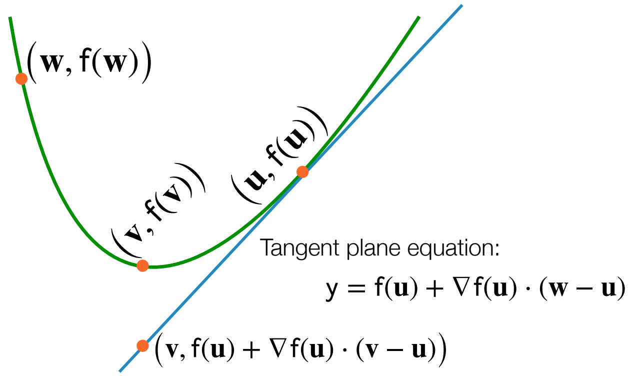

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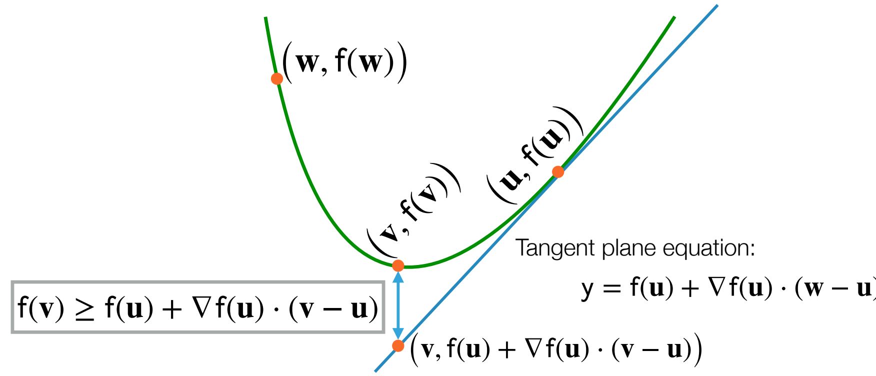

First Order Conditions

- Function $f : \mathbf{R}^d \rightarrow \mathbf{R}$ is convex iff:
  - For $\forall \alpha \in [0,1], \mathbf{u} \in \mathbf{R}^d, \mathbf{v} \in \mathbf{R}^d$:

$$f\left(\alpha \mathbf{u} + (1-\alpha)\mathbf{v}\right) \leq \alpha f(\mathbf{u}) + (1-\alpha) f(\mathbf{v})$$

  - $f(\mathbf{v}) \geq f(\mathbf{u}) + \nabla f(\mathbf{u}) \cdot (\mathbf{v} - \mathbf{u})$
  - Fix $\mathbf{u} \in \mathbf{R}^d, \mathbf{v} \in \mathbf{R}^d$ and define $h : \mathbf{R} \rightarrow \mathbf{R}$ as $h(t) = f(\mathbf{u} + t\mathbf{v})$ then $h(t)$ is a convex univariate function $\left(h''(t) \geq 0 \right)$

Second Order Conditions

Hessian of $f : \mathbf{R}^d \rightarrow \mathbf{R}$ is $d \times d$ matrix of second order derivatives $\nabla^2 f$:

$$H_{ij} = \frac{\partial^2 f}{\partial w_i \, \partial w_j}$$

f is convex iff:

$$\forall \mathbf{u} : \ \mathbf{u}^T H \, \mathbf{u} \geq 0$$

This means that the smallest Eigen value of H is non-negative

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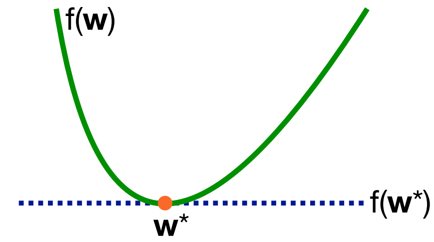


