High-dimensional integration without Markov chains

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High-dimensional integration by:

- Nonparametric statistics
- Computational geometry
- Computational physics
- Monte Carlo methods
- Machine learning
- ...

…but NOT Markov chains.

The problem

Compute $$I = \int f(x)dx$$

where $$x \in \Re^D, D >> 1$$

$$f(x) \geq 0$$

We can evaluate f(x) at any x. But we have no other special knowledge about f.

Often: $$I = \frac{\int g(x)f(x)dx}{\int f(x)dx}$$

Often f(x) expensive to evaluate.

Motivating example: Bayesian inference on large datasets

Curse of dimensionality

Quadrature doesn't extend: $O(m^D)$.

How to get the job done (Monte Carlo):

1. Importance sampling (IS) [not general]
2. Markov Chain Monte Carlo (MCMC)

Often:

$$M = \{x \mid f(x) > \varepsilon\}$$

$$d_M << D$$

MCMC
(Metropolis-Hastings algorithm)

1. Start at random x
2. Sample x^{new} from $N(x,s)$
3. Draw $u \sim U[0,1]$
4. If $u < \min(f(x^{new})/f(x),1)$, set x to x^{new}
5. Return to step 2.

MCMC (Metropolis-Hastings algorithm)

Do this a huge number of times. Analyze the stream of x's so far by hand to see if you can stop the process.

If you jump around f long enough (make a sequence long enough) and draw x's from it uniformly, these x's act as if drawn iid from f.

Then $$\int f(x)dx \approx E[f(x)] = \frac{1}{N}\sum_{i}^{N} f(x_i)$$

Good

Really cool:

- Ultra-simple
- Requires only evaluations of f
- Faster than quadrature in high dimensions

→ gave us the bomb (??)

→ listed in “Top 10 algorithms of all time”

Bad

Really unfortunate:

1. No reliable way to choose the scale s; yet, its choice is critical for good performance
2. With multiple modes, can get stuck
3. Correlated sampling is hard to characterize in terms of error
4. Prior knowledge can be incorporated only in simple ways
5. No way to reliably stop automatically

→ Requires lots of runs/tuning/guesswork. Many workarounds, for different knowledge about f. (Note that in general case, almost nothing has changed.)

→ Must become an MCMC expert just to do integrals.

→ (…and the ugly) In the end, we can't be quite sure about our answer.

Black art. Not yet in Numerical Recipes.

Let's try to make a new method

Goal:

- Simple like MCMC
- Weak/no requirements on f()
- Principled and automatic choice of key parameter(s)
- Real error bounds
- Better handling of isolated modes
- Better incorporation of prior knowledge
- Holy grail: automatic stopping rule

Importance sampling

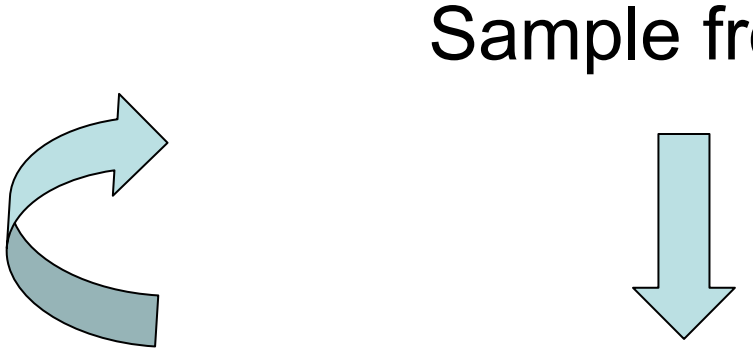
$$I = \int \frac{f(x)}{q(x)} q(x) dx$$

$$\hat{I} = \sum_{i}^{N} \frac{f(x_i)}{q(x_i)}$$

- Choose q() close to f() if you can; try not to underestimate f()
- Unbiased
- Error is easier to analyze/measure
- *But: not general (need to know something about f)*

Adaptive importance sampling

Idea: can we improve q() as go along?



By the way…

Now we're doing integration by *statistical inference*.

NAIS [Zhang, JASA 1996]

Assume f() is a density.

1. Generate x's from an initial q()
2. Estimate density f^{hat} from the x's, using kernel density estimation (KDE):

$$\hat{f}(x_i) = \frac{1}{N} \sum_{j \neq i}^{N} K_h(\|x_i - x_j\|)$$

3. Sample x's from f^{hat}.
4. Return to step 2.

Some attempts for q()

- Kernel density estimation [e.g. Zhang, JASA 1996]
  - $O(N^2)$; choice of bandwidth
- Gaussian process regression [e.g. Rasmussen-Ghahramani, NIPS 2002]
  - $O(N^3)$; choice of bandwidth
- Mixtures (of Gaussians, betas…) [e.g. Owen-Zhou 1998]
  - nonlinear unconstrained optimization is itself time-consuming and contributes variance; choice of k, …
- Neural networks [e.g. JSM 2003]
  - (let's get serious) awkward to sample from; like mixtures but worse

Bayesian quadrature: right idea but not general

None of these works

(i.e. is a viable alternative to MCMC)

Tough questions

- Which q()?
  - ability to sample from it
  - efficiently computable
  - reliable and automatic parameter estimation
- How to avoid getting trapped?
- Can we actively choose where to sample?
- How to estimate error at any point?
- When to stop?
- How to incorporate prior knowledge?

What's the *right* thing to do?

(i.e. what *objective function* should we be optimizing?)

Is this active learning (aka optimal experiment design)?

Basic framework:

bias-variance decomposition of least-squares objective function

→ minimize only variance term

Seems reasonable, but:

- Is least-squares really the optimal thing to do for our problem (integration)?

Observation #1:

$$\int [f(x) - q(x)]^2 dx$$

Least-squares is somehow not exactly right.

- It says to approximate well everywhere.
- Shouldn't we somehow focus more on regions where f() is large?

Back to basics

$$I = \int \frac{f(x)}{q(x)} q(x) dx$$

$$\hat{I} = \sum_{i}^{N} \frac{f(x_i)}{q(x_i)}, \quad x_i \sim q()$$

Estimate
(unbiased)

Back to basics

$$V(\hat{I}_q) = E\left[\left(\hat{I}_q - E\left[\hat{I}_q\right]\right)^2\right]$$ Variance

$$= \frac{1}{N}\left[\int \frac{f(x)^2}{q(x)}dx - I^2\right]$$

$$= \frac{1}{N}\left[\int f(x)\left(\frac{f(x)}{q(x)}\right)dx - I^2\right]$$

Back to basics

$$V(\hat{I}_q) = \frac{1}{N}\left[\int \frac{f(x)^2}{q(x)}dx - I^2\right] = 0$$

$$q^*(x) = \frac{f(x)}{I}$$

Optimal q()

$$V(\hat{I}_q) = \frac{1}{N}\int \frac{\left[f(x) - Iq(x)\right]^2}{q(x)}dx$$

Idea #1:
Minimize importance sampling error

$$\min_{q()} \int \frac{[f(x) - Iq(x)]^2}{q(x)} dx$$

Error estimate

$$\hat{V}(\hat{I}_q) = \frac{1}{N^2} \sum_i^N \frac{\left[f(x_i) - \hat{I}_q q(x_i) \right]^2}{q(x_i)}, \quad x_i \sim q()$$

cf. [Neal 1996]: Use $\hat{V}\left(\frac{w_i}{\sum_i w_i} \right), \quad w_i = \frac{f(x_i)}{q(x_i)}$

- indirect and approximate argument
- can use for stopping rule

What *kind* of estimation?

Observation #2:

Regression, not density estimation. (even if f() is a density)

- Supervised learning vs unsupervised.
- Optimal rate for regression is faster than that of density estimation (kernel estimators, finite-sample)

Idea #2: Use Nadaraya-Watson regression (NWR) for q()

$$E[Y \mid X = x] = \int y f(y \mid x) dy = \frac{\int y f(x, y) dy}{\int f(x, y) dy}$$

$$\hat{f}(x_i) = \frac{\frac{1}{N} \sum_{j \neq i}^{N} y_j K_h(\|x_i - x_j\|)}{\frac{1}{N} \sum_{j \neq i}^{N} K_h(\|x_i - x_j\|)}$$

Why Nadaraya-Watson?

- Nonparametric
- Good estimator (though not best) – optimal rate
- No optimization procedure needed
- Easy to add/remove points
- Easy to sample from – choose x_i with probability

$$p_i = \frac{\hat{f}(x_i)}{\sum_i \hat{f}(x_i)}$$

  then draw from $N(x_i, h^*)$
- Guassian kernel makes non-zero everywhere, sample more widely

How can we avoid getting trapped?

Idea #3:
Use defensive mixture for q()

$$q(x) = (1-\alpha)\hat{f}(x) + \alpha f_0(x)$$

$$V(\hat{I}_q) \leq \frac{1}{N\alpha}\left[\sigma^2 + (1-\alpha)I^2\right]$$

This also answered:
“How can we incorporate prior knowledge”?

Can we do NWR tractably?

Observation #3:

NWR is a '*generalized N-body problem*'.

- distances between n-tuples [pairs] of points in a metric space [Euclidean]
- modulated by a (symmetric) positive monotonic kernel [pdf]
- decomposable operator [summation]

Idea #4:

1. Use fast KDE alg. for denom.
2. Generalize to handle numer.

$$\hat{f}(x_i) = \frac{\frac{1}{N}\sum_{j \neq i}^{N} y_j K_h(\|x_i - x_j\|)}{\frac{1}{N}\sum_{j \neq i}^{N} K_h(\|x_i - x_j\|)}$$

Extension from KDE to NWR

- First: allow weights on each point
- Second: allow those weights to be negative
- Not hard

Okay, so we can compute NWR efficiently with accuracy.

How do we find the bandwidth (accurately and efficiently)?

What about an analytical method?

Bias-variance decomposition

has many terms that can be estimated (if very roughly)

→But the real problem is D.

Thus, this is not reliable in our setting.

Idea #5:
'Least-IS-error' cross-validation

$$h^* = \min_{h \in \{h_i\}} \left\{ \frac{[f(x_i) - Iq_h(x_i)]^2}{q_h(x_i)} \right\}$$

Idea #6:
Incremental cross-validation

$$h^*_{new} = \min_{h \in \{\frac{2}{3}h^*, h^*, \frac{3}{2}h^*\}} \left\{ \frac{[f(x_i) - Iq_h(x_i)]^2}{q_h(x_i)} \right\}$$

Idea #7: Simultaneous-bandwidth N-body algorithm

We can share work between bandwidths.

[Gray and Moore, 2003]

Idea #8: Use ‘equivalent kernels’ transformation

- Epanechnikov kernel (optimal) has finite extent

$$t = \|x - x_i\|^2 / h^2 \qquad K(x, x_i) = \begin{matrix} 1 - t^{2a} & 0 \le t < 1 \\ 0 & t \ge 1 \end{matrix}$$

- 2-3x faster than Gaussian kernel

How can we pick samples in a *guided* fashion?

- Go where we're uncertain?
- Go by the f() value, to ensure low intrinsic dimension for the N-body algorithm?

Idea #9: Sample more where the error was larger

- Choose new x_i with probability p_i

$$v_i = \frac{\left[f(x_i) - \hat{I}_q q(x_i)\right]^2}{q(x_i)}, \quad p_i = \frac{v_i}{\sum_i v_i}$$

- Draw from $N(x_i, h^*)$

Should we forget old points?

I tried that. It doesn't work.

So I remember all the old samples.

