15-830 – Machine Learning 1: Linear Regression

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Motivation

- How much energy will we consume tommorrow?
  - Difficult to estimate from "a priori" models
  - But, we have lots of data from which to build a model

Energy 101

- Energy: "ability to do work" (apply force through a distance)
- Unit of energy: joule (J), (also btu, kilowatt hour)

$$\begin{aligned} 1 \text{ joule} &= 1 \text{ newton} \cdot 1 \text{ meter} \\ &= \frac{1 \text{ kilogram} \cdot 1 \text{ meter}^2}{1 \text{ second}^2} \end{aligned}$$

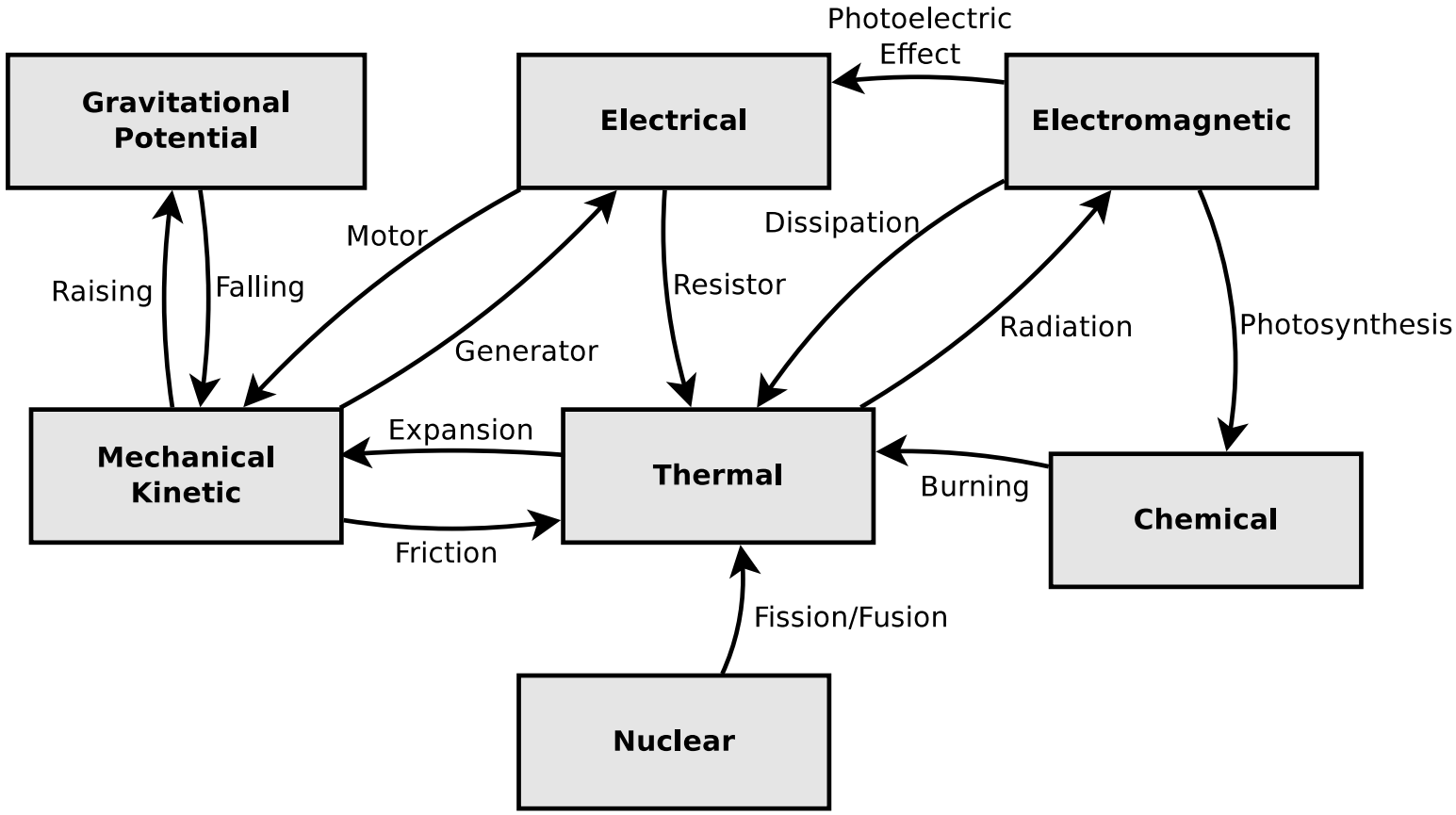
- Power is a *rate* of energy use
- Unit of power: watt (W) (commonly kilo/mega/gigawatt)