- $\mathbf{w}^*$ minimum (vector) of f:

$$f(\mathbf{w}^\star) \leq f(\mathbf{w}) \text{ for all } b \neq a^*$$

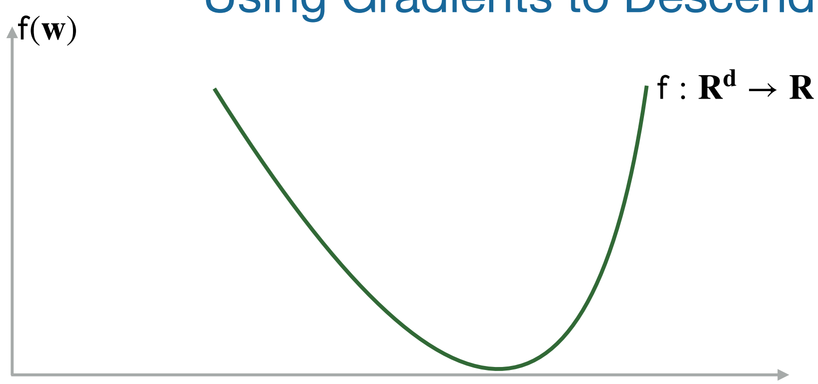
- Gradient of $f(\mathbf{w})$ at $\mathbf{w}^*$ is zero

$$\nabla f(\mathbf{w})\Big|_{\mathbf{w}=\mathbf{w}^\star} = (0, 0, \ \ldots \ , 0) = \mathbf{0}$$

- Almost always no closed form solution for:

$$\nabla f(\mathbf{w}) = \mathbf{0}$$

Using Gradients to Descend



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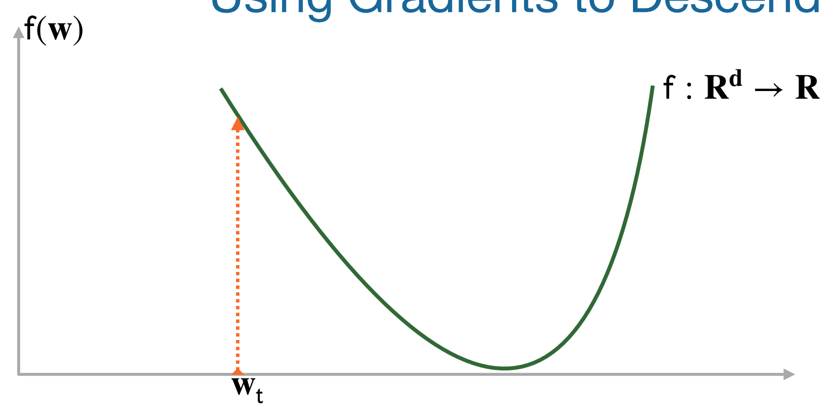

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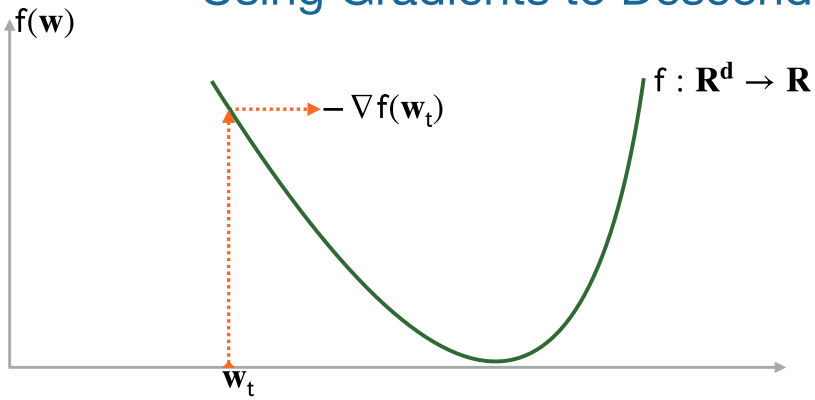