Idea #10:
Incrementally update estimates

$$\hat{I}_q = \left(\hat{I}_q N_{tot} + \sum_i^N \frac{f(x_i)}{q(x_i)} \right) / \left(N_{tot} + N \right)$$

$$\hat{V}(\hat{I}_q) = \left(\hat{V}(\hat{I}_q) N_{tot}^2 + \sum_i^N \frac{\left[f(x_i) - \hat{I}_q q(x_i) \right]^2}{q(x_i)} \right) / \left(N_{tot} + N \right)^2$$

Overall method: FIRE

Repeat:

1. Resample N points from $\{x_i\}$ using $v_i = \frac{\left[f(x_i) - \hat{I}_q q(x_i)\right]^2}{q(x_i)}$
   $p_i = \frac{v_i}{\sum_i v_i}$
   Add to training set. $\{\tilde{x}_i\}$
   Build/update $T_{\{\tilde{x}_i\}}$
2. Compute $h^*_{new} = \min_{h \in \{\frac{2}{3}h^*, h^*, \frac{3}{2}h^*\}} \left\{ \frac{\left[f(\tilde{x}_i) - \hat{I}_q q_h(\tilde{x}_i)\right]^2}{q_h(\tilde{x}_i)} \right\}$
3. Sample N points $\{x_i\}$ from $q() = (1-\alpha)\hat{f}() + \alpha f_0()$
4. For each x_i compute $\hat{f}_{h^*}(x_i)$, using $T_{\{x_i\}}$
5. Update I and V

Properties

- Because FIRE is importance sampling:
  - consistent
  - unbiased
- The NWR estimate approaches f(x)/I
- Somewhat reminiscent of particle filtering; EM-like; like N interacting Metropolis samplers

Test problems

- **Thin region**

  Anisotropic Gaussian

  a s^2 in off-diagonals

  a={0.99,0.9,0.5}, D={5,10,25,100}

- **Isolated modes**

  Mixture of two normals

  0.5*N*(4,1) + 0.5*N*(4+b,1)

  b={2,4,6,8,10}, D={5,10,25,100}

Competitors

- Standard Monte Carlo
- MCMC (Metropolis-Hastings)
  - starting point [Gelman-Roberts-Gilks 95]
  - adaptation phase [Gelman-Roberts-Gilks 95]
  - burn-in time [Geyer 92]
  - multiple chains [Geyer 92]
  - thinning [Gelman 95]

How to compare

Look at its relative error over many runs

When to stop it?

1. Use its actual stopping criterion
2. Use a fixed wall-clock time

Anisotropic Gaussian (a=0.9,D=10)

- MCMC
  - started at center of mass
  - when it wants to stop: >2 hours
  - after 2 hours
    - with best s: rel. err {24%,11%,3%,62%}
    - small s and large s: >250% errors
    - automatic s: {59%,16%,93%,71%}
  - ~40M samples
- FIRE
  - when it wants to stop: ~1 hour
  - after 2 hours: rel. err {1%,2%,1%,1%}
  - ~1.5M samples

Mixture of Gaussians (b=10,D=10)

- MCMC
  - started at one mode
  - when it wants to stop: ~30 minutes
  - after 2 hours:
    - with best s: rel. err {54%,42%,58%,47%}
    - small s, large s, automatic s: similar
  - ~40M samples
- FIRE
  - when it wants to stop: ~10 minutes
  - after 2 hours: rel. err {<1%,1%,32%,<1%}
  - ~1.2M samples

Extension #1

Non-positive functions

Positivization [Owen-Zhou 1998]

Extension #2

More defensiveness, and accuracy

Control variates [Veach 1997]

Extension #3

More accurate regression

Local linear regression

Extension #4 (maybe)

Fully automatic stopping

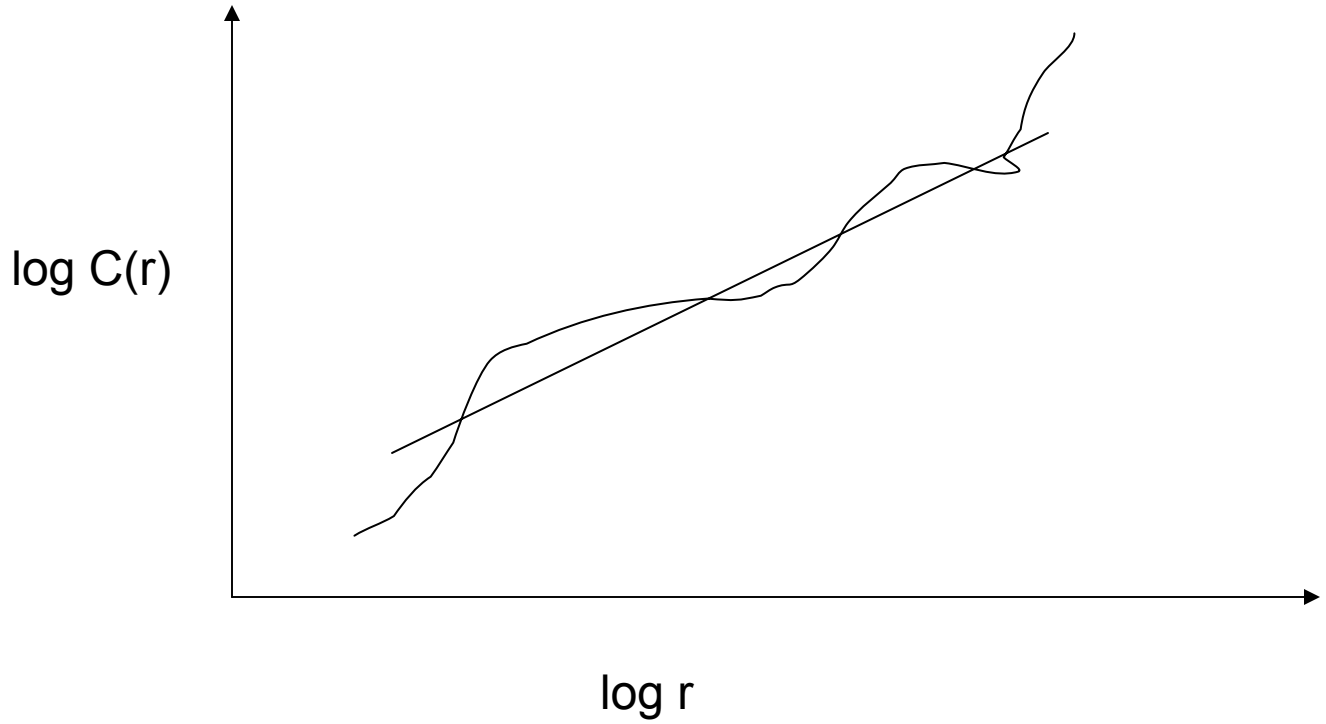
Function-wide confidence bands

stitch together pointwise bands, control with FDR

Summary

- We can do high-dimensional integration without Markov chains, by statistical inference
- Promising alternative to MCMC
  - safer (e.g. isolated modes)
  - not a black art
  - faster
- Intrinsic dimension - multiple viewpoints
- MUCH more work needed – please help me!

One notion of intrinsic dimension



‘Correlation dimension’

Similar: notion in metric analysis

N-body problems

- **Coulombic**

  (high accuracy required)

$$K(x, x_i) = \frac{mm_i}{\left\| x - x_i \right\|^a}$$

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$$K(x, x_i) = \frac{mm_i}{\|x - x_i\|^a}$$

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$$K(x, x_i) = e^{-\|x - x_i\|^2 / 2\sigma^2}$$

$$t = \|x - x_i\|^2 / \sigma^2$$

$$K(x, x_i) = \begin{cases} 1 - t^{2a} & 0 \le t < 1 \\ 0 & t \ge 1 \end{cases}$$

(only moderate accuracy required, often high-D)

N-body problems

- **Coulombic**

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$$K(x, x_i) = \frac{m m_i}{\|x - x_i\|^a}$$

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  (only moderate accuracy required, often high-D)

- **SPH** (smoothed particle hydrodynamics)

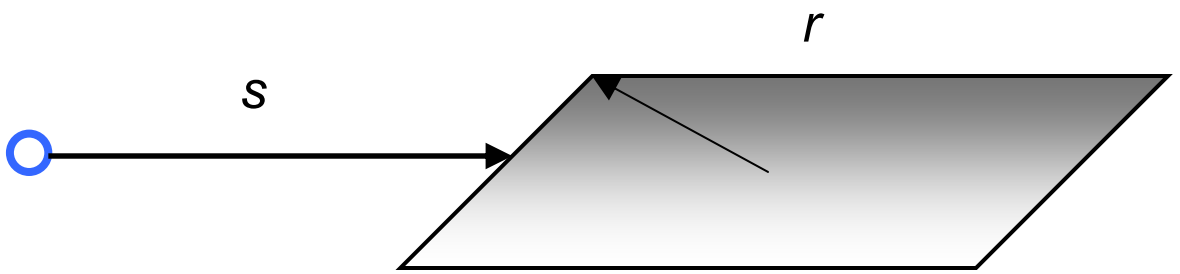
$$K(x, x_i) = \begin{cases} 4 - 6t^2 + 3t^3 & 0 \le t < 1 \\ (2 - t)^3 & 1 \le t < 2 \\ 0 & t \ge 2 \end{cases}$$

  (only moderate accuracy required)

Also: different for every point, non-isotropic, edge-dependent, …

N-body methods: Approximation

- **Barnes-Hut**



$$\sum_i K(x, x_i) \approx N_R K(x, \mu_R) \quad \text{if} \quad s > \frac{r}{\theta}$$

N-body methods: Approximation

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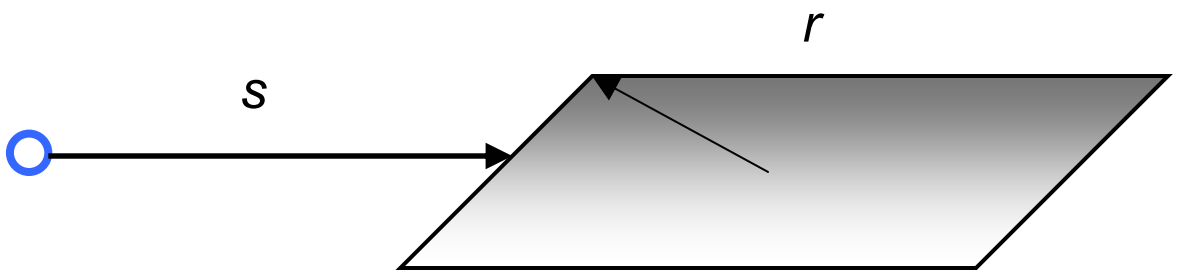
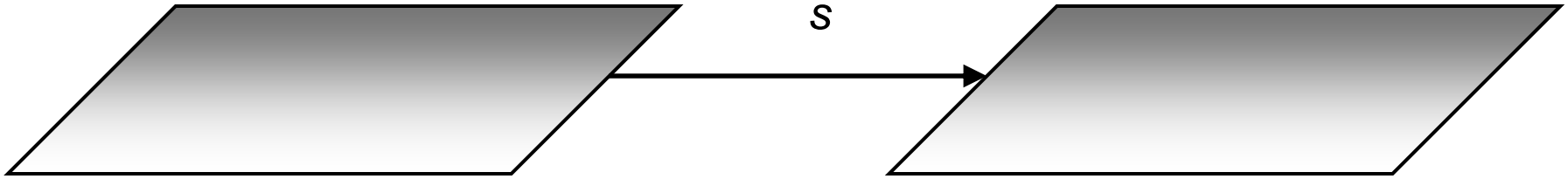


$$\sum_i K(x, x_i) \approx N_R K(x, \mu_R) \quad \text{if} \quad s > \frac{r}{\theta}$$

- **FMM**



$$\forall x, \sum_i K(x, x_i) \approx \text{multipole/Taylor expansion of order } p \quad \text{if} \quad s > r$$

N-body methods: Runtime

- **Barnes-Hut** $\approx O(N \log N)$

  non-rigorous, $\approx$ uniform distribution

- **FMM** $\approx O(N)$

  non-rigorous, $\approx$ uniform distribution

N-body methods: Runtime

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- **FMM** $\approx O(N)$

  non-rigorous, $\approx$ uniform distribution

[Callahan-Kosaraju 95]: *O(N)* is impossible for log-depth tree (in the worst case)

Expansions

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- Adds much complexity (software, human time)
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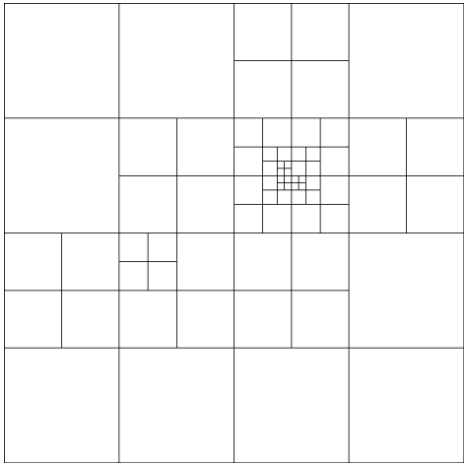
- BUT: Needed to achieve *O(N)* (?)
  Needed to achieve high accuracy (?)
  Needed to have hard error bounds (?)