$$1 \text{ watt} = \frac{1 \text{ joule}}{1 \text{ second}}$$

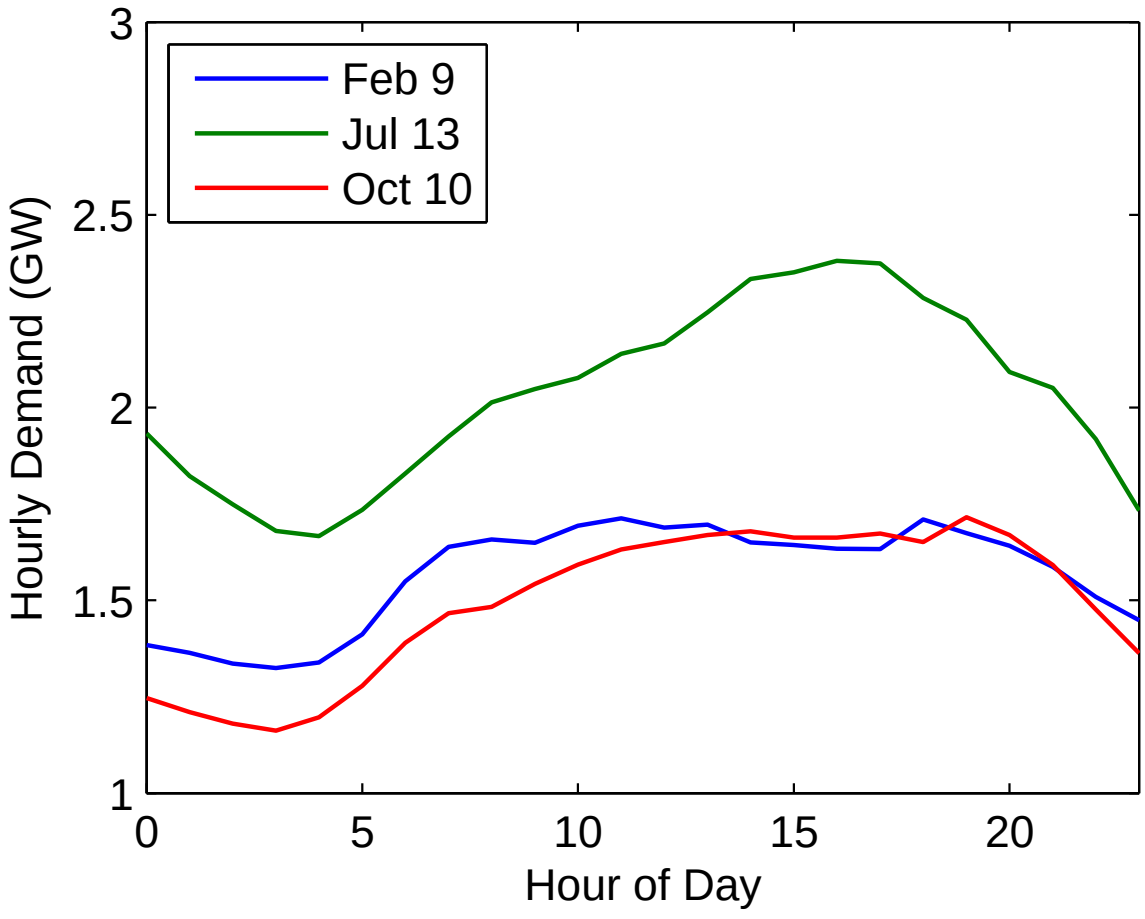
Forms of energy

- Mechanical kinetic energy: $E = \frac{1}{2}mv^2$
- Gravitational potential energy: $E = mgh$
- Thermal energy: $E = \frac{3}{2}NkT$
- Electrical energy: $E = VQ$
- Electromagnetic energy: $E = hf$
- Chemical energy
- Nuclear energy: $E = mc^2$

