Conjugate Gradient Method

- direct and indirect methods
- positive definite linear systems
- Krylov sequence
- derivation of the Conjugate Gradient Method
- spectral analysis of Krylov sequence
- preconditioning

Three classes of methods for linear equations

methods to solve linear system $Ax = b$, $A \in \mathbf{R}^{n \times n}$

- **dense direct** (factor-solve methods)
  - runtime depends only on size; independent of data, structure, or sparsity
  - work well for n up to a few thousand

- **sparse direct** (factor-solve methods)
  - runtime depends on size, sparsity pattern; (almost) independent of data
  - can work well for n up to 10^4 or 10^5 (or more)
  - requires good heuristic for ordering

- **indirect** (iterative methods)
  - runtime depends on data, size, sparsity, required accuracy
  - requires tuning, preconditioning, . . .
  - good choice in many cases; only choice for $n = 10^6$ or larger

Symmetric positive definite linear systems

SPD system of equations

$$Ax = b, \qquad A \in \mathbf{R}^{n \times n}, \qquad A = A^T \succ 0$$

examples

- Newton/interior-point search direction: $\nabla^2 \phi(x) \Delta x = -\nabla \phi(x)$
- least-squares normal equations: $(A^T A)x = A^T b$
- regularized least-squares: $(A^T A + \mu I)x = A^T b$
- minimization of convex quadratic function $(1/2)x^T Ax - b^T x$
- solving (discretized) elliptic PDE ($e.g.$, Poisson equation)

- analysis of resistor circuit: $Gv = i$
  - v is node voltage (vector), i is (given) source current
  - G is circuit conductance matrix

$$G_{ij} = \begin{cases} \text{total conductance incident on node } i & i = j \\ -(\text{conductance between nodes } i \text{ and } j) & i \neq j \end{cases}$$

CG overview

- proposed by Hestenes and Stiefel in 1952 (as direct method)
- solves SPD system $Ax = b$
  - in theory ($i.e.$, exact arithmetic) in n iterations
  - each iteration requires a few inner products in $\mathbf{R}^n$, and one matrix-vector multiply $z \rightarrow Az$
- for A dense, matrix-vector multiply $z \rightarrow Az$ costs n^2, so total cost is n^3, same as direct methods
- get advantage over dense if matrix-vector multiply is cheaper than n^2
- with roundoff error, CG can work poorly (or not at all)
- but for some A (and b), can get good approximate solution in $\ll n$ iterations

Solution and error

- $x^\star = A^{-1}b$ is solution
- $x^\star$ minimizes (convex function) $f(x) = (1/2)x^TAx - b^Tx$
- $\nabla f(x) = Ax - b$ is gradient of f
- with $f^\star = f(x^\star)$, we have

$$\begin{aligned} f(x) - f^\star &= (1/2)x^TAx - b^Tx - (1/2)x^{\star T}Ax^\star + b^Tx^\star \\ &= (1/2)(x - x^\star)^TA(x - x^\star) \\ &= (1/2)\|x - x^\star\|_A^2 \end{aligned}$$

i.e., $f(x) - f^\star$ is half of squared A-norm of error $x - x^\star$

- a relative measure (comparing x to 0):

$$\tau = \frac{f(x) - f^\star}{f(0) - f^\star} = \frac{\|x - x^\star\|_A^2}{\|x^\star\|_A^2}$$

(fraction of maximum possible reduction in f, compared to $x = 0$)

Residual

- $r = b - Ax$ is called the **residual** at x
- $r = -\nabla f(x) = A(x^\star - x)$
- in terms of r, we have

$$\begin{aligned} f(x) - f^\star &= (1/2)(x - x^\star)^T A(x - x^\star) \\ &= (1/2) r^T A^{-1} r \\ &= (1/2)\|r\|_{A^{-1}}^2 \end{aligned}$$

- a commonly used measure of relative accuracy: $\eta = \|r\|/\|b\|$
- $\tau \leq \kappa(A)\eta^2$ (η is easily computable from x; τ is not)

Krylov subspace

(a.k.a. controllability subspace)

$$\begin{aligned} \mathcal{K}_k &= \operatorname{span}\{b, Ab, \ldots, A^{k-1}b\} \\ &= \{p(A)b \mid p \text{ polynomial}, \ \deg p < k\} \end{aligned}$$

we define the *Krylov sequence* $x^{(1)}, x^{(2)}, \ldots$ as

$$x^{(k)} = \operatorname*{argmin}_{x \in \mathcal{K}_k} \ f(x) = \operatorname*{argmin}_{x \in \mathcal{K}_k} \ \|x - x^\star\|_A^2$$

the CG algorithm (among others) generates the Krylov sequence

Properties of Krylov sequence

- $f(x^{(k+1)}) \leq f(x^{(k)})$ (but $\|r\|$ can increase)
- $x^{(n)} = x^\star$ ($i.e.$, $x^\star \in \mathcal{K}_n$ even when $\mathcal{K}_n \neq \mathbf{R}^n$)
- $x^{(k)} = p_k(A)b$, where p_k is a polynomial with $\deg p_k < k$
- less obvious: there is a *two-term recurrence*

$$x^{(k+1)} = x^{(k)} + \alpha_k r^{(k)} + \beta_k (x^{(k)} - x^{(k-1)})$$

  for some α_k, β_k (basis of CG algorithm)