N-body methods: Adaptivity

- **Barnes-Hut** **recursive**
  → can use any kind of tree

- **FMM** **hand-organized control flow**
  → requires grid structure

quad-tree/oct-tree	not very adaptive
kd-tree	adaptive
ball-tree/metric tree	very adaptive

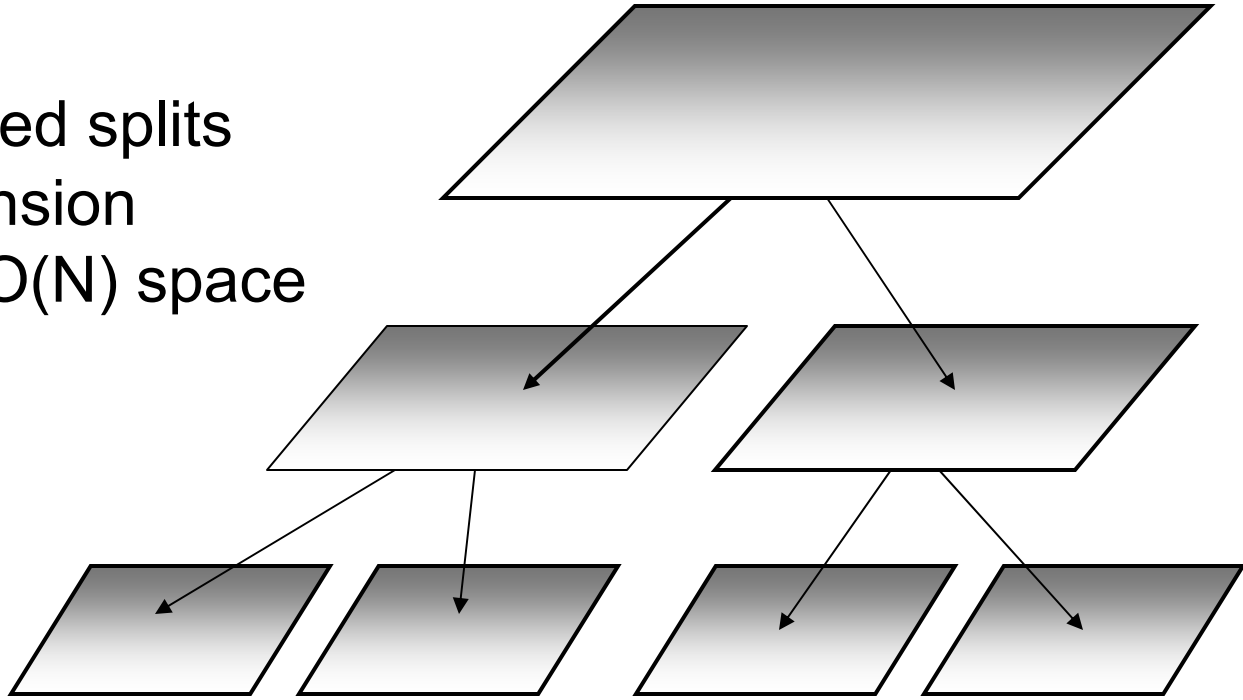


kd-trees:

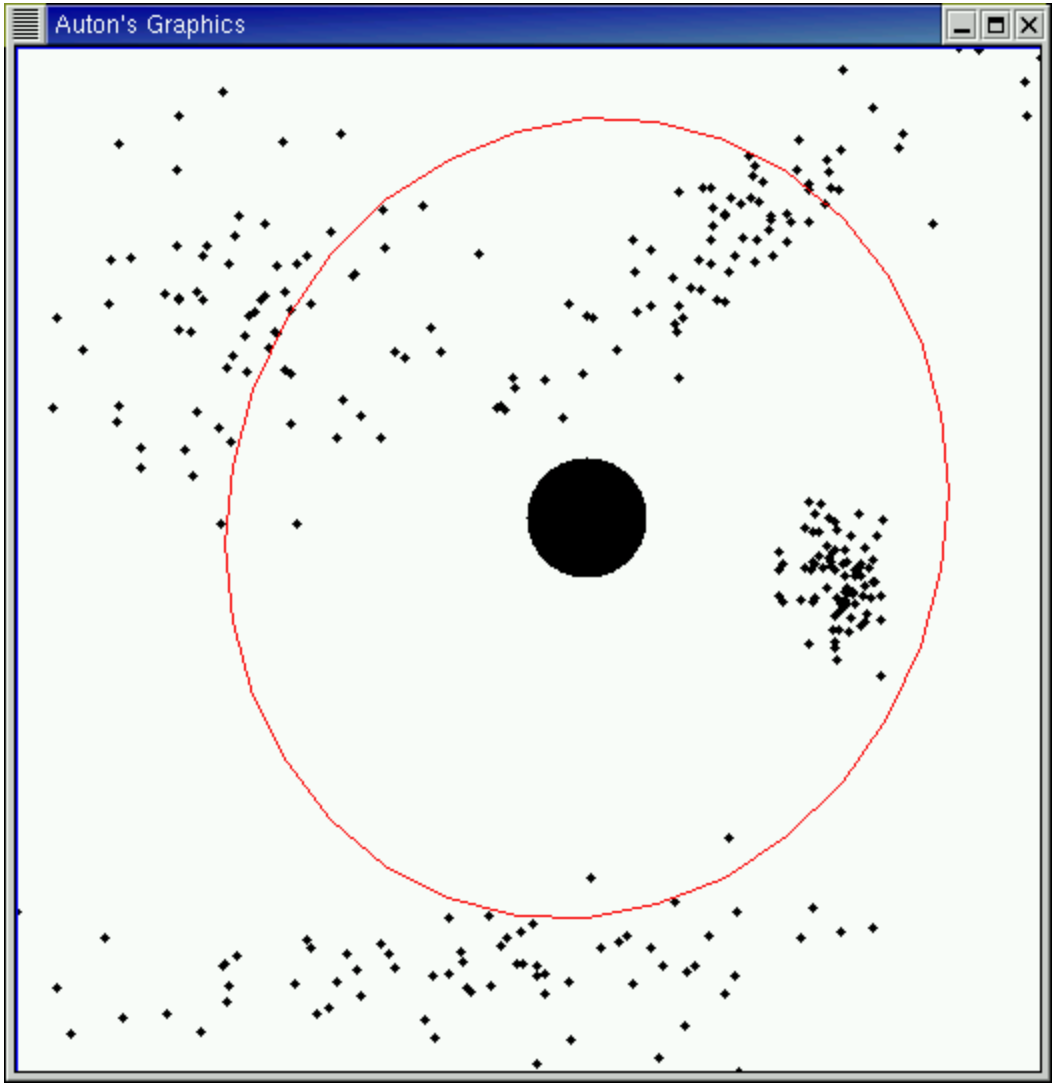
most widely-used space-partitioning tree

[Friedman, Bentley & Finkel 1977]

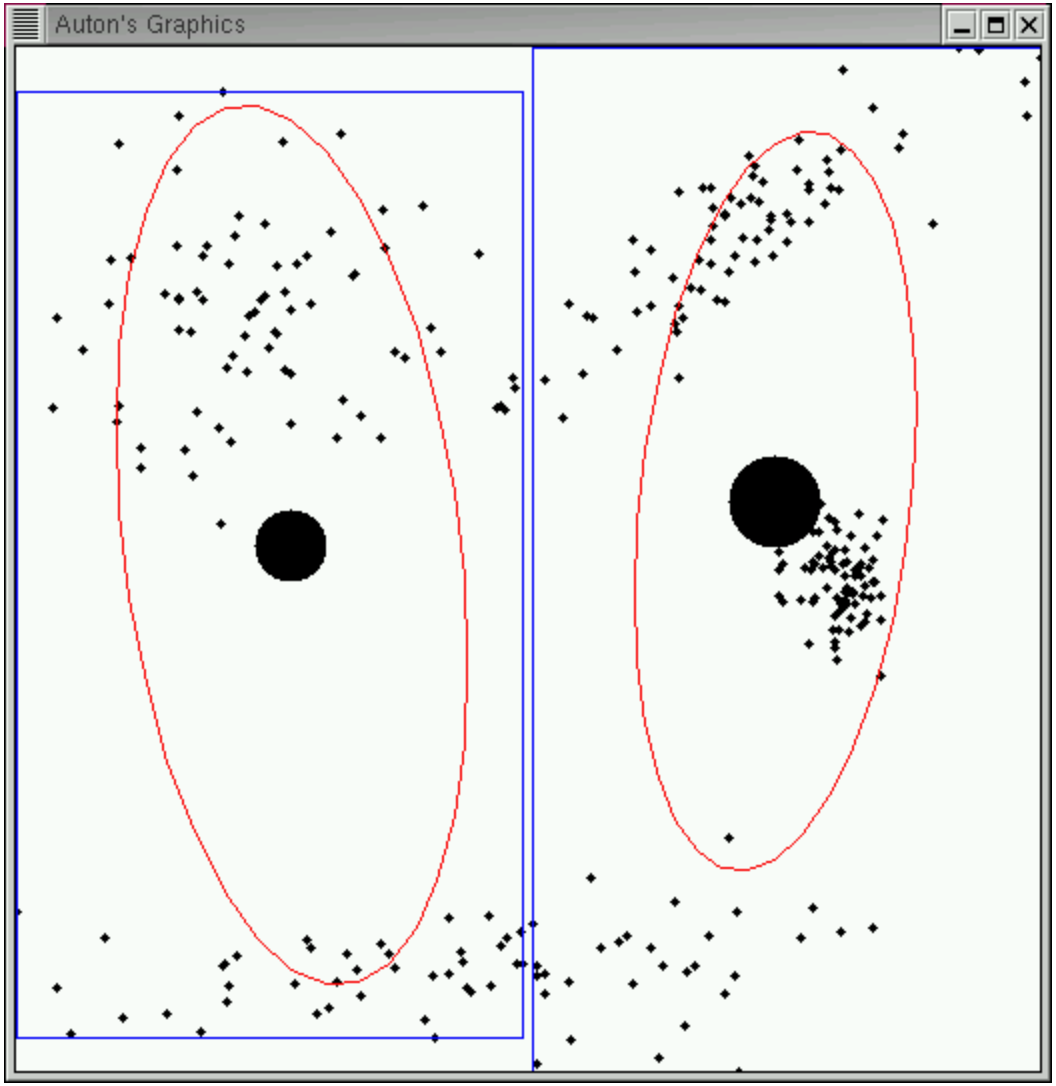
- Univariate axis-aligned splits
- Split on widest dimension
- O(N log N) to build, O(N) space



