CS260: Machine Learning Algorithms

Lecture 2: Linear regression and classification

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Linear Regression

Regression

- Classification:

  Customer record $\Rightarrow$ Yes/No

- Regression: predicting credit limit

  Customer record $\Rightarrow$ dollar amount

Input

age	23
Annual salary	30,000
Year in residence	1
Year in job	1
...	...

Output

4000

$\mathbf{x}$ $\quad$ $h(\mathbf{x})$

Regression

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Input

age	23
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...	...

Output

4000

x

h(**x**)

Linear Regression: $h(\boldsymbol{x}) = \sum_{i=0}^{d} w_i x_i = \boldsymbol{w}^T \boldsymbol{x}$

The data set

- Training data:

$$(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_N, y_N)$$

$\boldsymbol{x}_n \in \mathbb{R}^d$: feature vector for a sample

$y_n \in \mathbb{R}$: observed output (real number)

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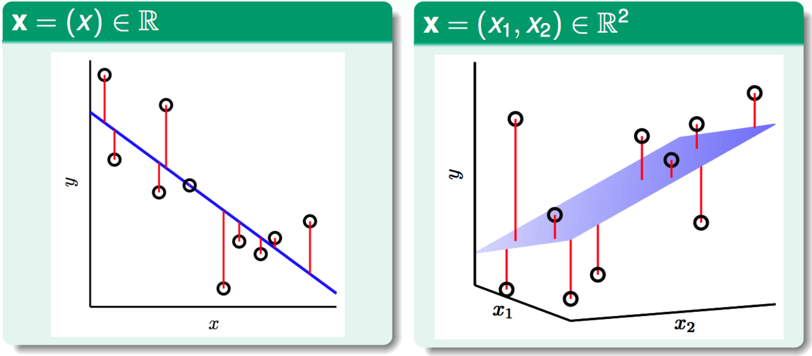
- Linear regression: find a function $h(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x}$ to approximate y
- Measure the error by $(h(\boldsymbol{x}) - y)^2$ (square error)

$$\text{Training error :} E_{\text{train}}(h) = \frac{1}{N} \sum_{n=1}^{N} (h(\boldsymbol{x}_n) - y_n)^2$$

Illustration



Linear regression: find linear function with small residual

Matrix form of E_{train}

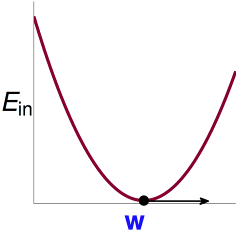
$$\begin{aligned}
E_{\text{train}}(\mathbf{w}) &= \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n^T\mathbf{w} - y_n)^2 \\
&= \frac{1}{N}\left\| \begin{bmatrix} \mathbf{x}_1^T\mathbf{w} - y_1 \\ \mathbf{x}_2^T\mathbf{w} - y_2 \\ \vdots \\ \mathbf{x}_N^T\mathbf{w} - y_N \end{bmatrix} \right\|^2 \\
&= \frac{1}{N}\left\| \begin{bmatrix} -\,-\ \mathbf{x}_1^T\ -\,- \\ -\,-\ \mathbf{x}_2^T\ -\,- \\ \vdots \\ -\,-\ \mathbf{x}_N^T\ -\,- \end{bmatrix} \mathbf{w} - \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \right\|^2 \\
&= \frac{1}{N}\|\underbrace{X}_{N\times d}\mathbf{w} - \underbrace{\mathbf{y}}_{N\times 1}\|^2
\end{aligned}$$

Minimize E_{train}

$$\min_{\boldsymbol{w}} f(\boldsymbol{w}) = \|X\boldsymbol{w} - \mathbf{y}\|^2$$

- E_{train}: continuous, differentiable, convex
- Necessary condition of optimal $\boldsymbol{w}$:

$$\nabla f(\boldsymbol{w}^*) = \begin{bmatrix} \frac{\partial f}{\partial w_0}(\boldsymbol{w}^*) \\ \vdots \\ \frac{\partial f}{\partial w_d}(\boldsymbol{w}^*) \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}$$