Cayley-Hamilton theorem

characteristic polynomial of A:

$$\chi(s) = \det(sI - A) = s^n + \alpha_1 s^{n-1} + \cdots + \alpha_n$$

by Caley-Hamilton theorem

$$\chi(A) = A^n + \alpha_1 A^{n-1} + \cdots + \alpha_n I = 0$$

and so

$$A^{-1} = -(1/\alpha_n)A^{n-1} - (\alpha_1/\alpha_n)A^{n-2} - \cdots - (\alpha_{n-1}/\alpha_n)I$$

in particular, we see that $x^\star = A^{-1}b \in \mathcal{K}_n$

Deriving the Conjugate Gradient Method

- suppose $\{d_0, ..., d_{k-1}\}$ is an orthogonal basis for $\mathcal{K}_k$ under the $A-$inner product, i.e., $(d_i)^T A d_j = 0 \, \forall i \neq j$

- let $x^{(k)} = \sum_{i=0}^{k-1} \alpha_i d_i$

$$\begin{aligned} f(x^{(k)}) &= \frac{1}{2}(x^{(k)})^T A x^{(k)} - b^T x^{(k)} \\ &= \frac{1}{2}\Big(\sum_{i=0}^{k-1} \alpha_i d_i\Big) A \Big(\sum_{i=0}^{k-1} \alpha_i d_i\Big) - b^T \Big(\sum_{i=0}^{k-1} \alpha_i d_i\Big) \\ &= \frac{1}{2}\sum_{i=0}^{k-1} \alpha_i^2 (d_i)^T A d_i - \alpha_i b^T d_i \end{aligned}$$

- decomposable problem, optimal $\alpha_i^* = b^T d_i / \|d_i\|_A^2 \, \forall i$

Constructing the basis (slow)

- suppose $\{d_0, ..., d_{k-1}\}$ is an orthogonal basis for $\mathcal{K}_k$
- extend $\{d_0, ..., d_{k-1}\}$ to a basis of $\mathcal{K}_{k+1}$ using Gram-Schmidt procedure

$$d^k = g - \sum_{j=0}^{k-1} d_j \frac{(d_j)^T A g}{(d_j)^T A d_j}$$

- where we can pick any $g \in \mathcal{K}_{k+1}$ such that $g \notin \mathcal{K}_k$, e.g., $g = A^k b$
- after constructing the basis, set $x^{(k)} = \sum_{j=0}^{k-1} \alpha_j^* d_j = \sum_{j=0}^{k} \frac{b^T d_j}{(d_j)^T A d_j} d_j$
- Conjugate Gradient method constructs the basis online by picking $g := -\nabla f(x^{(k)}) = b - Ax^{(k)}$

Simplifying Gram-Schmidt procedure

- initialize at $x^{(0)} = 0$

$$d_0 = -\nabla f(x^{(k)}) = b - Ax^{(0)} = b$$

$$d_1 = (b - Ax^{(1)}) - d_0 \frac{(d^0)^T A(b - Ax^{(1)})}{(d_0)^T A d_0}$$

$$d_2 = (b - Ax^{(2)}) - d_1 \frac{(d_1)^T A(b - Ax^{(2)})}{(d_1)^T A d_1} - d_0 \frac{(d_0)^T A(b - Ax^{(2)})}{(d_0)^T A d_0}$$

$$d_3 = (b - Ax^{(3)}) - d_2 \frac{(d_2)^T A(b - Ax^{(3)})}{(d_2)^T A d_3} - d_1 \frac{(d_1)^T A(b - Ax^{(3)})}{(d_1)^T A d_1} - d_0 \frac{(d_0)^T A(b - Ax^{(3)})}{(d_0)^T A d_0}$$

$$\vdots$$

- turns out red terms are zero due to orthogonality

- since $x^{(k)} = \sum_{j=0}^{k} \alpha_j^* d_j$ we have $x^{(k+1)} = x^{(k)} + \alpha_k^* d_k$