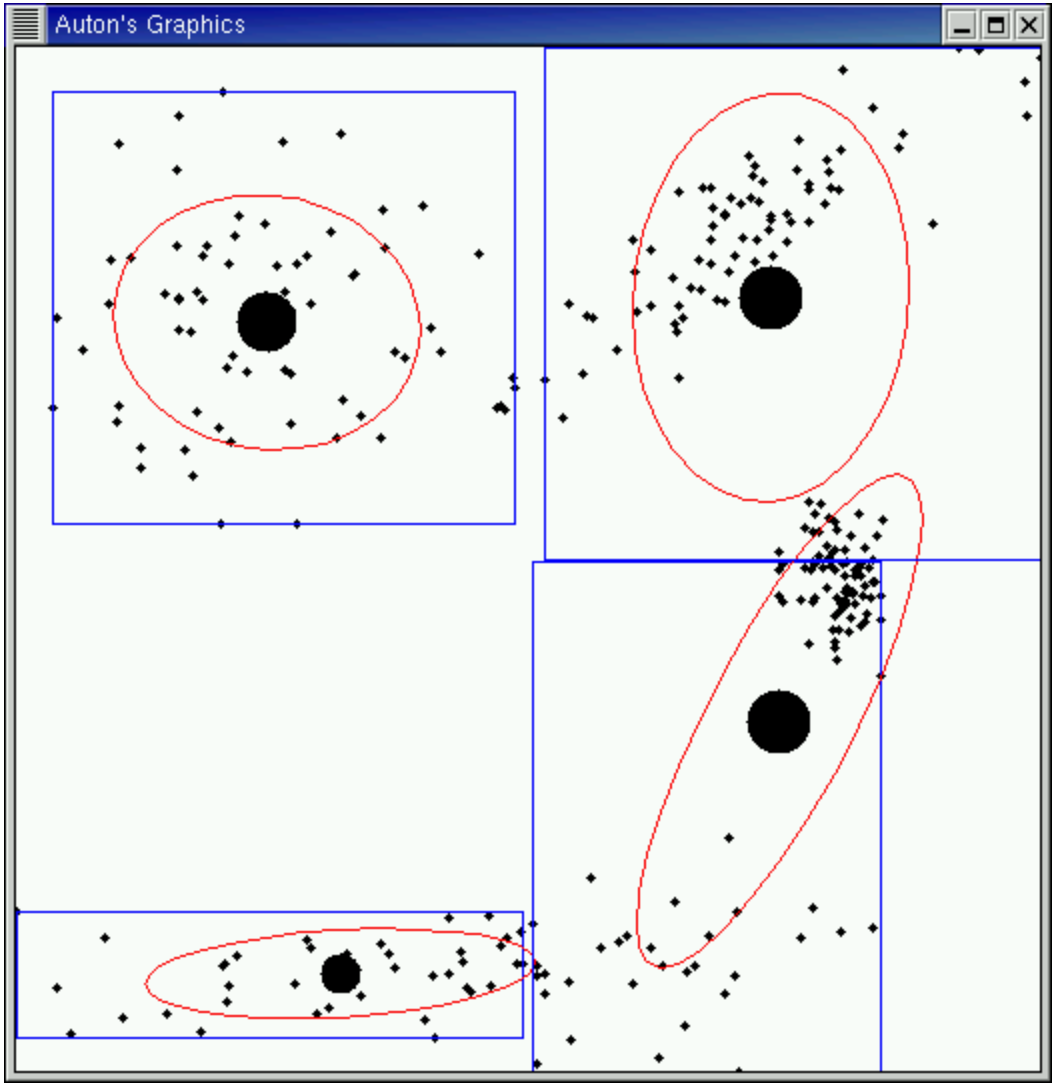
A *kd*-tree: level 1



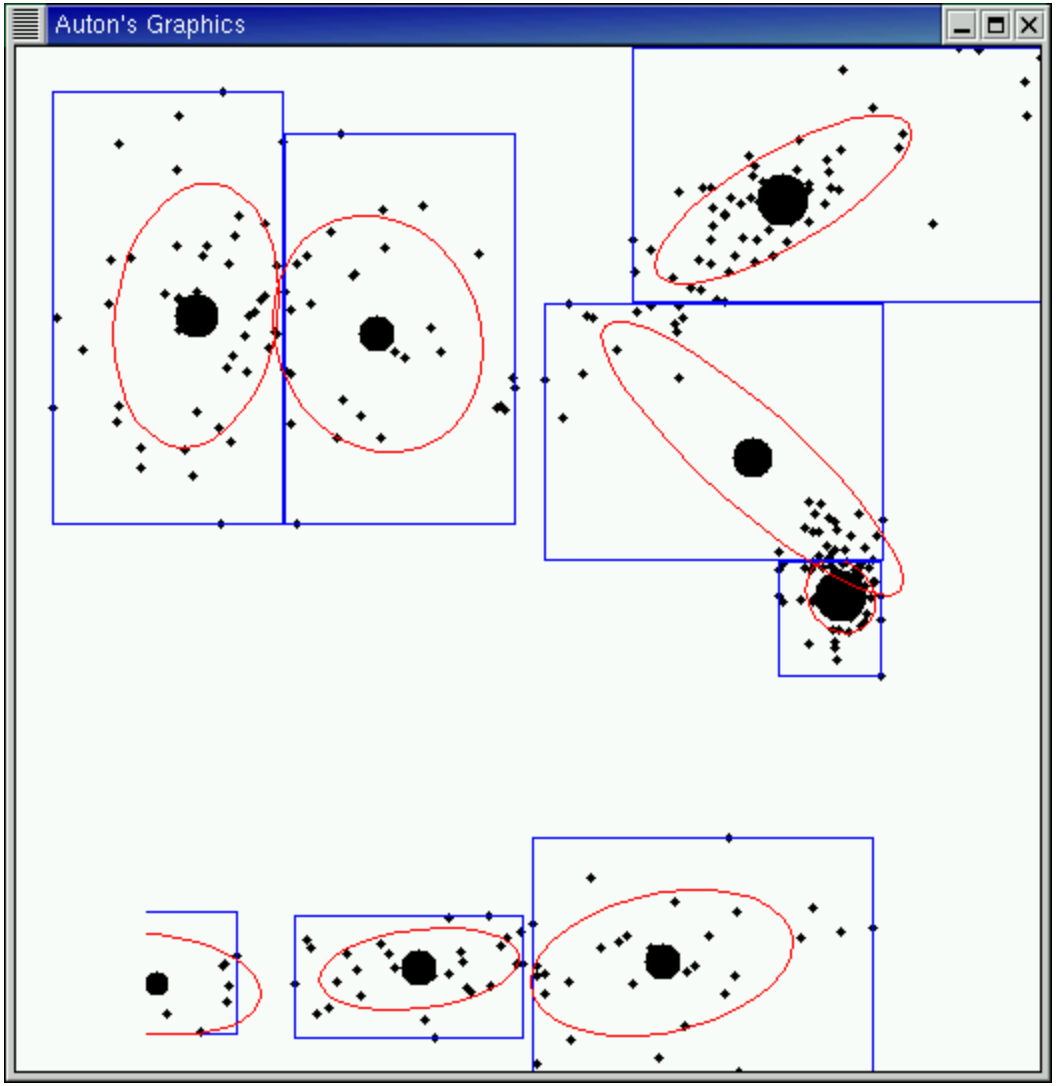
A *kd*-tree: level 2



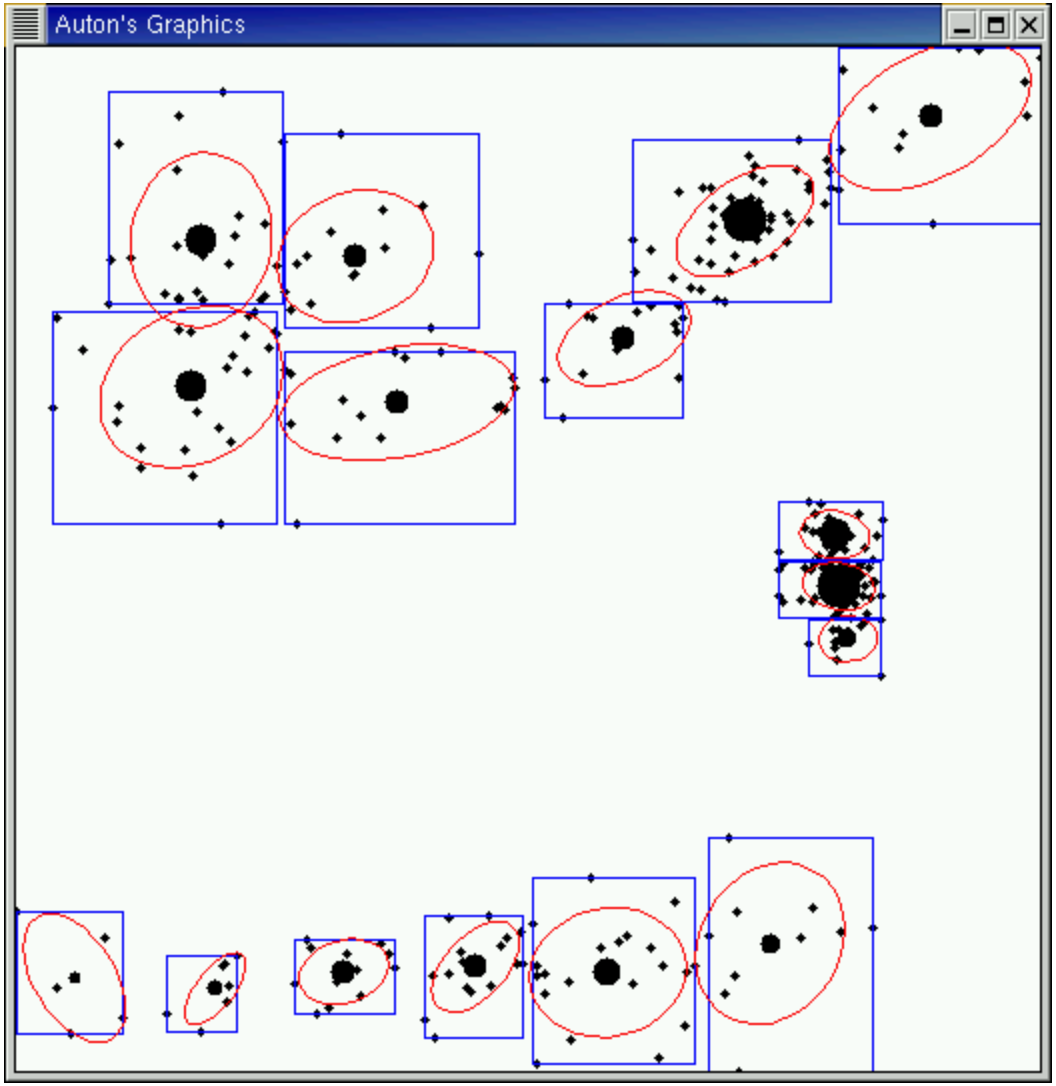
A *kd*-tree: level 3



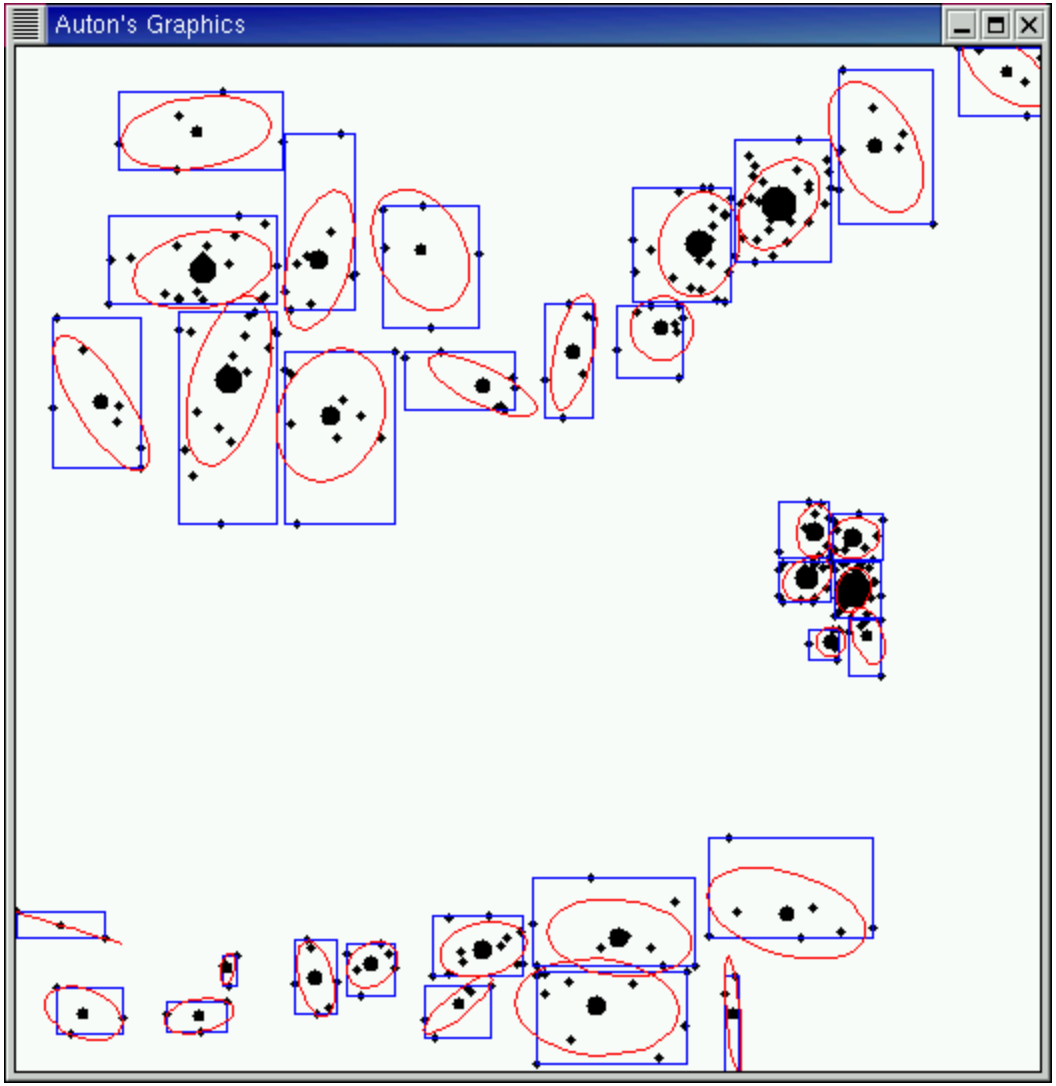
A *kd*-tree: level 4