Minimizing f

$$f(\boldsymbol{w}) = \|X\boldsymbol{w} - \mathbf{y}\|^2 = \boldsymbol{w}^T X^T X \boldsymbol{w} - 2\boldsymbol{w}^T X^T \mathbf{y} + \mathbf{y}^T \mathbf{y}$$

$$\nabla f(\boldsymbol{w}) = 2(X^T X \boldsymbol{w} - X^T \mathbf{y})$$

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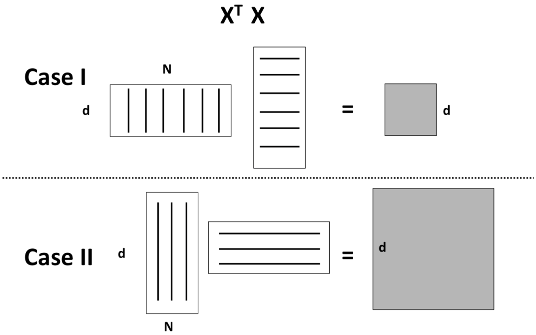
$$\Rightarrow \boldsymbol{w}^* = (X^T X)^{-1} X^T \mathbf{y} \quad ??$$

More on Linear Regression Solutions

- Case I: $X^T X$ is invertible $\Rightarrow$ Unique solution
  - Often when $N > d$
  - Yes, $\boldsymbol{w}^* = (X^T X)^{-1} X^T \mathbf{y}$
- Case II: $X^T X$ is non-invertible $\Rightarrow$ Many solutions
  - Often when $d > N$



Linear System Solver

- A "linear system":

$$\text{Find the minimum 2-norm solution of } \min_{\boldsymbol{w}} \|X\boldsymbol{w} - \mathbf{y}\|$$

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- Let $X = U\Sigma V^T$ be the Singular Value Decomposition (SVD) of X:
  - U: $m \times m$ orthonormal matrix ($U^T U = I$)
  - V: $n \times n$ orthonormal matrix ($V^T V = I$)
  - $\Sigma = \text{diag}[\sigma_1, \sigma_2, \cdots, \sigma_r, 0, \cdots, 0]$ $(\sigma_1, \cdots, \sigma_r > 0)$
  - Solution:

$$\boldsymbol{w}^+ = X^+\mathbf{y},$$

where $X^+ = V\Sigma^+U^T$, $\Sigma^+ = \text{diag}[1/\sigma_1, 1/\sigma_2, \cdots, 1/\sigma_r, 0, \cdots, 0]$

Linear System Solver

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    ($\sigma_1, \cdots, \sigma_r > 0$)
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    where $X^+ = V\Sigma^+U^T$, $\Sigma^+ = \text{diag}[1/\sigma_1, 1/\sigma_2, \cdots, 1/\sigma_r, 0, \cdots, 0]$
  - X^+: pseudo-inverse of X

Why? (details in lecture note)

- Show $X^+\mathbf{y}$ satisfies the normal equation

- Is this the minimum 2-norm solution?

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  Overall complexity: $O(d^2 N + d^3)$

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- What if $d, N \approx$ millions?