Energy conversion

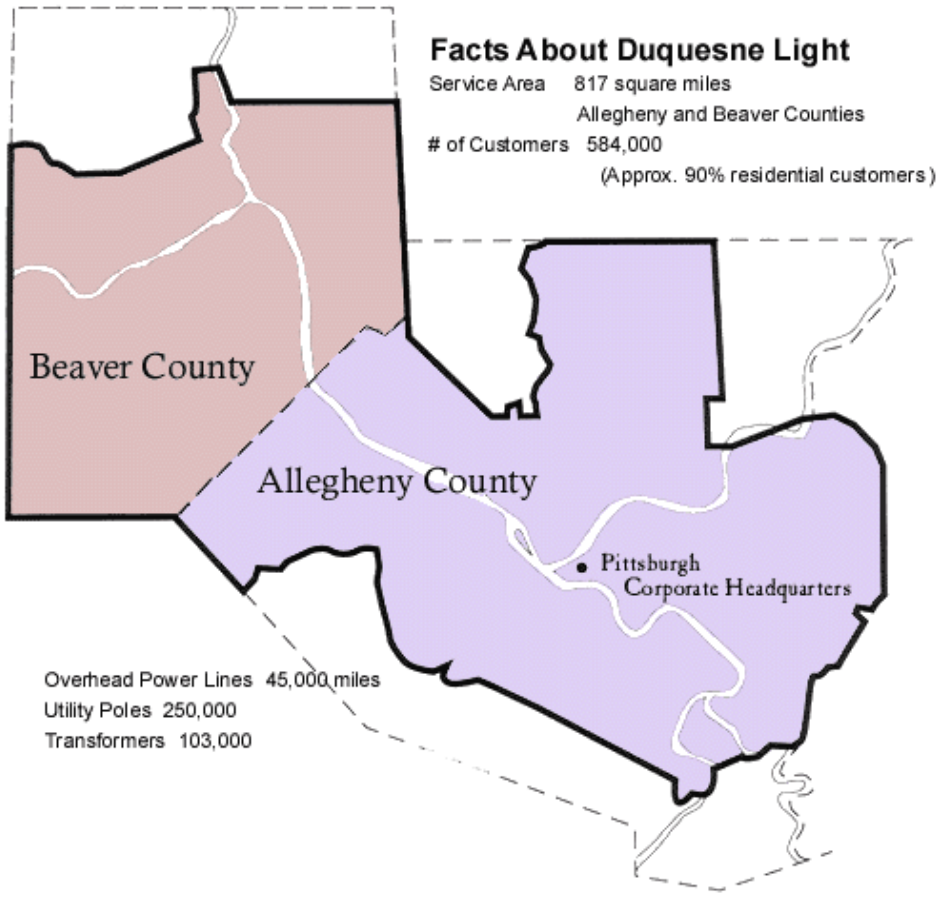


Duquesne Light electricity consumption



Data: PJM `http://www.pjm.com`

Duquesne Light electricity consumption

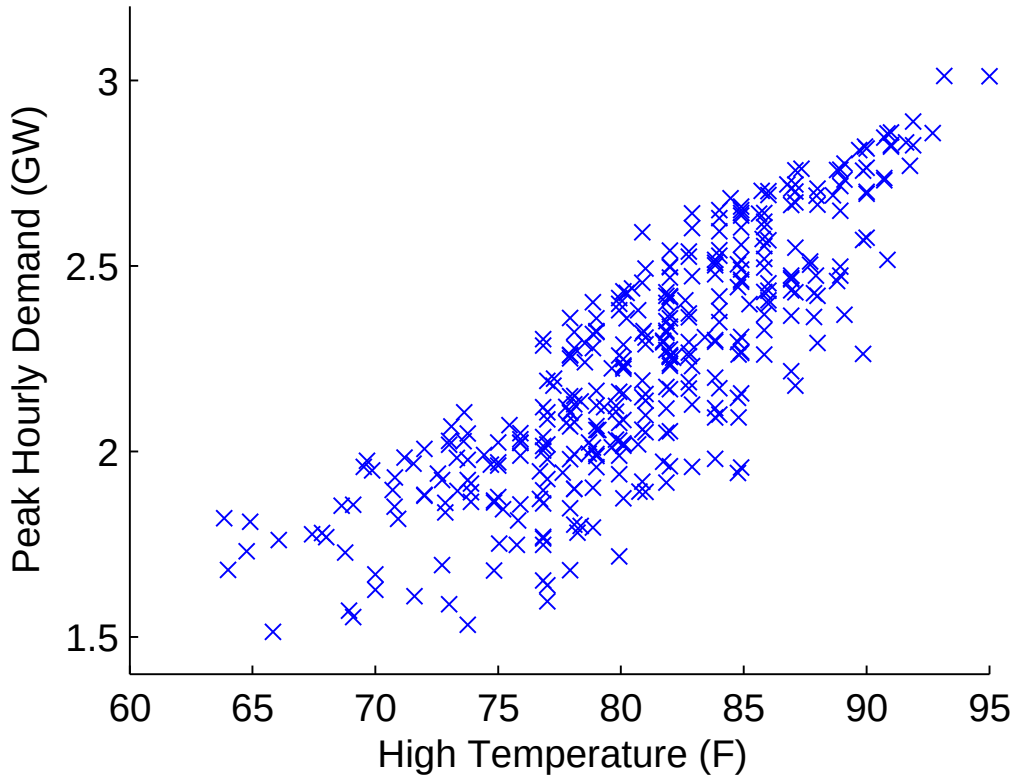


Source: Duquesne Light `http://www.duquesnelight.com`

Predict peak demand from high temperature

- What will peak demand be tomorrow?