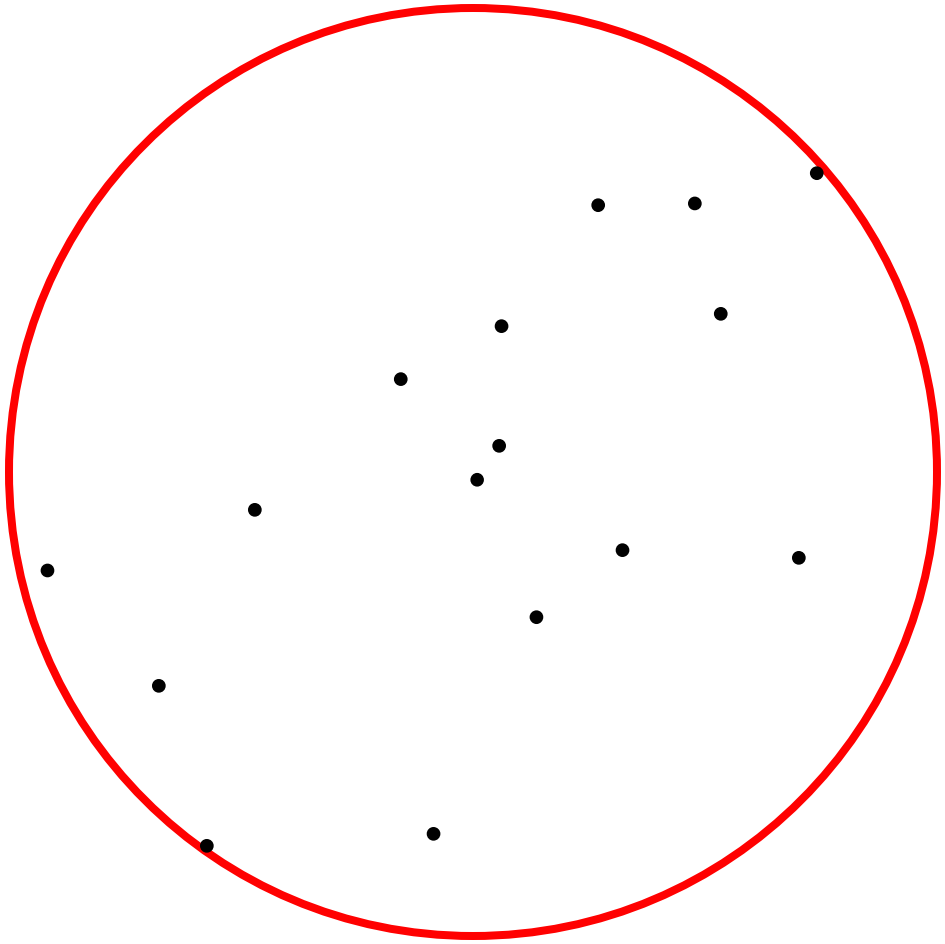


A *kd*-tree: level 5



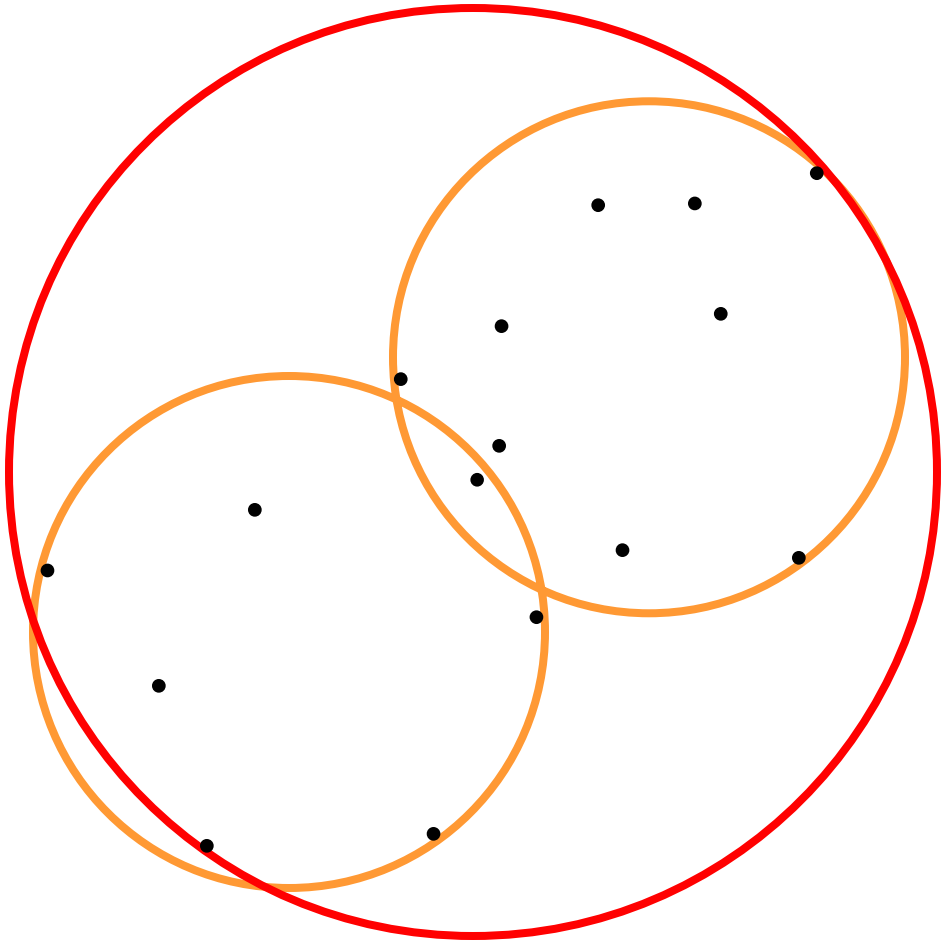
A *kd*-tree: level 6



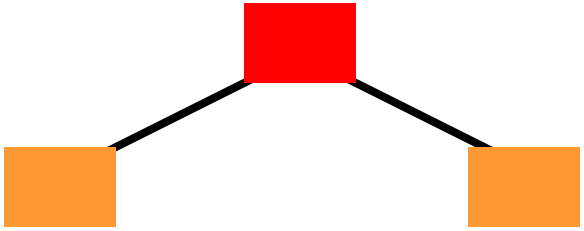


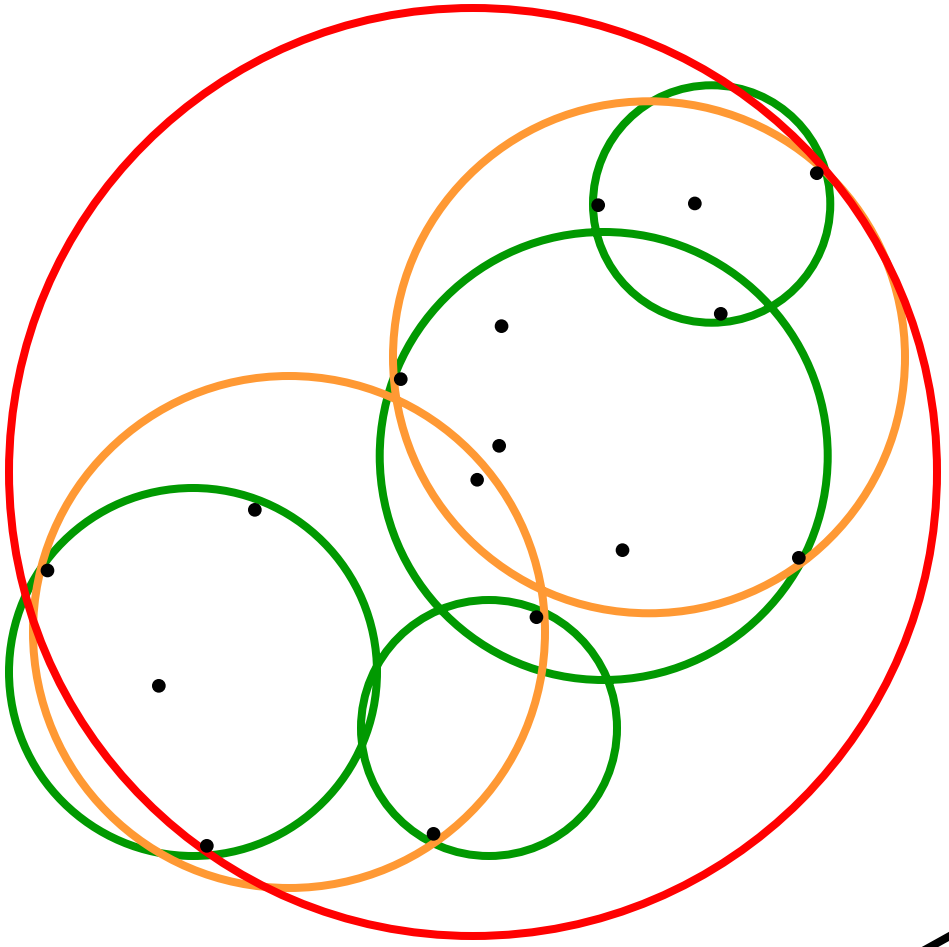
A ball-tree: level 1

[Uhlmann 1991], [Omohundro 1991]