  (use iterative algorithms, next class)

Logistic Regression

Binary Classification

- Input: training data $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n \in \mathbb{R}^d$ and corresponding outputs $y_1, y_2, \ldots, y_n \in \{+1, -1\}$
- Training: compute a function f such that $\text{sign}(f(\boldsymbol{x}_i)) \approx y_i$ for all i
- Prediction: given a testing sample $\tilde{\boldsymbol{x}}$, predict the output as $\text{sign}(f(\tilde{\boldsymbol{x}}))$

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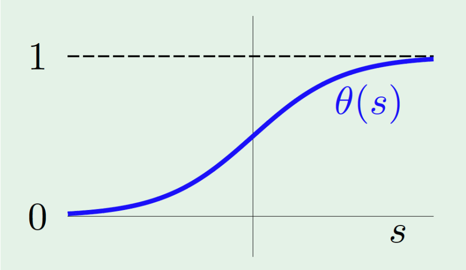
where $\theta(s) = \frac{e^s}{1+e^s} = \frac{1}{1+e^{-s}}$



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- Therefore, $P(y \mid \boldsymbol{x}) = \theta(y\boldsymbol{w}^T\boldsymbol{x})$

Maximizing the likelihood

- Likelihood of $\mathcal{D} = (\boldsymbol{x}_1, y_1), \cdots, (\boldsymbol{x}_N, y_N)$:

$$\Pi_{n=1}^{N} P(y_n \mid \boldsymbol{x}_n) = \Pi_{n=1}^{N} \theta(y_n \boldsymbol{w}^T \boldsymbol{x}_n)$$

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- Find $\boldsymbol{w}$ to maximize the likelihood!

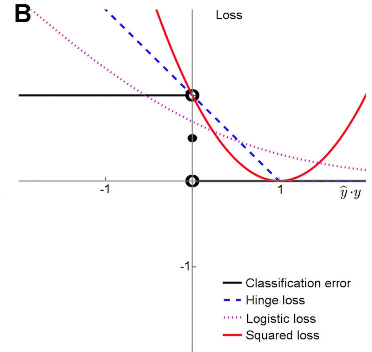
$$\begin{aligned}
&\max_{\boldsymbol{w}} \Pi_{n=1}^{N} \theta(y_n \boldsymbol{w}^T \boldsymbol{x}_n) \\
\Leftrightarrow &\max_{\boldsymbol{w}} \log(\Pi_{n=1}^{N} \theta(y_n \boldsymbol{w}^T \boldsymbol{x}_n)) \\
\Leftrightarrow &\min_{\boldsymbol{w}} -\sum_{n=1}^{N} \log(\theta(y_n \boldsymbol{w}^T \boldsymbol{x}_n)) \\
\Leftrightarrow &\min_{\boldsymbol{w}} \sum_{n=1}^{N} \log(1 + e^{-y_n \boldsymbol{w}^T \boldsymbol{x}_n})
\end{aligned}$$

Empirical Risk Minimization (linear)

- Linear classification/regression:

$$\min_{\boldsymbol{w}} \frac{1}{N}\sum_{n=1}^{N} \text{loss}(\underbrace{\boldsymbol{w}^T\boldsymbol{x}_n}_{\hat{y}_n\text{:the predicted score}}, y_n)$$

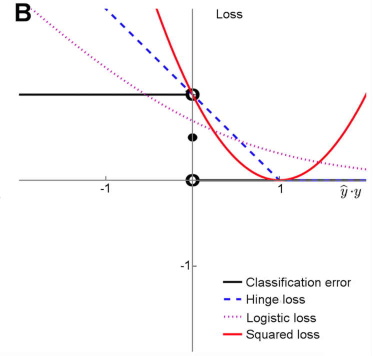
  - Linear regression: $\text{loss}(h(\boldsymbol{x}_n), y_n) = (\boldsymbol{w}^T\boldsymbol{x}_n - y_n)^2$
  - Logistic regression: $\text{loss}(h(\boldsymbol{x}_n), y_n) = \log(1 + e^{-y_n\boldsymbol{w}^T\boldsymbol{x}_n})$



(Linear) Support Vector Machines

- Replace the logistic loss by hinge loss:

$$\min_{\boldsymbol{w}} \frac{1}{N} \sum_{n=1}^{N} \max(0, 1 - y_n \boldsymbol{w}^T \boldsymbol{x}_n)$$



Empirical Risk Minimization (general)