- we pick $d_0 = -\nabla f(x^{(0)})$ and for $k = 1, ..., n-1$

$$d_k = -\nabla f(x^{(k)}) - \sum_{j=0}^{k-1} d_j \frac{d_j^T A(-\nabla f(x^{(k)}))}{d_j^T A d_j}$$

- it holds that $d_j^T \nabla f(x^{(k)}) = 0$ and $\nabla f(x^{(j)})^T \nabla f(x^{(k)}) = 0 \ \forall j < k$

  proof: we have $d_0^T \nabla f(x^{(1)}) = d_0^T (\underbrace{Ax_0}_{0} - b) + \alpha_0^* d_0^T A d_0 = 0$ and

  $d_j^T \nabla f(x^{(k+1)}) = d_j^T (Ax^{(k)} + \alpha_k d_k - b) = d_j^T \nabla f(x^{(k)}) - \alpha_k^* \underbrace{d_j^T A d_k}_{0 \text{ for } j \neq k}$

  in addition $\textbf{span}(d_0, ..., d_k) = \textbf{span}(\nabla f(x^{(0)}, ..., \nabla f(x^{(k)}))$

Simplifying CG update

- finally, note that

$$\nabla f(x^{(j+1)}) - \nabla f(x^{(j)}) = A(x^{(j)} + \alpha_j^* d_j) - b - (Ax^{(j)} - b) = \alpha_j^* A d_j$$

- simplify the basis update

$$\begin{aligned} d_k &= -\nabla f(x^{(k)}) - \sum_{j=0}^{k-1} d_j \frac{d_j^T A(-\nabla f(x^{(k)}))}{d_j^T A d_j} \\ &= -\nabla f(x^{(k)}) - \sum_{j=0}^{k-1} d_j \frac{(\nabla f(x^{(j+1)}) - \nabla f(x^{(j)}))^T(-\nabla f(x^{(k)}))}{(\nabla f(x^{(j+1)}) - \nabla f(x^{(j)}))^T d_j} \\ &= -\nabla f(x^{(k)}) - d_{k-1} \frac{\nabla f(x^{(k)})^T(-\nabla f(x^{(k)}))}{(-\nabla f(x^{(k-1)}))^T d_{k-1}} \end{aligned}$$

Final CG update rule

- CG algorithm simplifies to

$$d_k \quad = \quad -\nabla f(x^{(k)}) + d_{k-1} \frac{\|\nabla f(x^{(k)})\|_2^2}{\|\nabla f(x^{(k-1)})\|_2^2}$$

- $x^{(k+1)} = x^{(k)} + \alpha_k^* d_k$ where $\alpha^* = \arg\min_\alpha f(x_k + \alpha d_k) = \frac{b^T d_k}{d_k^T A d_k}$

  since we have $f(x^{(k-1)})^T d_{k-1} = -\|\nabla f(x^{(k-1)})\|_2^2$. **Proof:**

$$\begin{aligned} \nabla f(x^{(k)})^T d_k &= \nabla f(x^{(k)})^T \big(-\nabla f(x^{(k)}) - d_{k-1} \frac{\nabla f(x^{(k)})^T (-\nabla f(x^{(k)}))}{(-\nabla f(x^{(k-1)}))^T d_{k-1}} \big) \\ &= -\nabla f(x^{(k)})^T \nabla f(x^{(k)}) \end{aligned}$$

Spectral analysis of Krylov sequence

- $A = Q\Lambda Q^T$, Q orthogonal, $\Lambda = \mathbf{diag}(\lambda_1, \ldots, \lambda_n)$
- define $y = Q^T x$, $\bar{b} = Q^T b$, $y^\star = Q^T x^\star$
- in terms of y, we have

$$\begin{aligned} f(x) = \bar{f}(y) &= (1/2)x^T Q\Lambda Q^T x - b^T Q Q^T x \\ &= (1/2)y^T \Lambda y - \bar{b}^T y \\ &= \sum_{i=1}^{n} \left((1/2)\lambda_i y_i^2 - \bar{b}_i y_i\right) \end{aligned}$$

so $y_i^\star = \bar{b}_i/\lambda_i$, $f^\star = -(1/2)\sum_{i=1}^n \bar{b}_i^2/\lambda_i$