- If we know something else about tomorrow (like the high temperature), we can use this to *predict* peak demand

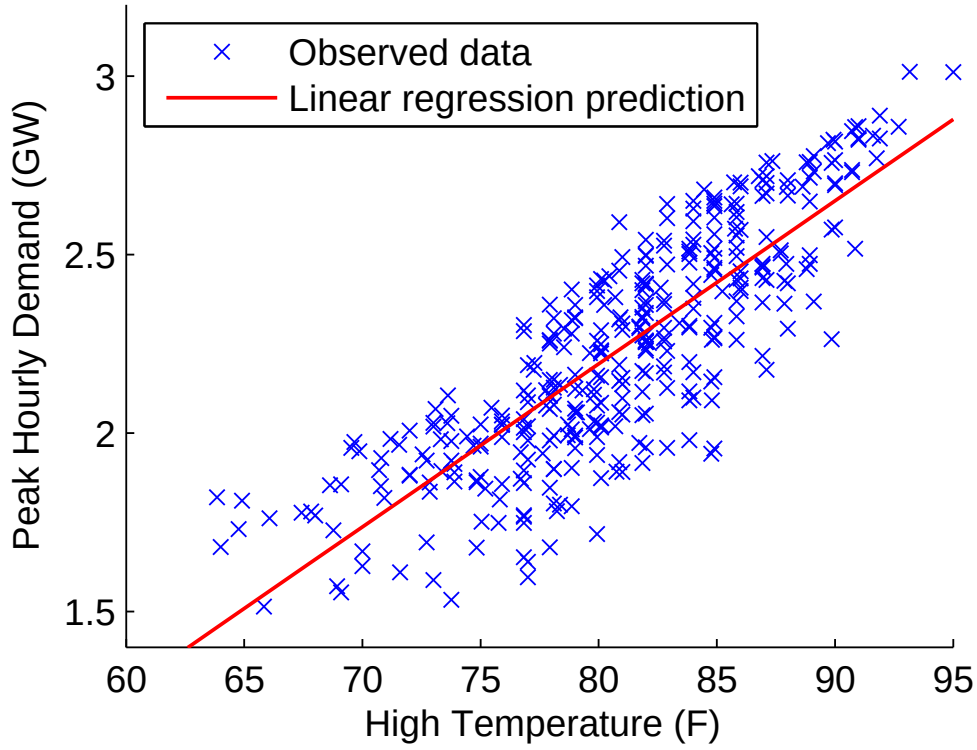


Data: PJM, Weather Underground (summer months, June-August)

A simple model

- A linear model that predicts demand:

$$\text{predicted peak demand} = \theta_1 \cdot (\text{high temperature}) + \theta_2$$



- *Parameters* of model: $\theta_1, \theta_2 \in \mathbb{R}$ $(\theta_1 = 0.046,\ \theta_2 = -1.46)$