- Assume $f_W(\boldsymbol{x})$ is the decision function to be learned (W is the parameters of the function)
- General empirical risk minimization:

$$\min_{W} \frac{1}{N} \sum_{n=1}^{N} \text{loss}(f_W(\boldsymbol{x}_n), y_n)$$

- Example: Neural network ($f_W(\cdot)$ is the network)

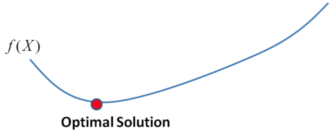
Gradient descent and SGD

Optimization

- Goal: find the minimizer of a function

$$\min_{\boldsymbol{w}} f(\boldsymbol{w})$$

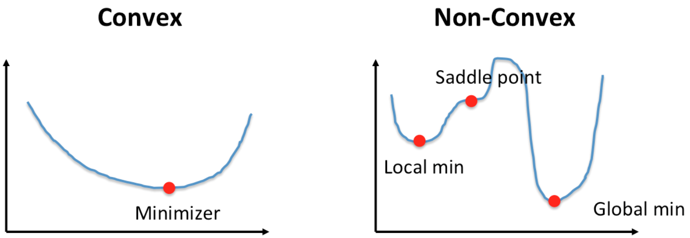
For now we assume f is twice differentiable



Convex vs Nonconvex

- Convex function:
  - $\nabla f(\boldsymbol{x}) = 0 \Leftrightarrow$ Global minimum
  - A function is convex if $\nabla^2 f(\boldsymbol{x})$ is positive definite
  - Example: linear regression, logistic regression, $\cdots$
- Non-convex function:
  - $\nabla f(\boldsymbol{x}) = 0 \Leftrightarrow$ Global min, local min, or saddle point

    most algorithms only converge to gradient$= 0$
  - Example: neural network, $\cdots$



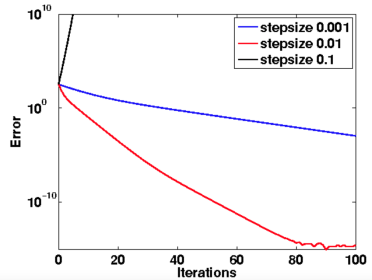
Gradient Descent

- Gradient descent: repeatedly do

$$\boldsymbol{w}^{t+1} \leftarrow \boldsymbol{w}^{t} - \alpha \nabla f(\boldsymbol{w}^{t})$$

  $\alpha > 0$ is the step size

- Step size too large $\Rightarrow$ diverge; too small $\Rightarrow$ slow convergence



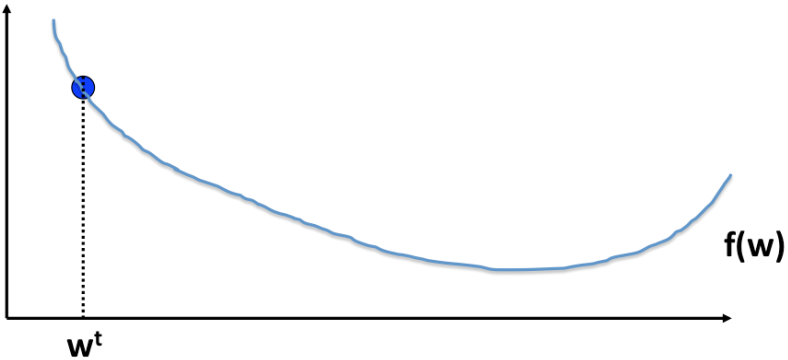
Why gradient descent?