Krylov sequence in terms of y

$$y^{(k)} = \operatorname*{argmin}_{y \in \bar{\mathcal{K}}_k} \bar{f}(y), \qquad \bar{\mathcal{K}}_k = \operatorname{span}\{\bar{b}, \Lambda\bar{b}, \ldots, \Lambda^{k-1}\bar{b}\}$$

$$y_i^{(k)} = p_k(\lambda_i)\bar{b}_i, \qquad \deg p_k < k$$

$$p_k = \operatorname*{argmin}_{\deg p < k} \sum_{i=1}^{n} \bar{b}_i^2 \left((1/2)\lambda_i p(\lambda_i)^2 - p(\lambda_i)\right)$$

$$
\begin{aligned}
f(x^{(k)}) - f^\star &= \bar{f}(y^{(k)}) - f^\star \\
&= \min_{\deg p<k} (1/2) \sum_{i=1}^{n} \bar{b}_i^2 \frac{(\lambda_i p(\lambda_i) - 1)^2}{\lambda_i} \\
&= \min_{\deg p<k} (1/2) \sum_{i=1}^{n} \bar{y}_i^{\star 2} \lambda_i (\lambda_i p(\lambda_i) - 1)^2 \\
&= \min_{\deg q\leq k,\ q(0)=1} (1/2) \sum_{i=1}^{n} \bar{y}_i^{\star 2} \lambda_i q(\lambda_i)^2 \\
&= \min_{\deg q\leq k,\ q(0)=1} (1/2) \sum_{i=1}^{n} \bar{b}_i^2 \frac{q(\lambda_i)^2}{\lambda_i}
\end{aligned}
$$

$$
\begin{aligned}
\tau_k &= \frac{\min_{\deg q \leq k,\ q(0)=1} \sum_{i=1}^n \bar{y}_i^{\star 2} \lambda_i q(\lambda_i)^2}{\sum_{i=1}^n \bar{y}_i^{\star 2} \lambda_i} \\
&\leq \min_{\deg q \leq k,\ q(0)=1} \left(\max_{i=1,\ldots,n} q(\lambda_i)^2 \right)
\end{aligned}
$$

- if there is a polynomial q of degree k, with $q(0) = 1$, that is small on the spectrum of A, then $f(x^{(k)}) - f^\star$ is small

- if eigenvalues are clustered in k groups, then $y^{(k)}$ is a good approximate solution

- if solution $x^\star$ is approximately a linear combination of k eigenvectors of A, then $y^{(k)}$ is a good approximate solution

A bound on convergence rate

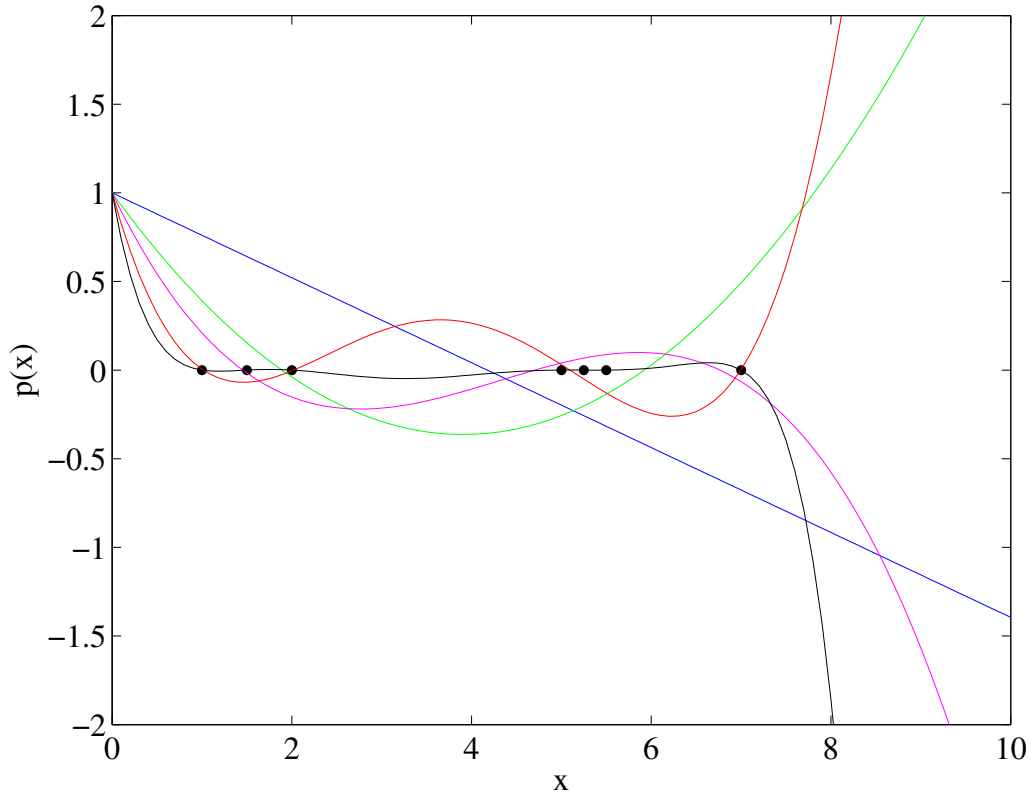
- taking q as Chebyshev polynomial of degree k, that is small on interval $[\lambda_{\min}, \lambda_{\max}]$, we get

$$\tau_k \leq \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k, \qquad \kappa = \lambda_{\max}/\lambda_{\min}$$