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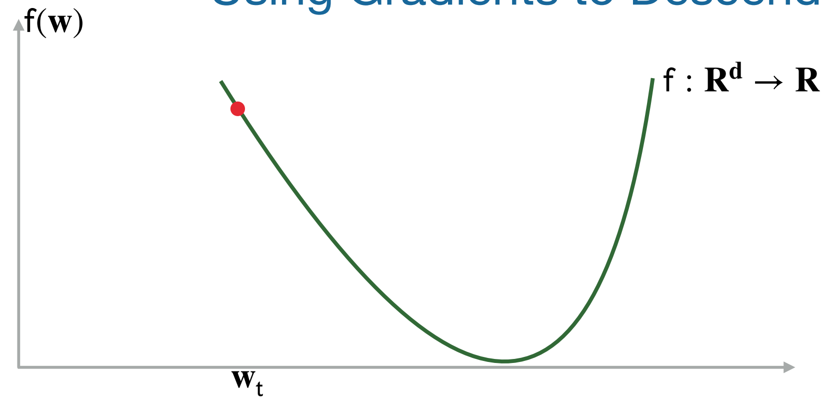

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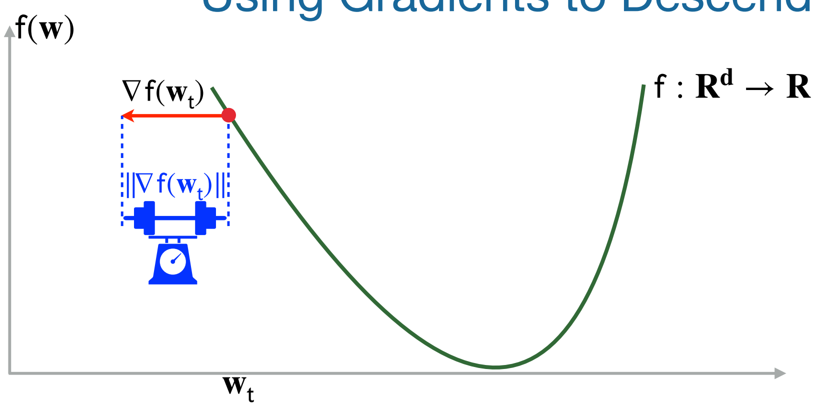

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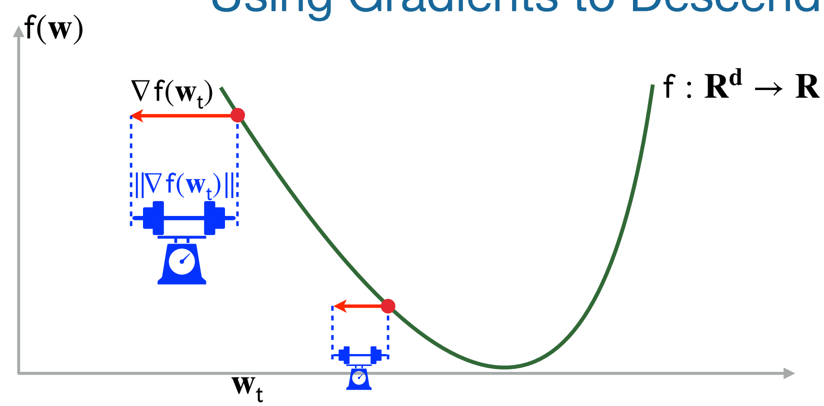

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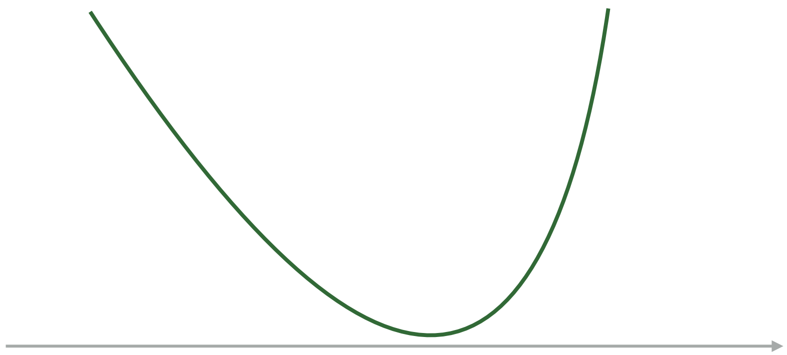