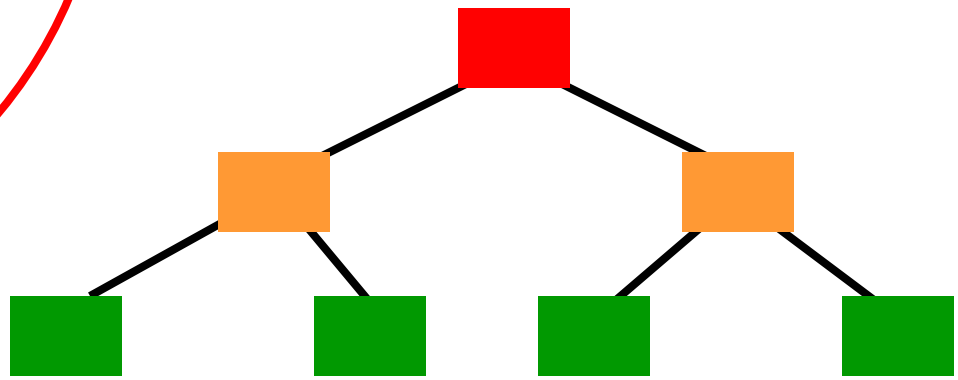


A ball-tree: level 2

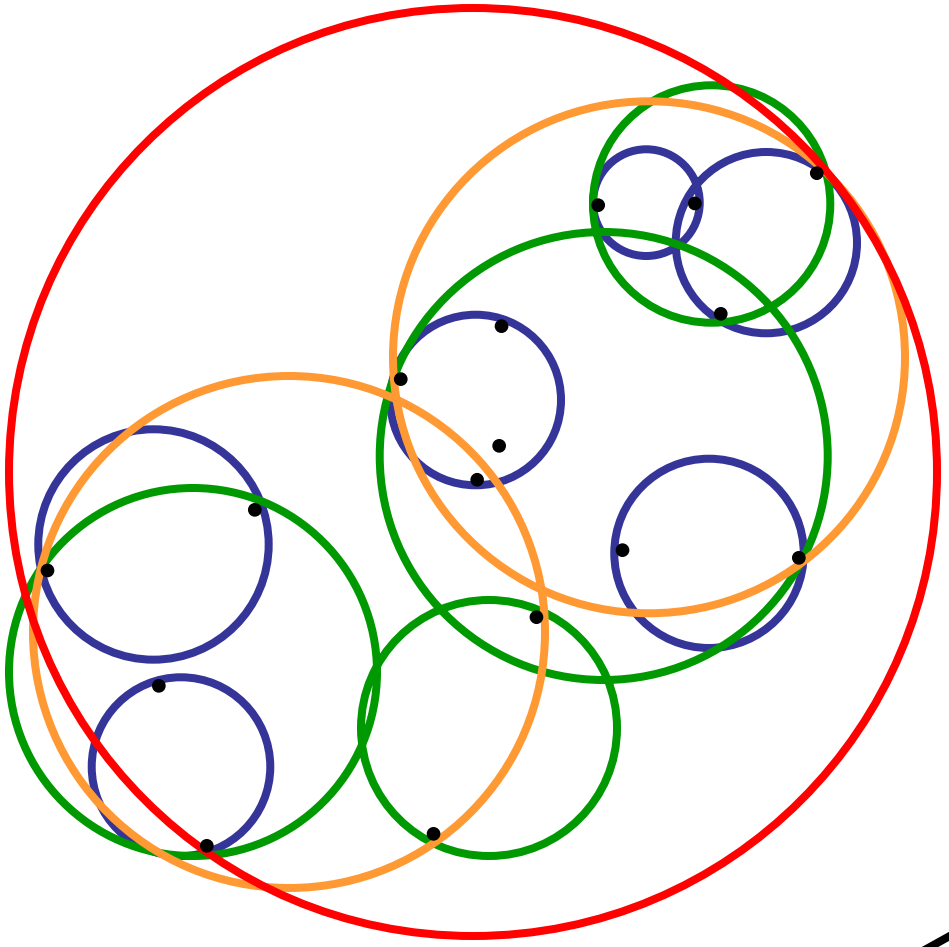


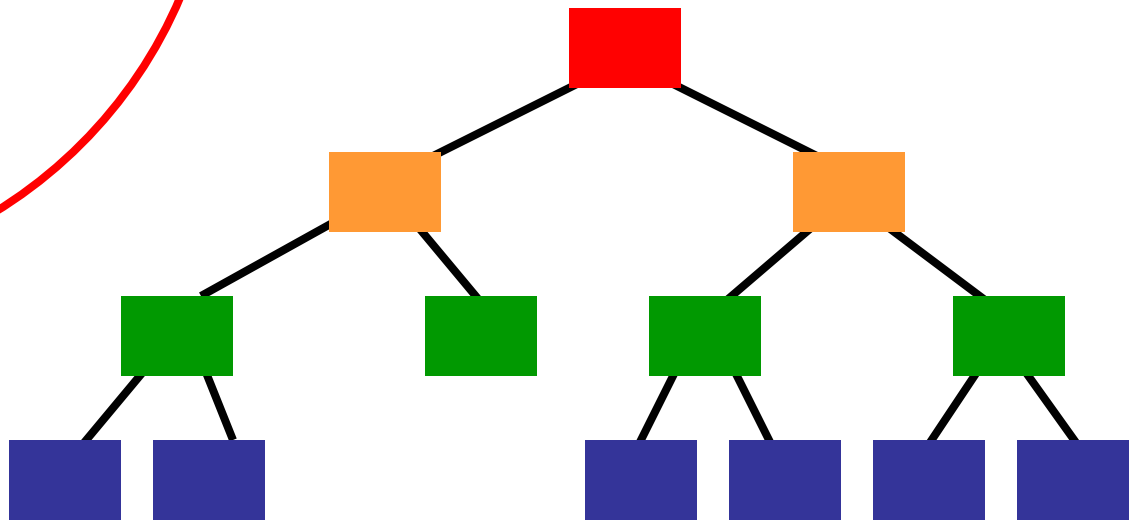


A ball-tree: level 3

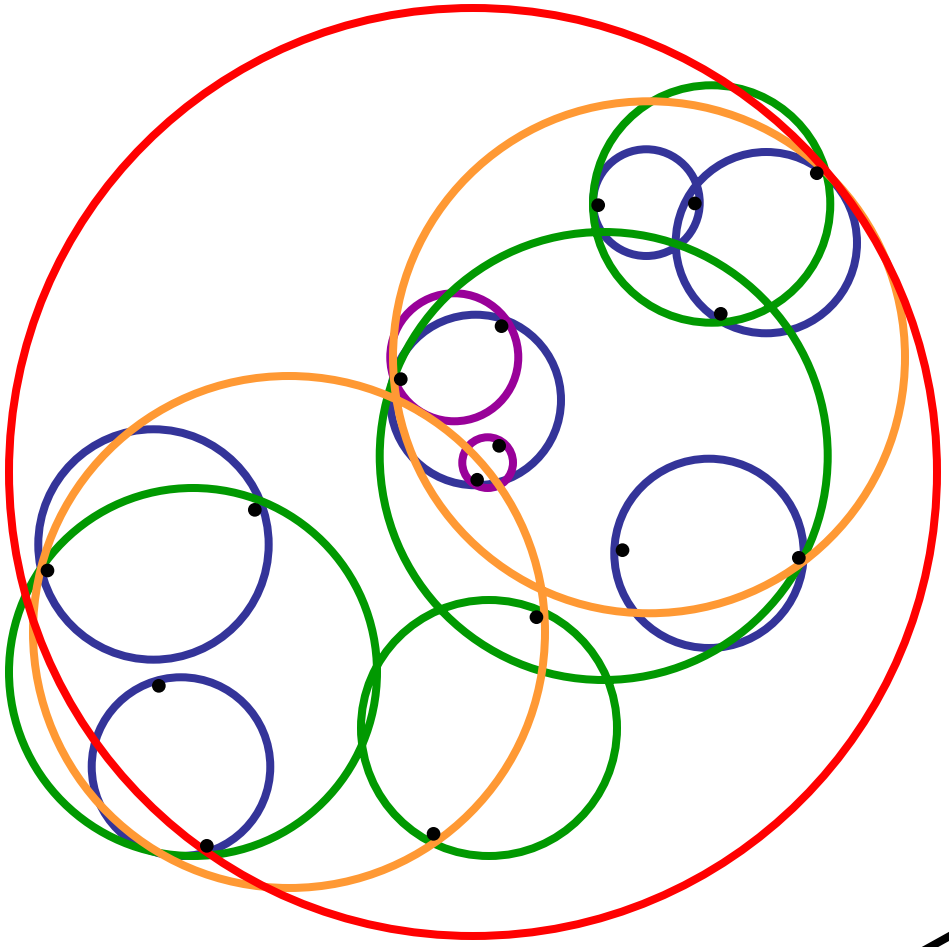


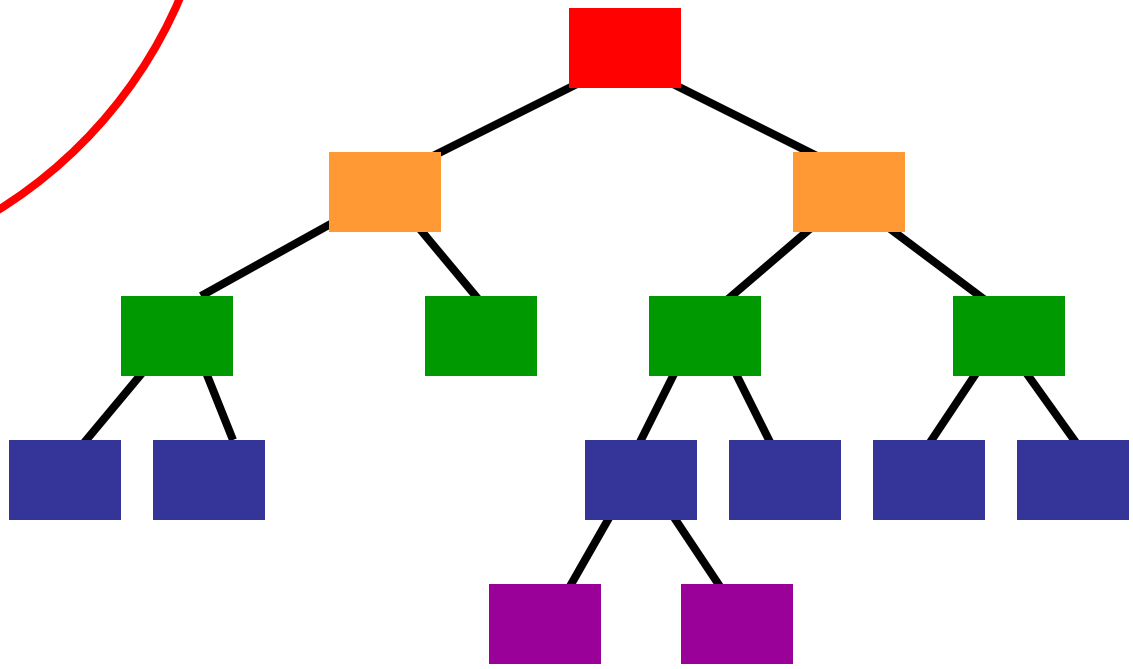
A ball-tree: level 4





A ball-tree: level 5





N-body methods: Comparison

	Barnes-Hut	**FMM**
runtime	$O(N \log N)$	*O(N)*
expansions	optional	required
simple,recursive?	yes	no
adaptive trees?	yes	no
error bounds?	no	yes

Questions

- What's the magic that allows *O(N)*?

  Is it really because of the expansions?

- Can we obtain an method that's:

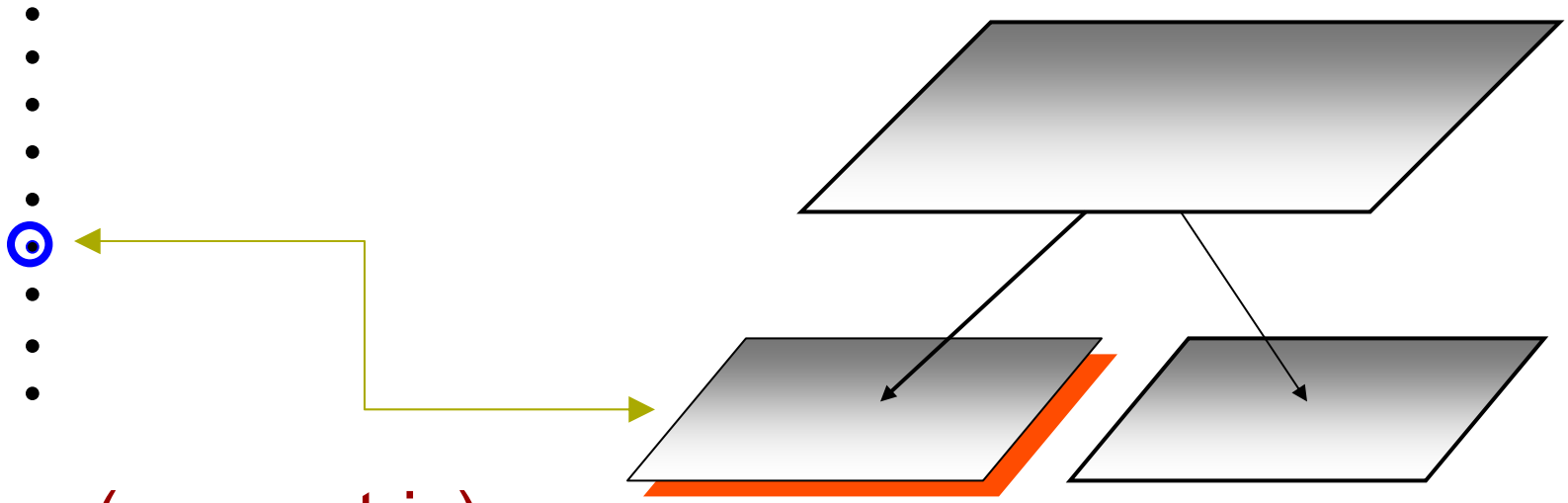
  1. *O(N)*
  2. lightweight: works with or without expansions

     simple, recursive

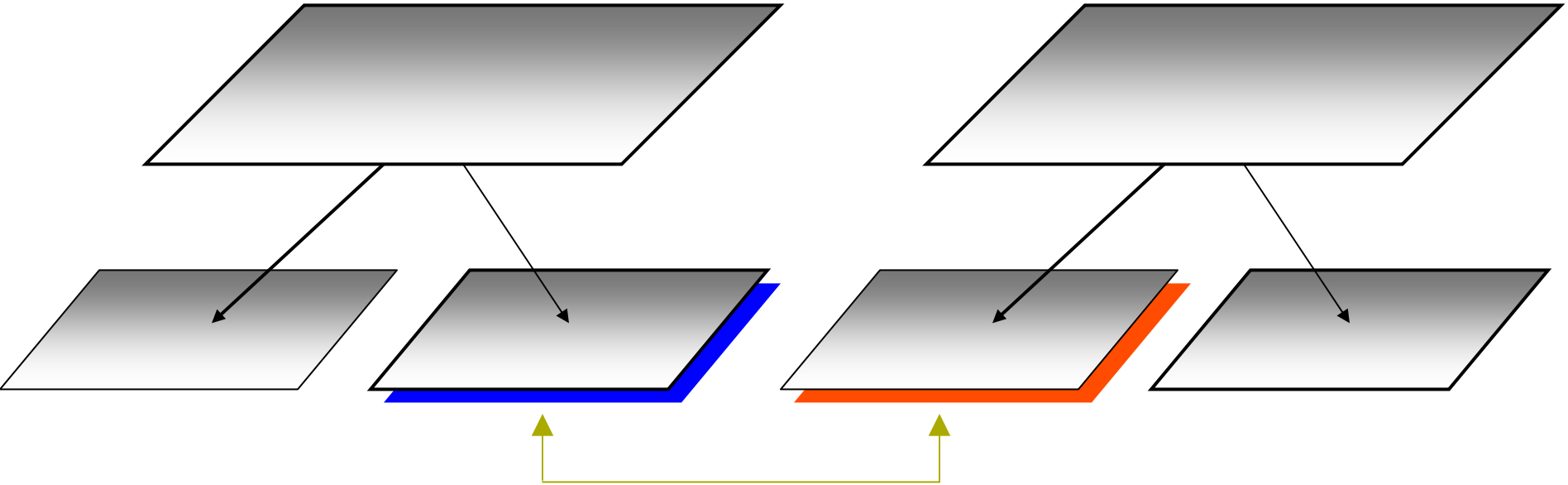
New algorithm

- Use an adaptive tree (*kd*-tree or ball-tree)
- Dual-tree recursion
- Finite-difference approximation