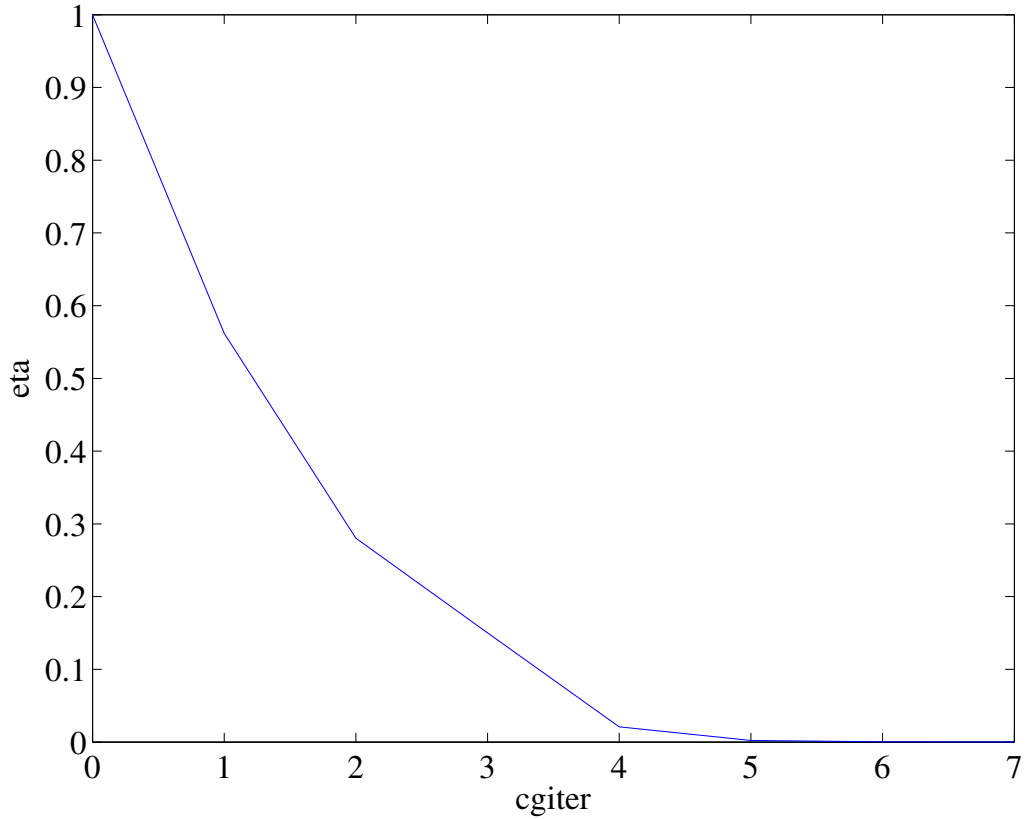
- convergence can be much faster than this, if spectrum of A is spread but clustered

Small example

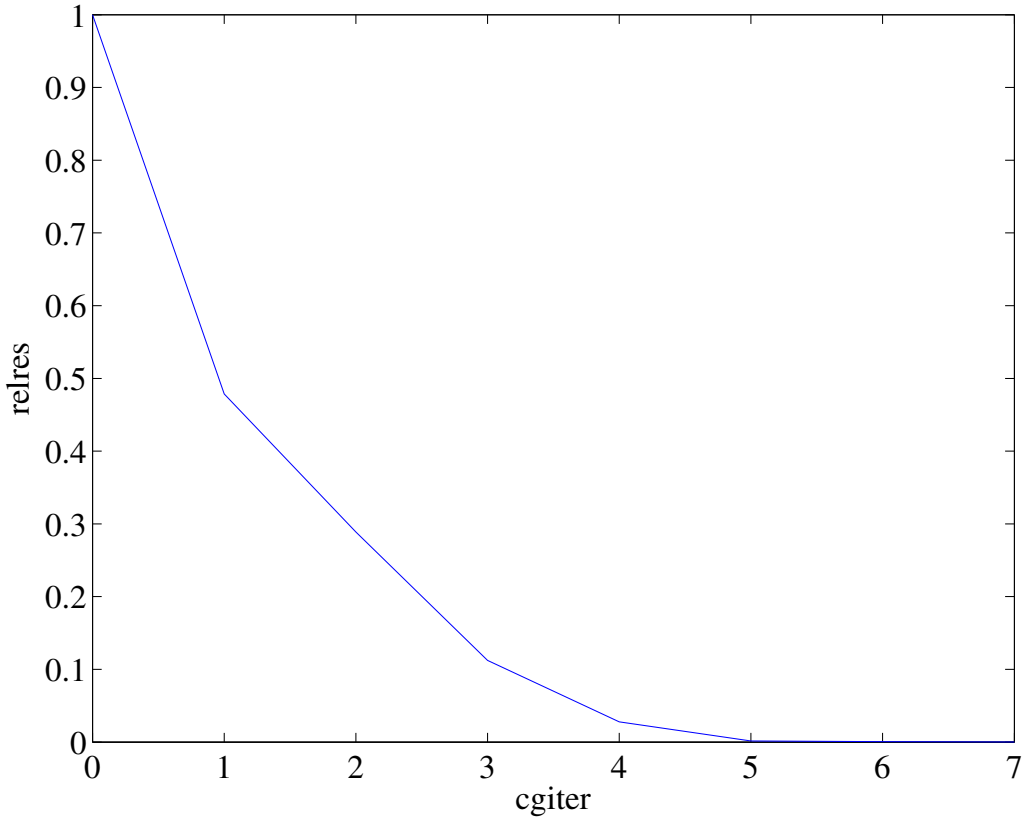
$A \in \mathbf{R}^{7\times 7}$, spectrum shown as filled circles; p_1, p_2, p_3, p_4, and p_7 shown