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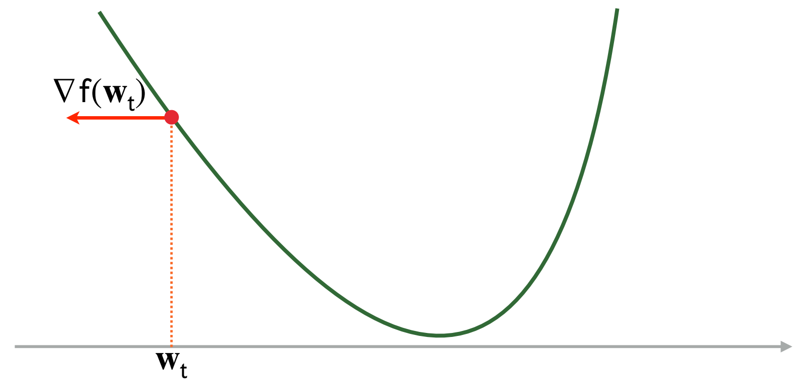

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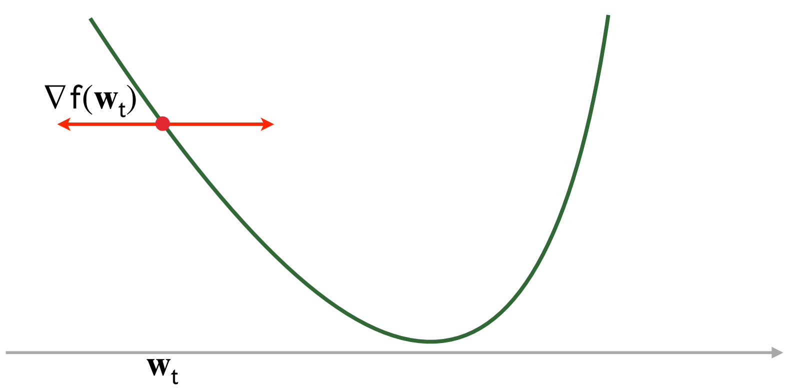

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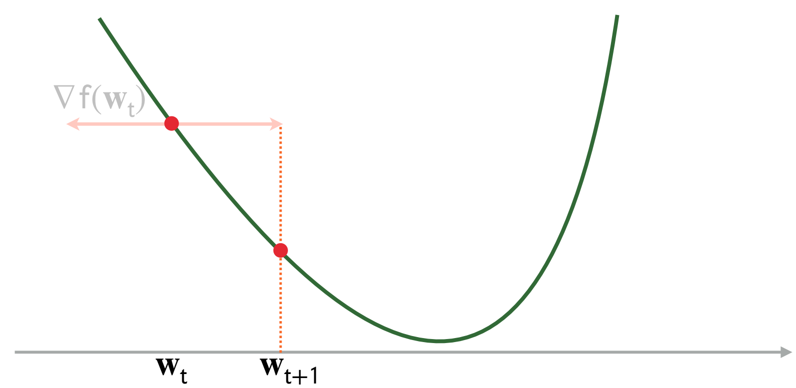

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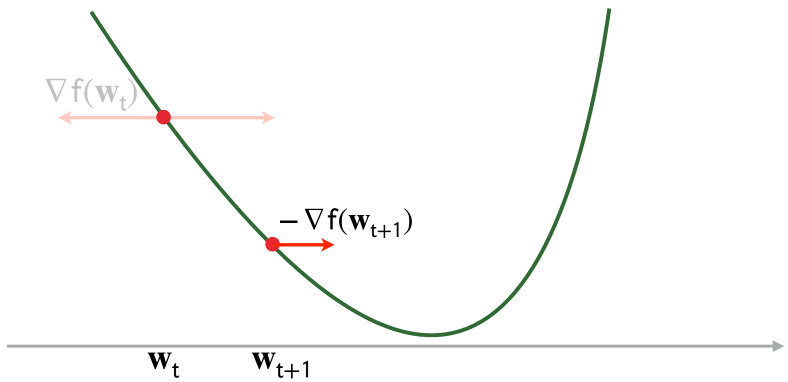