- At each iteration, form an approximation function of $f(\cdot)$:

$$f(\boldsymbol{w} + \boldsymbol{d}) \approx g(\boldsymbol{d}) := f(\boldsymbol{w}^t) + \nabla f(\boldsymbol{w}^t)^T \boldsymbol{d} + \frac{1}{2\alpha}\|\boldsymbol{d}\|^2$$

- Update solution by $\boldsymbol{w}^{t+1} \leftarrow \boldsymbol{w}^t + \boldsymbol{d}^*$
- $\boldsymbol{d}^* = \arg\min_{\boldsymbol{d}} g(\boldsymbol{d})$
  $\nabla g(\boldsymbol{d}^*) = 0 \Rightarrow \nabla f(\boldsymbol{w}^t) + \frac{1}{\alpha}\boldsymbol{d}^* = 0 \Rightarrow \boldsymbol{d}^* = -\alpha \nabla f(\boldsymbol{w}^t)$
- $\boldsymbol{d}^*$ will decrease $f(\cdot)$ if α (step size) is sufficiently small

Illustration of gradient descent



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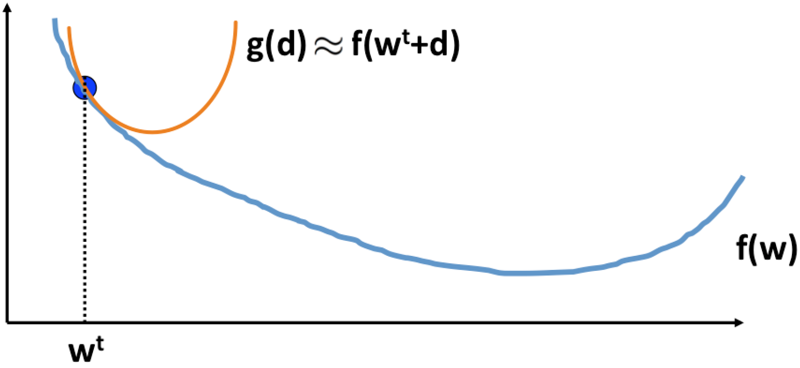

Form a quadratic approximation

$$f(\boldsymbol{w}^t + \boldsymbol{d}) \approx g(\boldsymbol{d}) = f(\boldsymbol{w}^t) + \nabla f(\boldsymbol{w}^t)^T \boldsymbol{d} + \frac{1}{2\alpha}\|\boldsymbol{d}\|^2$$

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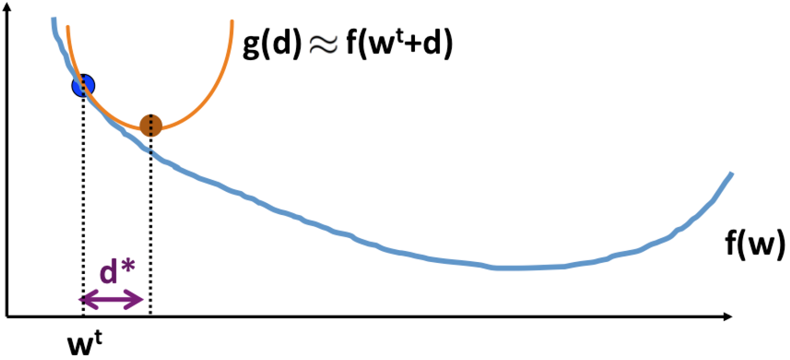

Minimize $g(\boldsymbol{d})$:

$$\nabla g(\boldsymbol{d}^*) = 0 \Rightarrow \nabla f(\boldsymbol{w}^t) + \frac{1}{\alpha}\boldsymbol{d}^* = 0 \Rightarrow \boldsymbol{d}^* = -\alpha \nabla f(\boldsymbol{w}^t)$$