A simple model

- We can use a model like this to make predictions
- What will be the peak demand for Duquense Light tomorrow?
  - I know from weather report that high temperature will be $80°$F (ignore, for the moment, that this too is a prediction)
- Then predicted peak demand is:

$$\theta_1 \cdot 80 + \theta_2 = 0.046 \cdot 80 - 1.46 = 2.19 \text{ GW}$$

Formal problem setting

- **Input**: $x_i \in \mathbb{R}^n, \;\; i = 1, \ldots, m$
  - E.g.: $x_i \in \mathbb{R}^1 = \{\text{high temperature for day } i\}$
- **Output**: $y_i \in \mathbb{R}$ (*regression* task)
  - E.g.: $y_i \in \mathbb{R} = \{\text{peak demand for day } i\}$
- **Model Parameters**: $\theta \in \mathbb{R}^k$
- **Predicted Output**: $\hat{y}_i \in \mathbb{R}$

$$\text{E.g.:} \;\; \hat{y}_i = \theta_1 \cdot x_i + \theta_2$$

- For convenience, we define a function that maps inputs to *feature vectors*

$$\phi : \mathbb{R}^n \to \mathbb{R}^k$$

- For example, in our task above, if we define

$$\phi(x_i) = \begin{bmatrix} x_i \\ 1 \end{bmatrix} \quad \text{(here } n = 1, \, k = 2\text{)}$$

  then we can write

$$\hat{y}_i = \sum_{j=1}^{k} \theta_j \cdot \phi_j(x_i) \equiv \theta^T \phi(x_i)$$

Loss functions

- Want a model that performs "well" on the data we have

$$\text{I.e., } \hat{y}_i \approx y_i, \quad \forall i$$

- We measure "closeness" of $\hat{y}_i$ and y_i using *loss function*

$$\ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R}_+$$

- Example: squared loss

$$\ell(\hat{y}_i, y_i) = (\hat{y}_i - y_i)^2$$

Finding model parameters, and optimization

- Want to find model parameters such that minimize sum of costs over all input/output pairs

$$J(\theta) = \sum_{i=1}^{m} \ell(\hat{y}_i, y_i) = \sum_{i=1}^{m} (\theta^T \phi(x_i) - y_i)^2$$

- Write our objective formally as

$$\underset{\theta}{\text{minimize}} \quad J(\theta)$$

simple example of an *optimization problem*; these will dominate our development of algorithms throughout the course

- Let's write $J(\theta)$ a little more compactly using matrix notation; define

$$\Phi \in \mathbb{R}^{m \times k} = \begin{bmatrix} — & \phi(x_1)^T & — \\ — & \phi(x_2)^T & — \\ & \vdots & \\ — & \phi(x_m)^T & — \end{bmatrix}, \quad y \in \mathbb{R}^m = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

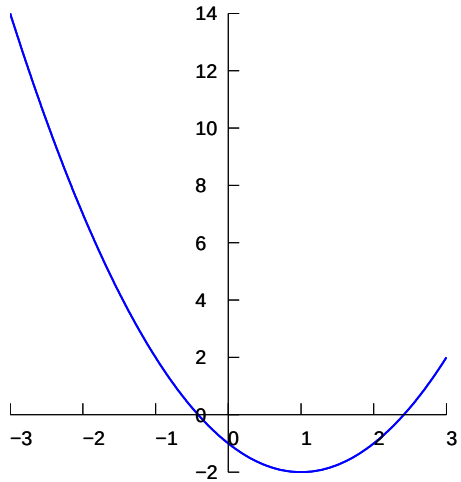
then

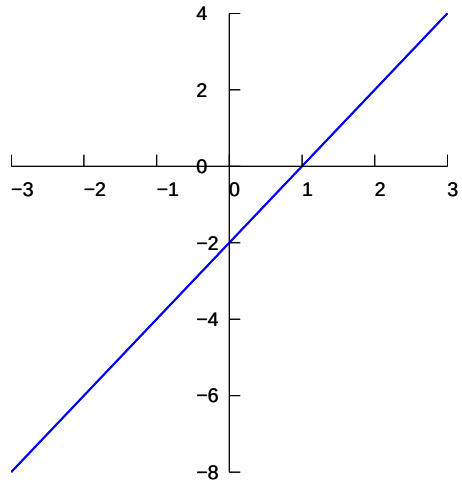
$$J(\theta) = \sum_{i=1}^{m} (\theta^T \phi(x_i) - y_i)^2 = \|\Phi\theta - y\|_2^2$$