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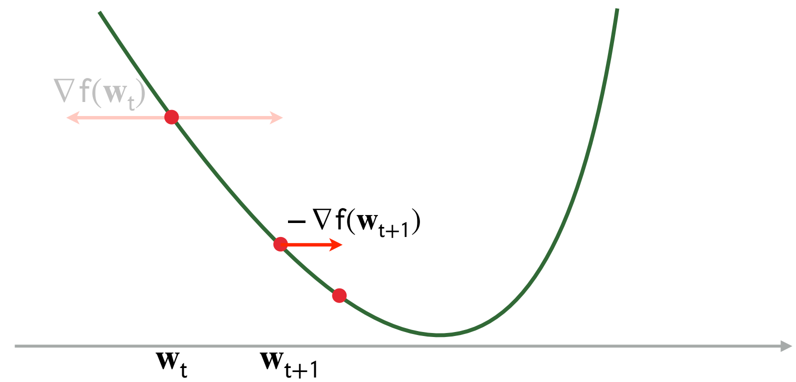

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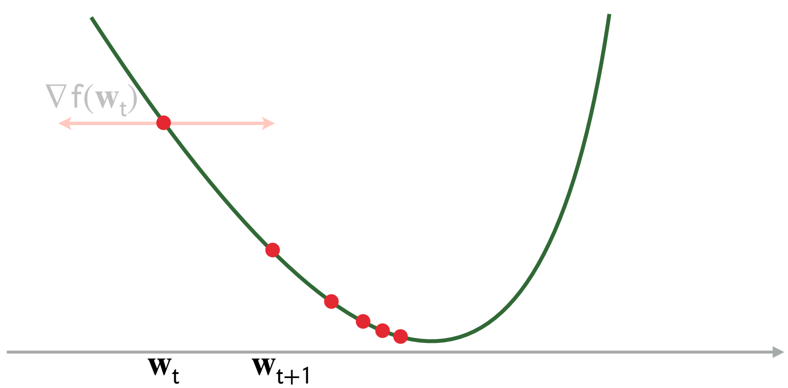

Gradient Descent Procedure

- Input: function $f : \mathbf{R} \to \mathbf{R}_+$
- Goal: find $\hat{\mathbf{w}}$ such that $f(\hat{\mathbf{w}}) - f(\mathbf{w}^\star) \leq \epsilon$
- Choose initial value $\mathbf{w}_1$
- Loop:
  - $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta_t \nabla f(\mathbf{w}_t)$
  - Until …

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  - Until …

☆learning rate
☆step size

Gradient Descent

```
def derivative_descent(w0, gradient_func, eta):
    T, d = len(eta) + 1, len(w0)
    w = w0
    for t in range(1, T):
        w = w - eta[t-1] * gradient_func(w)
    return w
```


Learning Rate

- Crucial in many learning problems
- Fixed learning-rate can be used in restricted circumstances
- Self-tuning procedure of learning-rate exist, notably AdaGrad
- In many applications:
  - Linear decrease $\eta_t = \dfrac{\eta_0}{b + st}$ where $\eta_0 \in [0.1, 1]$ (typically)
  - Sub-linear decrease $\eta_t \sim \dfrac{\eta_0}{\sqrt{t}}$

Generalized Linear Models

Loss for linear predictors $\mathscr{L}(\mathbf{w}) = \dfrac{1}{n} \sum_{i=1}^{n} \ell(y_i, h(\mathbf{w} \cdot \mathbf{x_i}))$

h: transfer (activation) function $h : \mathbf{R} \to \mathbf{R}$ and $\hat{y}_i = h(\mathbf{w} \cdot \mathbf{x_i})$

$\ell(y, \hat{y})$ binary function from to $\mathbf{R} \times \mathbf{R}$ to $\mathbf{R}_+$