Single-tree:



Dual-tree (symmetric):



Simple recursive algorithm

```
SingleTree(q,R)
{
   if approximate(q,R), return.

   if leaf(R), SingleTreeBase(q,R).
   else,
      SingleTree(q,R.left).
      SingleTree(q,R.right).
}
```

(NN or range-search: recurse on the closer node first)

Simple recursive algorithm

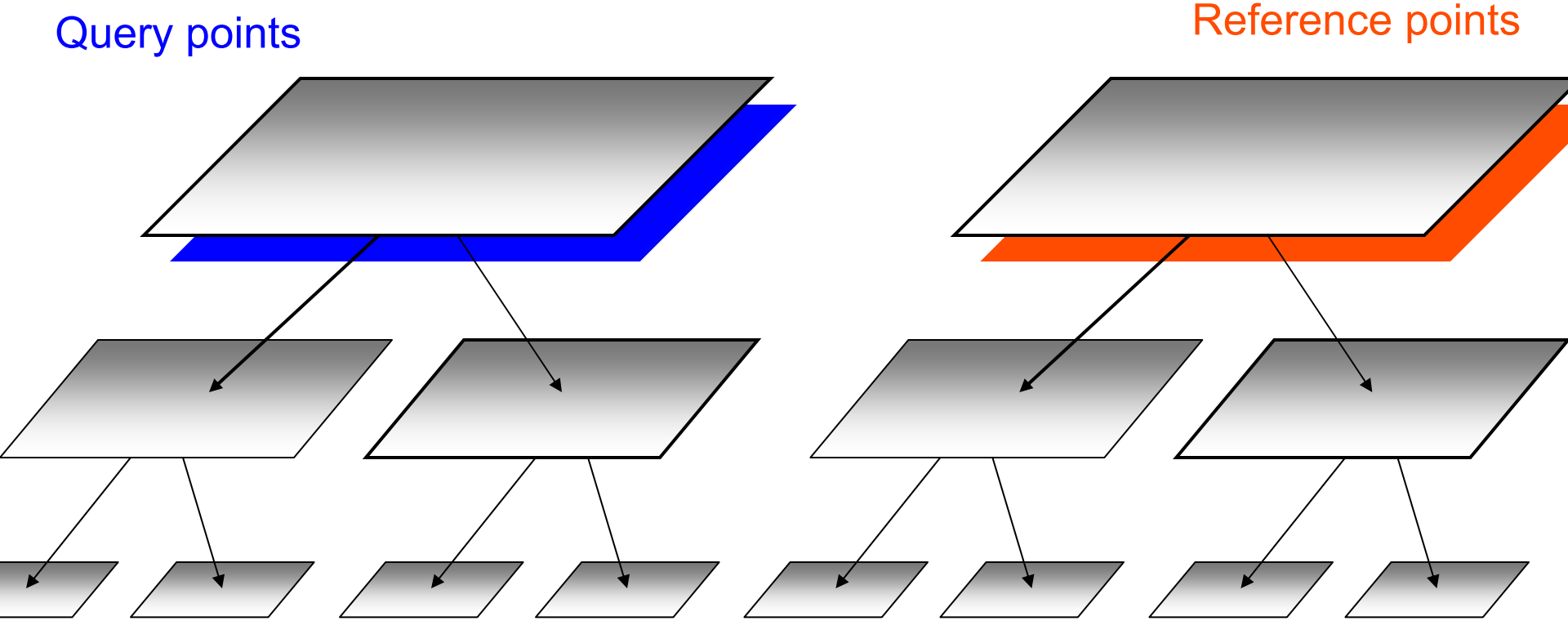
```
DualTree(Q,R)
{
   if approximate(Q,R), return.

   if leaf(Q) and leaf(R), DualTreeBase(Q,R).
   else,
      DualTree(Q.left,R.left).
      DualTree(Q.left,R.right).
      DualTree(Q.right,R.left).
      DualTree(Q.right,R.right).
}
```

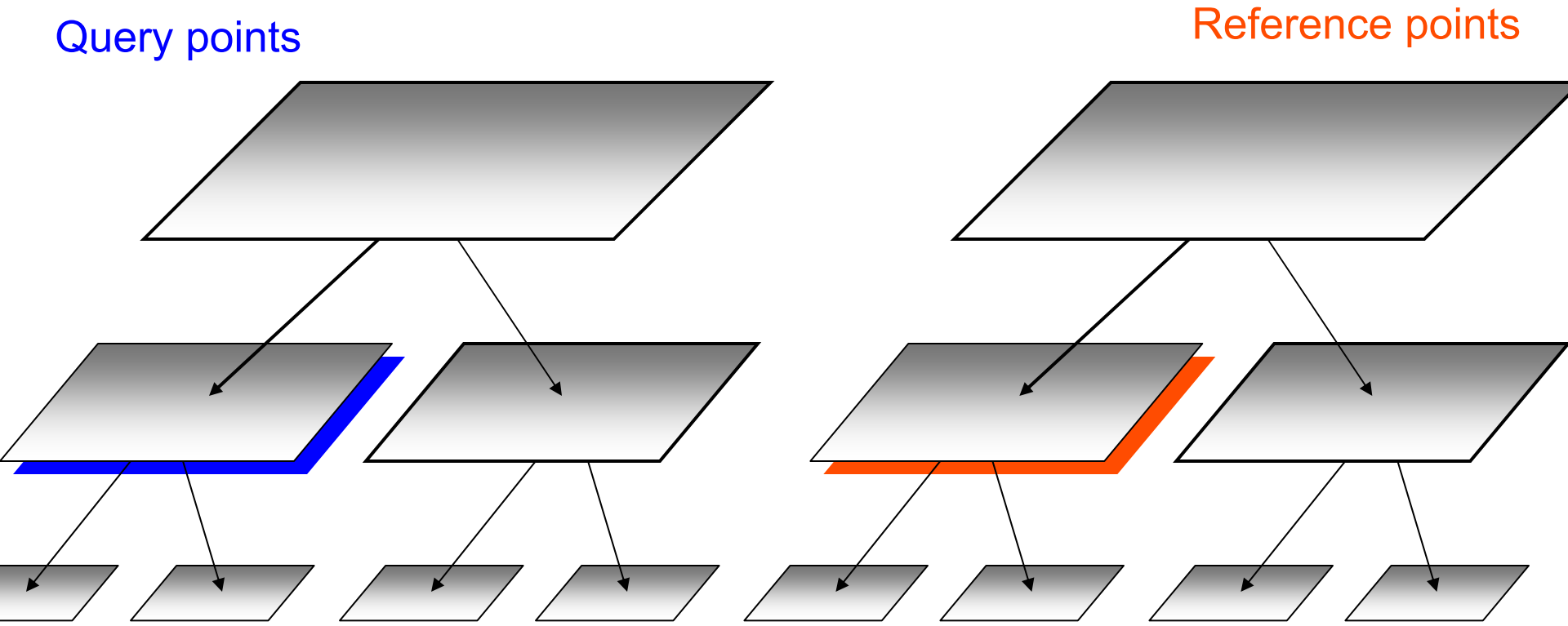
(NN or range-search: recurse on the closer node first)

Dual-tree traversal

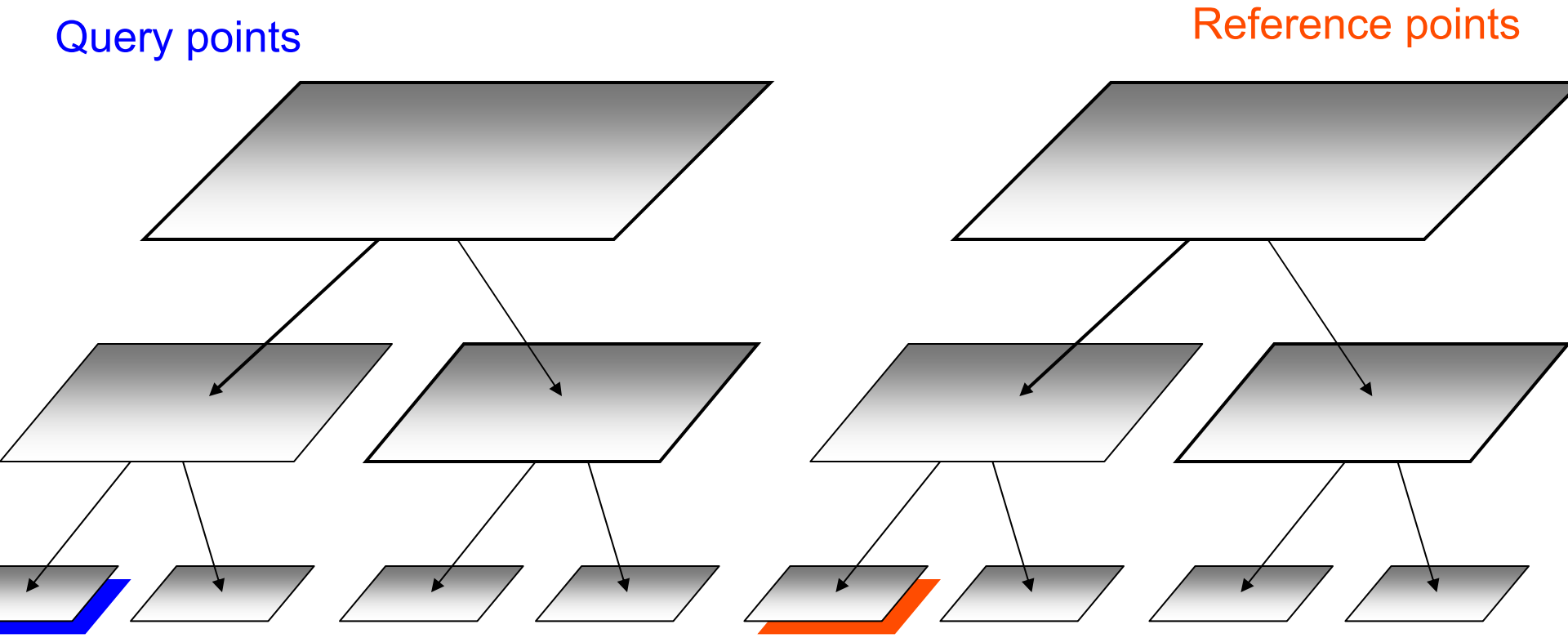
(depth-first)