Convergence



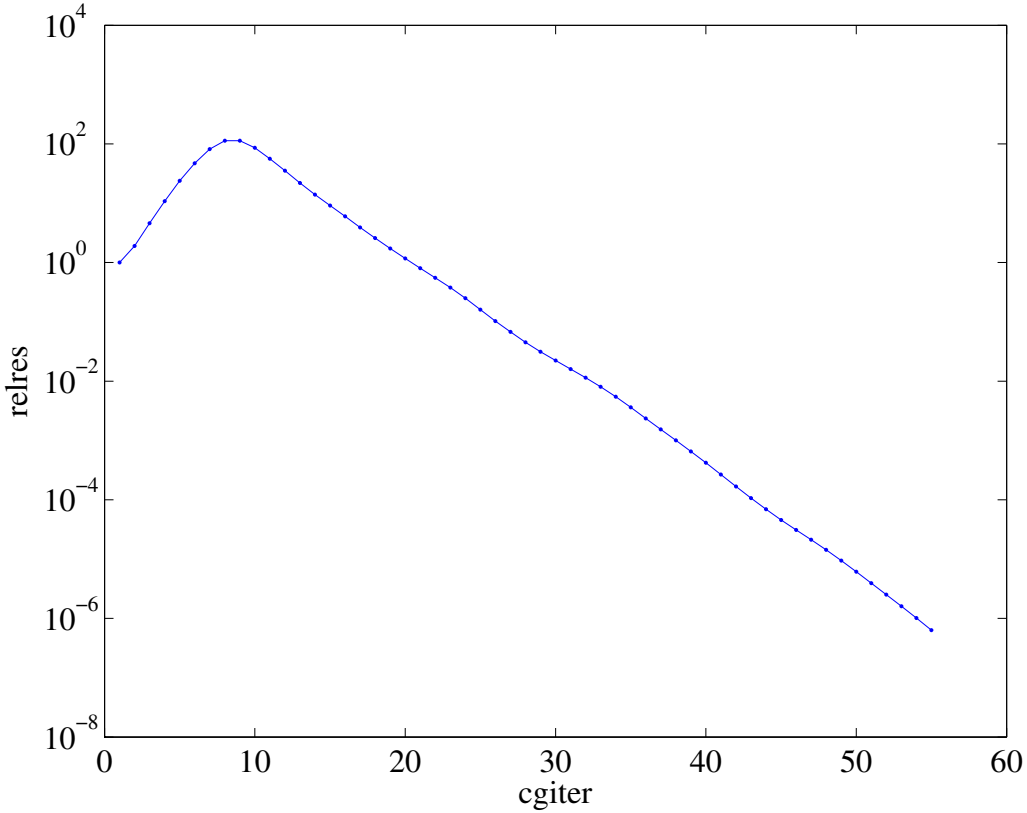
Residual convergence



Larger example

- solve $Gv = i$, resistor network with 10^5 nodes
- average node degree 10; around 10^6 nonzeros in G
- random topology with one grounded node
- nonzero branch conductances uniform on $[0, 1]$
- external current i uniform on $[0, 1]$
- sparse Cholesky factorization of G requires too much memory

Residual convergence



CG algorithm

(follows C. T. Kelley)