We can find $\mathbf{w}$ which (approximately) minimizes $\mathscr{L}(\mathbf{w})$ using GD and computing the gradient using chain rule

GLM: Examples

Linear regression:

$y \in \mathbf{R} \quad h(z) = z \quad \ell(y, \hat{y}) = (y - \hat{y})^2$

Classification with hinge-loss:

$y \in \{-1, +1\} \quad h(z) = z \quad \ell(y, \hat{y}) = [1 - y\hat{y}]_+$ where $[z]_+ = \max\{0, z\}$

Logistic regression:

$y \in \{0, 1\} \quad h(z) = \dfrac{1}{1 + e^{-z}} \quad \ell(y, \hat{y}) = -y\log(\hat{y}) - (1 - y)\log(1 - \hat{y})$

Gradients for GLM

$$\nabla \mathscr{L}(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n} \nabla_{\mathbf{w}}\, \ell(y_i, h(\mathbf{w} \cdot \mathbf{x_i}))$$

Given y_i derivative w.r.t $\hat{y}_i$ is $\ell'(y_i, \hat{y}_i) = \dfrac{d\,\ell(y_i, \hat{y}_i)}{d\hat{y}_i}$

Define $z_i = \mathbf{w} \cdot \mathbf{x}_i$ then derivative of h w.r.t. z_i is $h'(z_i)$

Finally $\nabla_{\mathbf{w}}\, z_i = \mathbf{x}_i$

Thus $\nabla \mathscr{L}(\mathbf{w}) = \dfrac{1}{n}\displaystyle\sum_{i=1}^{n} \ell'(y_i, \hat{y}_i)\, h'(z_i)\, \mathbf{x_i}$

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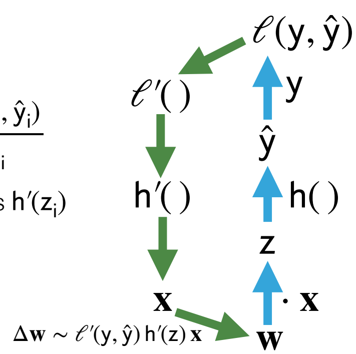

Gradient for Logistic Regression

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$$y \in \{0,1\} \quad h(z) = \frac{1}{1+e^{-z}} \quad \ell(y,\hat{y}) = -y\log(\hat{y}) - (1-y)\log(1-\hat{y})$$

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$$\ell'(y,\hat{y}) = \frac{1-y}{1-\hat{y}} - \frac{y}{\hat{y}} = \frac{\hat{y}-y}{\hat{y}(1-\hat{y})}$$

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$$h'(z) = h(z)\,(1-h(z)) = \hat{y}\,(1-\hat{y})$$

$$\Rightarrow \quad \ell'(y,\hat{y})\,h'(z) = \hat{y} - y$$

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$$\nabla \mathscr{L}(\mathbf{w}) = -\frac{1}{n}\sum_{i=1}^{n} (\hat{y}_i - y_i)\,\mathbf{x}_i$$

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$$\nabla \mathscr{L}(\mathbf{w}) = -\frac{1}{n}\sum_{i=1}^{n} \boxed{(\hat{y}_i - y_i)}\,\mathbf{x}_i$$

Interpretation?

Properties of GD

Assume that $\|\nabla \mathscr{L}(\mathbf{w})\| \le \gamma$

This typically amounts to $\forall i:\ \|\mathbf{x}_i\| \le c\gamma$

Assume that $\forall t:\ \|\mathbf{w}_t\| \le r$ and $\|\mathbf{w}^\star\| \le r$

Recall that from convexity $f(\mathbf{v}) \ge f(\mathbf{u}) + \nabla f(\mathbf{u}) \cdot (\mathbf{v} - \mathbf{u})$

Using $\mathbf{v} = \mathbf{w}^\star$ and $\mathbf{u} = \mathbf{w}_t$ we get

$$\mathscr{L}(\mathbf{w}_t) - \mathscr{L}(\mathbf{w}^\star) \le \nabla\mathscr{L}(\mathbf{w}_t) \cdot (\mathbf{w}_t - \mathbf{w}^\star)$$