($\|z\|_2$ is ℓ_2 norm of a vector: $\|z\|_2 \equiv \sqrt{\sum_{i=1}^{n} z_i^2} = \sqrt{z^T z}$)

- Called *least-squares* objective function

- How do we optimize a function? 1-D case ($\theta \in \mathbb{R}$):





$$J(\theta) = \theta^2 - 2\theta - 1 \qquad \frac{dJ}{d\theta} = 2\theta - 2$$

$$\begin{aligned} \theta^\star \text{ minimum} &\iff \left.\frac{dJ}{d\theta}\right|_{\theta^\star} = 0 \\ &\iff 2\theta^\star - 2 = 0 \\ &\iff \theta^\star = 1 \end{aligned}$$

- Multi-variate case: $\theta \in \mathbb{R}^k$, $J : \mathbb{R}^k \to \mathbb{R}$

$$\text{Generalized condition:} \quad \nabla_\theta J(\theta)|_{\theta^\star} = 0$$

- $\nabla_\theta J(\theta)$ denotes *gradient* of J with respect to θ

$$\nabla_\theta J(\theta) \in \mathbb{R}^n \equiv \begin{bmatrix} \frac{\partial J}{\partial \theta_1} \\ \frac{\partial J}{\partial \theta_2} \\ \vdots \\ \frac{\partial J}{\partial \theta_k} \end{bmatrix}$$

- Some important rules and common gradient

$$\nabla_\theta(af(\theta) + bg(\theta)) = a\nabla_\theta f(\theta) + b\nabla_\theta g(\theta), \quad (a, b \in \mathbb{R})$$
$$\nabla_\theta(\theta^T A\theta) = (A + A^T)\theta, \quad (A \in \mathbb{R}^{k\times k})$$
$$\nabla_\theta(b^T\theta) = b, \quad (b \in \mathbb{R}^k)$$

- Optimizing least-squares objective

$$\begin{aligned} J(\theta) &= \|\Phi\theta - y\|_2^2 \\ &= (\Phi\theta - y)^T(\Phi\theta - y) \\ &= \theta^T\Phi^T\Phi\theta - 2y^T\Phi\theta + y^Ty \end{aligned}$$

- Using the previous gradient rules

$$\begin{aligned} \nabla_\theta J(\theta) &= \nabla_\theta(\theta^T\Phi^T\Phi\theta - 2y^T\Phi\theta + y^Ty) \\ &= \nabla_\theta(\theta^T\Phi^T\Phi\theta) - 2\nabla_\theta(y^T\Phi\theta) + \nabla_\theta(y^Ty) \\ &= 2\Phi^T\Phi\theta - 2\Phi^Ty \end{aligned}$$

- Setting gradient equal to zero

$$2\Phi^T\Phi\theta^\star - 2\Phi^Ty = 0 \iff \theta^\star = (\Phi^T\Phi)^{-1}\Phi^Ty$$

known as the *normal equations*

- Let's see how this looks in MATLAB code

```
X = load('high_temperature.txt');
y = load('peak_demand.txt');
n = size(X,2);
m = size(X,1);
Phi = [X ones(m,1)];
theta = inv(Phi' * Phi) * Phi' * y;

theta =
    0.0466
   -1.4600
```

- The normal equations are so common that MATLAB has a special operation for them

```
% same as inv(Phi' * Phi) * Phi' * y
theta = Phi \ y;
```

Aside: general optimization problems

- In this class we'll consider general optimization problems

$$\begin{aligned} \underset{\theta}{\text{minimize}} \;\; & J(\theta) \\ \text{subject to} \;\; & g_i(\theta) \leq 0, \quad i = 1, \ldots, N_i \\ & h_i(\theta) = 0, \quad i = 1, \ldots, N_e \end{aligned}$$

  A *constrained* optimization problem; g_i terms are the inequality constraints; h_i terms are the equality constraints.

- Many different classifications of optimization problems (linear programming, quadratic programming, semidefinite programming, integer programming), depending on the form of J, the g_i's and the h_i's.