$x := 0, \quad r := b, \quad \rho_0 := \|r\|^2$

for $k = 1, \ldots, N_{\max}$

quit if $\sqrt{\rho_{k-1}} \leq \epsilon \|b\|$

if $k = 1$ then $p := r$; else $p := r + (\rho_{k-1}/\rho_{k-2})p$

$w := Ap$

$\alpha := \rho_{k-1}/p^T w$

$x := x + \alpha p$

$r := r - \alpha w$

$\rho_k := \|r\|^2$

Efficient matrix-vector multiply

- sparse A
- structured ($e.g.$, sparse) plus low rank
- products of easy-to-multiply matrices
- fast transforms (FFT, wavelet, . . .)
- inverses of lower/upper triangular (by forward/backward substitution)
- fast Gauss transform, for $A_{ij} = \exp(-\|v_i - v_j\|^2/\sigma^2)$ (via multipole)

Shifting

- suppose we have guess $\hat{x}$ of solution $x^\star$
- we can solve $Az = b - A\hat{x}$ using CG, then get $x^\star = \hat{x} + z$
- in this case $x^{(k)} = \hat{x} + z^{(k)} = \underset{x \in \hat{x} + \mathcal{K}_k}{\operatorname{argmin}} f(x)$

  ($\hat{x} + \mathcal{K}_k$ is called *shifted Krylov subspace*)
- same as initializing CG alg with $x := \hat{x}$, $r := b - Ax$
- good for 'warm start', $i.e.$, solving $Ax = b$ starting from a good initial guess ($e.g.$, the solution of another system $\tilde{A}x = \tilde{b}$, with $A \approx \tilde{A}$, $b \approx \tilde{b}$)

Preconditioned conjugate gradient algorithm

- idea: apply CG after linear change of coordinates $x = Ty$, $\det T \neq 0$
- use CG to solve $T^T A T y = T^T b$; then set $x^\star = T^{-1} y^\star$
- T or $M = TT^T$ is called *preconditioner*
- in naive implementation, each iteration requires multiplies by T and T^T (and A); also need to compute $x^\star = T^{-1} y^\star$ at end
- can re-arrange computation so each iteration requires one multiply by M (and A), and no final solve $x^\star = T^{-1} y^\star$
- called *preconditioned conjugate gradient* (PCG) algorithm

Choice of preconditioner

- if spectrum of $T^T AT$ (which is the same as the spectrum of MA) is clustered, PCG converges fast
- extreme case: $M = A^{-1}$
- trade-off between enhanced convergence, and extra cost of multiplication by M at each step
- goal is to find M that is cheap to multiply, and approximate inverse of A (or at least has a more clustered spectrum than A)

Some generic preconditioners

- diagonal: $M = \mathbf{diag}(1/A_{11}, \ldots, 1/A_{nn})$

- incomplete/approximate Cholesky factorization: use $M = \hat{A}^{-1}$, where $\hat{A} = \hat{L}\hat{L}^T$ is an approximation of A with cheap Cholesky factorization
  - compute Cholesky factorization of $\hat{A}$, $\hat{A} = \hat{L}\hat{L}^T$
  - at each iteration, compute $Mz = \hat{L}^{-T}\hat{L}^{-1}z$ via forward/backward substitution

- examples
  - $\hat{A}$ is central k-wide band of A
  - $\hat{L}$ obtained by sparse Cholesky factorization of A, ignoring small elements in A, or refusing to create excessive fill-in

Randomized preconditioning

- suppose $A = H^T H$, for some $H \in \mathbf{R}^{m \times n}$ and $m \gg n$

  example: Hessian of a convex objective, e.g., least squares problem $\mathrm{argmin}_x \frac{1}{2}\|Hx - y\|_2^2 = \mathrm{argmin}_x \frac{1}{2} x^T H^T H x - x^T y$

- QR decomposition $H = QR$ and the preconditioner $T = R^{-1}$ is ideal since $T^T A T = (HT)^T (HT) = Q^T Q = I$, whose condition number is 1

  however, QR decomposition on H costs $O(mn^2)$ operations

- **randomized preconditioner:** let $S \in \mathbf{R}^{s \times m}$ be a random matrix, e.g., i.i.d. ± 1, and apply QR decomposition as $SH = \tilde{Q}\tilde{R}$. Set $T = \tilde{R}^{-1}$

  computational cost is $O(sn^2)$+cost of forming the **sketch** SH

- S can be Randomized Hadamard Transform $(O(mn \log s))$

Preconditioned conjugate gradient

(with preconditioner $M \approx A^{-1}$ (hopefully))