Properties of GD (cont)

Going forward we abbreviate $\mathbf{g}_t = \nabla \mathscr{L}(\mathbf{w}_t)$ and thus we can write

$$\mathscr{L}(\mathbf{w}_t) - \mathscr{L}(\mathbf{w}^\star) \le \mathbf{g}_t \cdot (\mathbf{w}_t - \mathbf{w}^\star)$$

Define progress towards (unknown) optimum as $\Delta_t = \|\mathbf{w}_t - \mathbf{w}^\star\|^2$

From GD update & boundedness of gradients:

$$\Delta_{t+1} \le \Delta_t - 2\eta\mathbf{g}_t \cdot (\mathbf{w}_t - \mathbf{w}^\star) + \eta^2\gamma^2$$

Rearranging terms and dividing by 2η gives

$$\mathbf{g}_t \cdot (\mathbf{w}_t - \mathbf{w}^\star) \le \frac{1}{2\eta}(\Delta_t - \Delta_{t+1}) + \frac{\eta\gamma^2}{2}$$

Properties of GD (cont)

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We established that $\mathscr{L}(\mathbf{w}_t) - \mathscr{L}(\mathbf{w}^\star) \le \frac{1}{2\eta}(\Delta_t - \Delta_{t+1}) + \frac{\eta\gamma^2}{2}$

Taking the average from t=1 through T

$$\frac{1}{T}\sum_{t=1}^{T} \mathscr{L}(\mathbf{w}_t) - \mathscr{L}(\mathbf{w}^\star) \le \frac{1}{2\eta T}(\Delta_1 - \Delta_{T+1}) + \frac{\eta\gamma^2}{2} \le \frac{r^2}{\eta T} + \frac{\eta\gamma^2}{2}$$

Assume $\forall t : \mathscr{L}(\mathbf{w}_t) \le \mathscr{L}(\mathbf{w}_{t-1})$ then $\mathscr{L}(\mathbf{w}_T) - \mathscr{L}(\mathbf{w}^\star) \le \frac{r^2}{\eta T} + \frac{\eta\gamma^2}{2}$

Choosing $\eta = r/(\gamma\, T^{1/2})$ gives $\mathscr{L}(\mathbf{w}_T) - \mathscr{L}(\mathbf{w}^\star) \le \frac{2r\gamma}{\sqrt{T}}$

Convergence of GD

Assumptions:

$\|\nabla \mathscr{L}(\mathbf{w})\| \le \gamma$, $\forall t : \|\mathbf{w}_t\| \le r$, $\|\mathbf{w}^\star\| \le r$

$\mathscr{L}(\mathbf{w}_t)$ is monotonically decreasing

Using learning rate of $\eta = r/(\gamma\sqrt{t})$

Then $\mathscr{L}(\mathbf{w}_t)$ converges t to $\mathscr{L}(\mathbf{w}^\star)$ at a rate of $O\left(\gamma\, r\, t^{-1/2}\right)$

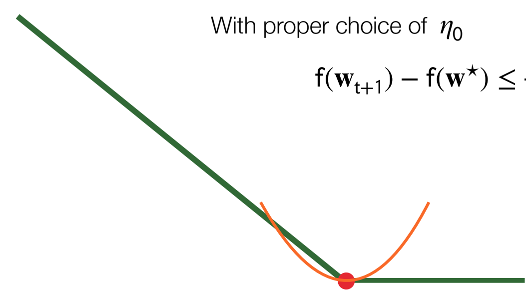
Summary: GD for Convex Losses

Learning rate goes to zero $\eta_0\, t^{-1/2}$

With proper choice of η_0

$$f(\mathbf{w}_{t+1}) - f(\mathbf{w}^\star) \le \frac{\kappa}{\sqrt{t}}$$

problem dependent



Next

When data is prevalent:

Stochastic Gradient Descent (SGD)

Solving multiclass problems with SGD

Beyond GLIM: deep learning