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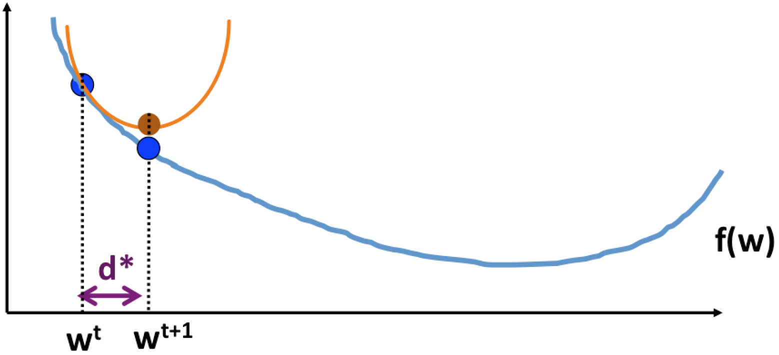

Update $\boldsymbol{w}$:

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^{t} + \boldsymbol{d}^{*} = \boldsymbol{w}^{t} - \alpha \nabla f(\boldsymbol{w}^{t})$$

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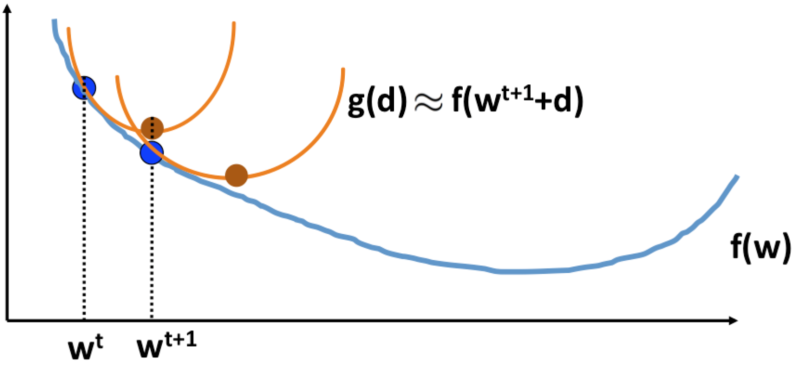

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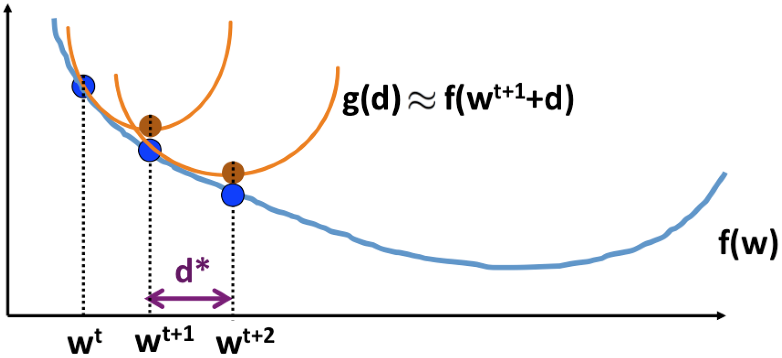

Convergence

- Let L be a constant such that $\nabla^2 f(\boldsymbol{x}) \preceq LI$ for all $\boldsymbol{x}$
- **Theorem:** gradient descent converges if $\alpha < \frac{1}{L}$
- In practice, we do not know $L \cdots$

  need to tune step size when running gradient descent

Applying to Logistic regression

gradient descent for logistic regression

- Initialize the weights $\boldsymbol{w}_0$
- For $t = 1, 2, \cdots$
  - Compute the gradient

$$\nabla f(\boldsymbol{w}) = -\frac{1}{N}\sum_{n=1}^{N} \frac{y_n \boldsymbol{x}_n}{1 + e^{y_n \boldsymbol{w}^T \boldsymbol{x}_n}}$$

  - Update the weights: $\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \nabla f(\boldsymbol{w})$
- Return the final weights $\boldsymbol{w}$

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When to stop?

- Fixed number of iterations, or
- Stop when $\|\nabla f(\boldsymbol{w})\| < \epsilon$

Conclusions

- Linear regression:
  - Square loss $\Rightarrow$ solving a linear system
  - Closed form solution
- Logistic regression:
  - A classification model based on a probability assumption
- Gradient descent: an iterative solver

Questions?