$x := 0, \quad r := b - Ax_0, \quad p := r \quad z := Mr, \quad \rho_1 := r^T z$

for $k = 1, \ldots, N_{\max}$

quit if $\sqrt{\rho_k} \leq \epsilon \|b\|_2$ or $\|r\| \leq \epsilon \|b\|_2$

$w := Ap$

$\alpha := \frac{\rho_k}{w^T p}$

$x := x + \alpha p$

$r := r - \alpha w$

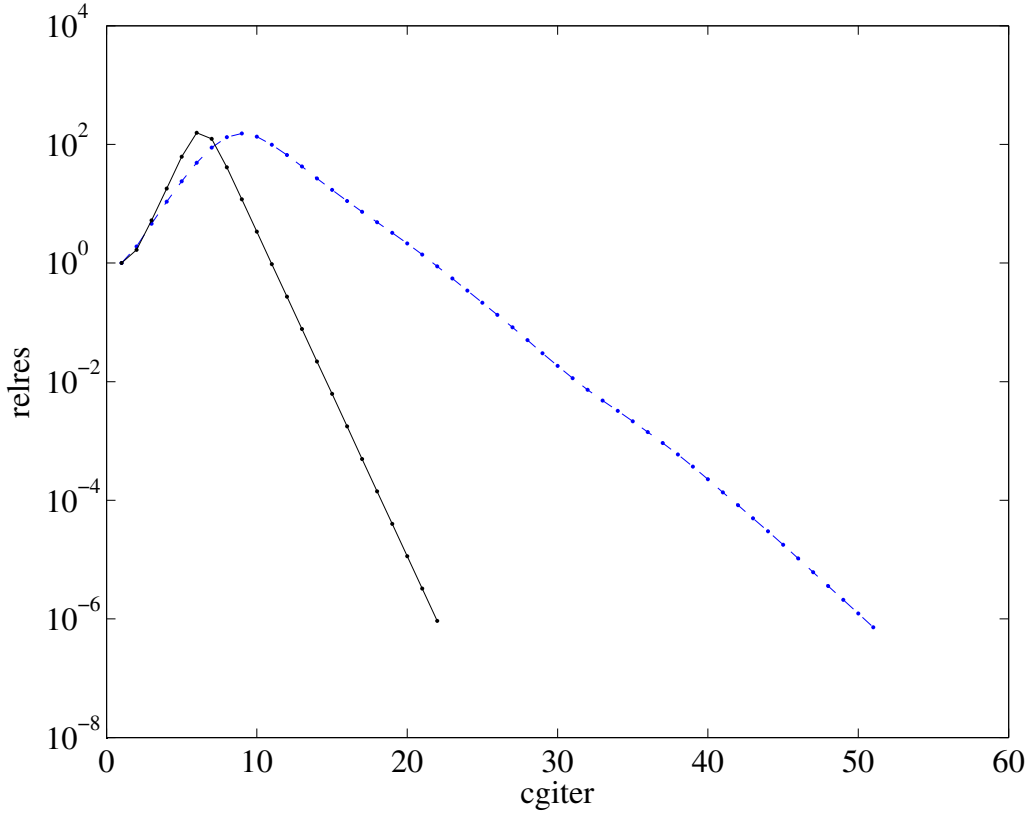
$z := Mr$

$\rho_{k+1} := z^T r$

$p := z + \frac{\rho_{k+1}}{\rho_k} p$

Larger example

residual convergence with and without diagonal preconditioning



The Fletcher-Reeves Method

CG can be adapted for arbitrary differentiable objectives:
set $d_0 = -\nabla f(x^{(0)})$ and

$$\begin{aligned} d_k &= -\nabla f(x^{(k)}) + d_{k-1}\frac{\|\nabla f(x^{(k)})\|_2^2}{\|\nabla f(x^{(k-1)})\|_2^2} \\ x^{(k+1)} &= x^{(k)} + \alpha_k^* d_k \quad \text{where} \quad \alpha^* = \arg\min_{\alpha} f(x_k + \alpha d_k) \end{aligned}$$

- exact line searches are replaced by practical line search procedures
- termination criterion is typically $\|\nabla f(x^{(k)})\|_2 \leq \epsilon$
- conjugacy of the search directions d_k is only achieved approximately

  hence, we may need to reset d_k to $-\nabla f(x^{(k)})$ periodically

CG summary

- in theory (with exact arithmetic) converges to solution in n steps
  - the bad news: due to numerical round-off errors, can take more than n steps (or fail to converge)
  - the good news: with luck ($i.e.$, good spectrum of A), can get good approximate solution in $\ll n$ steps
- each step requires $z \rightarrow Az$ multiplication
  - can exploit a variety of structure in A
  - in many cases, never form or store the matrix A
- compared to direct (factor-solve) methods, CG is less reliable, data dependent; often requires good (problem-dependent) preconditioner
- but, when it works, can solve extremely large systems