- Important distinctions in optimization is between *convex* (where J, g_i are convex and h_i linear) and *non-convex* problems

$$f \text{ convex} \Longleftrightarrow f(a\theta + (1-a)\theta') \leq af(\theta) + (1-a)f(\theta')$$

$$\text{for } 0 \leq a \leq 1$$

- Informally speaking, we can usually find *global* solutions of convex problems efficiently, while for non-convex problems we must settle for *local* solutions or time-consuming optimization

Solving optimization problems

- Many generic optimization libraries
- We will be using YALMIP (Yet Another Linear Matrix Inequality Parser): `http://users.isy.liu.se/johanl/yalmip/`
- YALMIP code for least squares optimization:

```
theta = sdpvar(n,1);
solvesdp([], sum((Phi*theta - y).^2));
double(theta)

ans =
    0.0466
   -1.4600
```

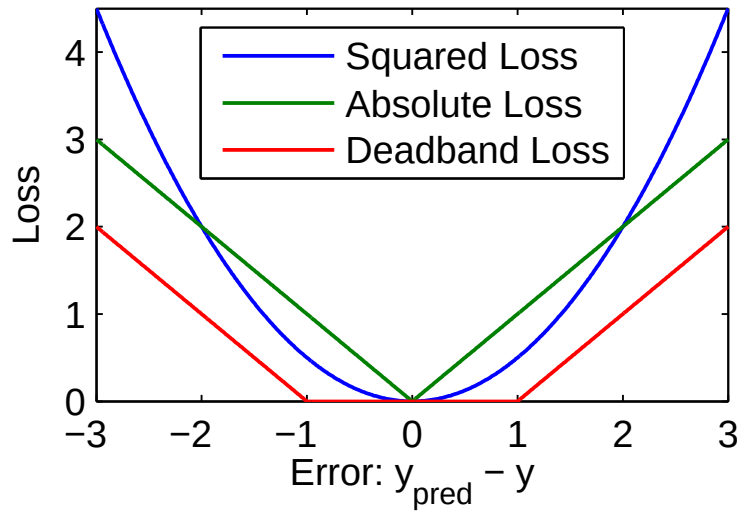
Alternative loss functions

- Nothing special about least-squares loss function $\ell(\hat{y}, y) = (\hat{y} - y)^2$.

- Some alternatives:

$$\text{Absolute loss:} \quad \ell(\hat{y}, y) = |\hat{y} - y|$$

$$\text{Deadband loss:} \quad \ell(\hat{y}, y) = \max\{0, |\hat{y} - y| - \epsilon\}, \ \epsilon \in \mathbb{R}_+$$



- How do we find parameters that minimize absolute loss?

$$\underset{\theta}{\text{minimize}} \quad \sum_{i=1}^{m} |\theta^T \phi(x_i) - y_i|$$

  - Non-differentiable, can't take gradient

- Solution: frame as a *constrained optimization problem*
  - Introduce new variables $\nu \in \mathbb{R}^m$, $(\nu_i \geq |\theta^T \phi(x_i) - y_i|)$

$$\begin{aligned} \underset{\theta,\nu}{\text{minimize}} \quad & \sum_{i=1}^{m} \nu_i \\ \text{subject to} \quad & -\nu_i \leq \theta^T \phi(x_i) - y_i \leq \nu_i \end{aligned}$$

- *Linear program* (LP): linear object and linear constraints

- To solve LPs, typically need to put them in standard form:

$$\begin{aligned} &\underset{z}{\text{minimize}} && c^T z \\ &\text{subject to} && Az \leq b \end{aligned}$$

  - $z \in \mathbb{R}^n$, $A \in \mathbb{R}^{N_i \times n}$, $b \in \mathbb{R}^{N_i}$

- For absolute loss LP

$$z = \begin{bmatrix} \theta \\ \nu \end{bmatrix}, \quad c = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad A = \begin{bmatrix} \Phi & -I \\ -\Phi & -I \end{bmatrix}, \quad b = \begin{bmatrix} y \\ -y \end{bmatrix}$$

- MATLAB code

```
c = [zeros(n,1); ones(m,1)];
A = [Phi -eye(m); -Phi -eye(m)];
b = [y; -y];
z = linprog(c,A,b);
theta = z(1:n)

theta =
    0.0477
   -1.5978
```

- The same solution in YALMIP:

```
theta = sdpvar(n,1);
solvesdp([], sum(abs((Phi*theta - y))));
double(theta)

theta =
    0.0477
   -1.5978
```

- Which loss function should we use?