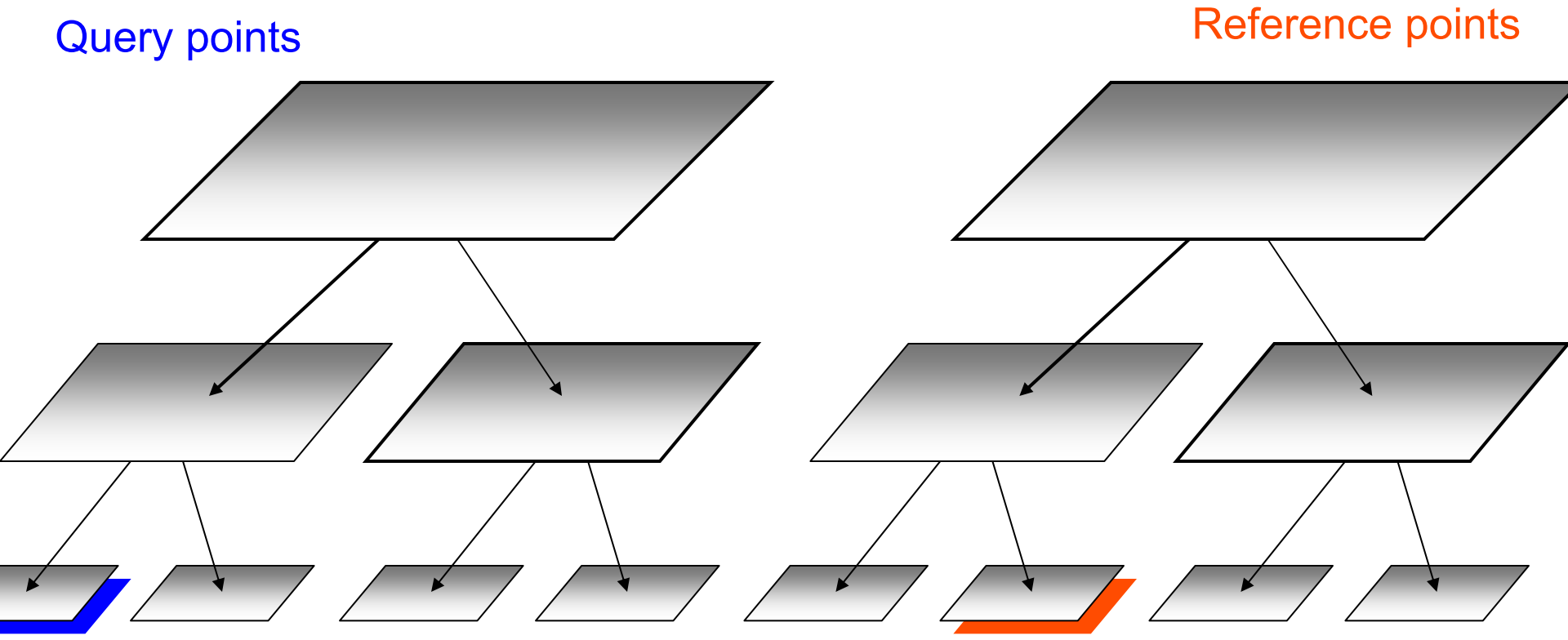
Dual-tree traversal



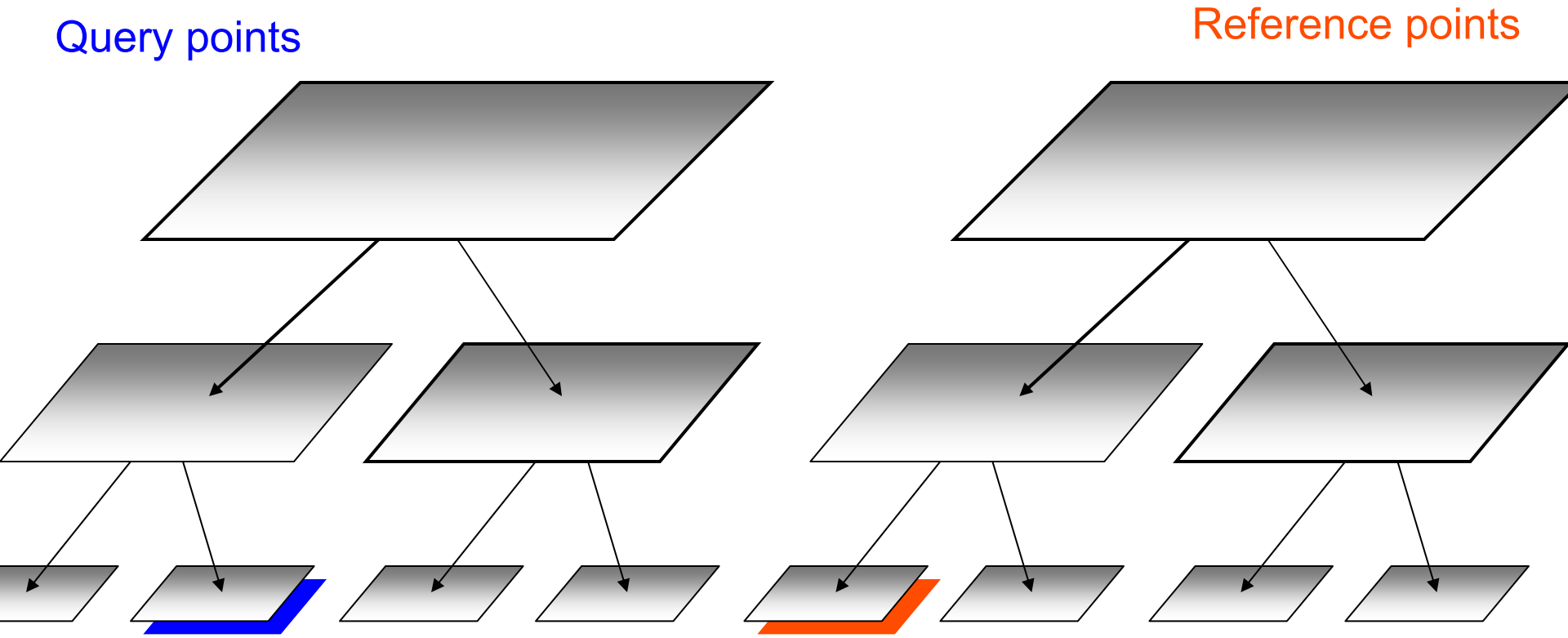
Dual-tree traversal



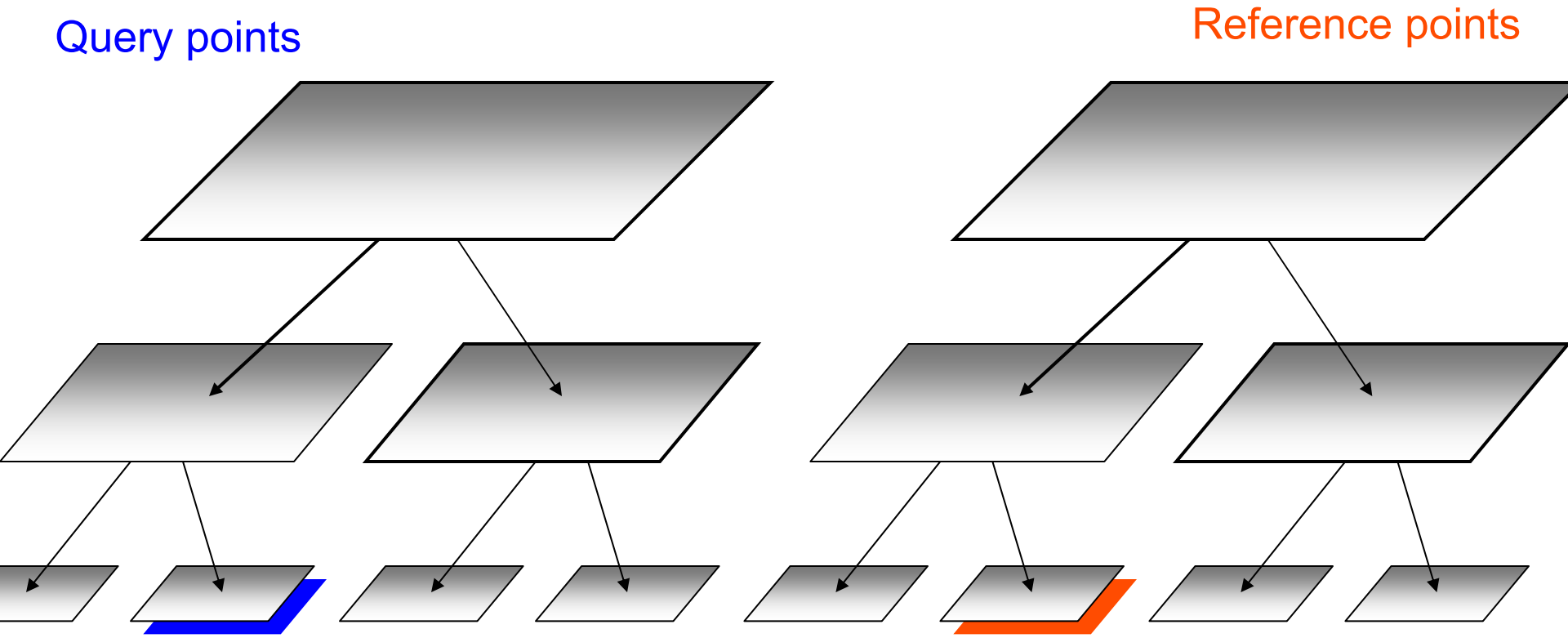
Dual-tree traversal



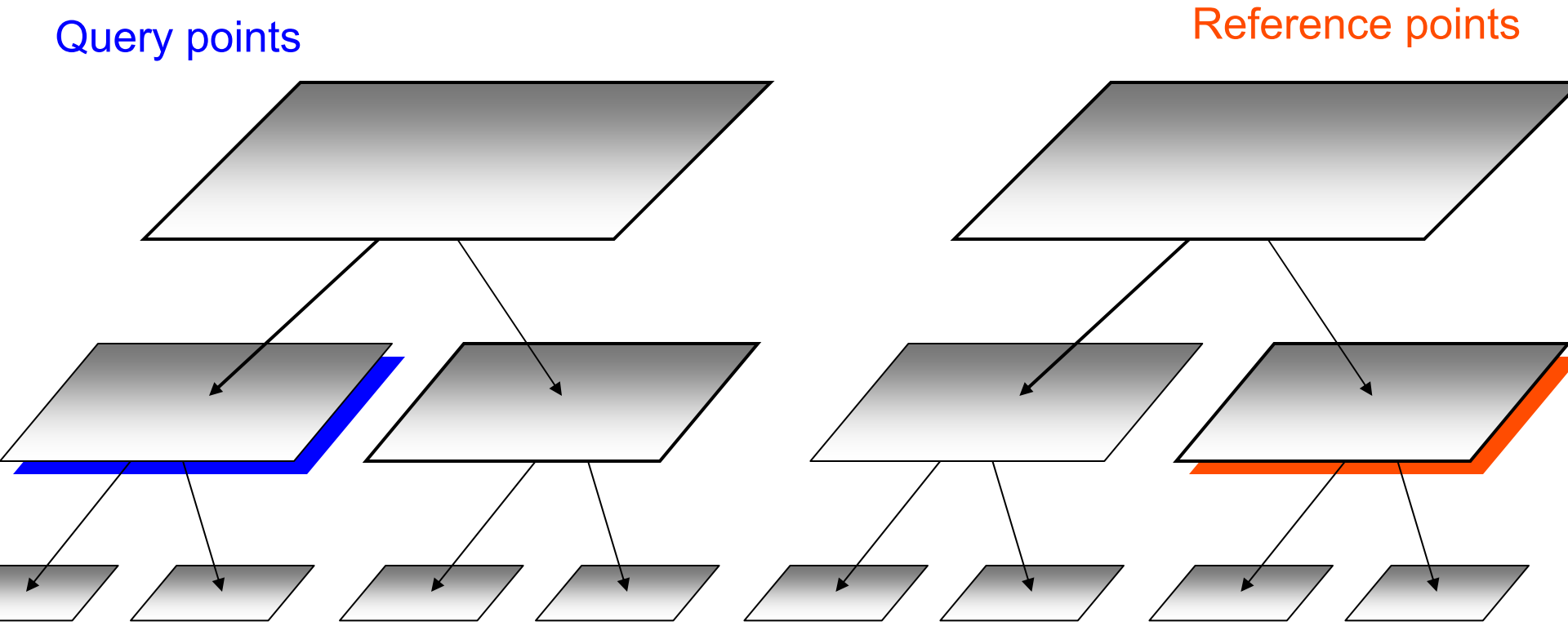
Dual-tree traversal



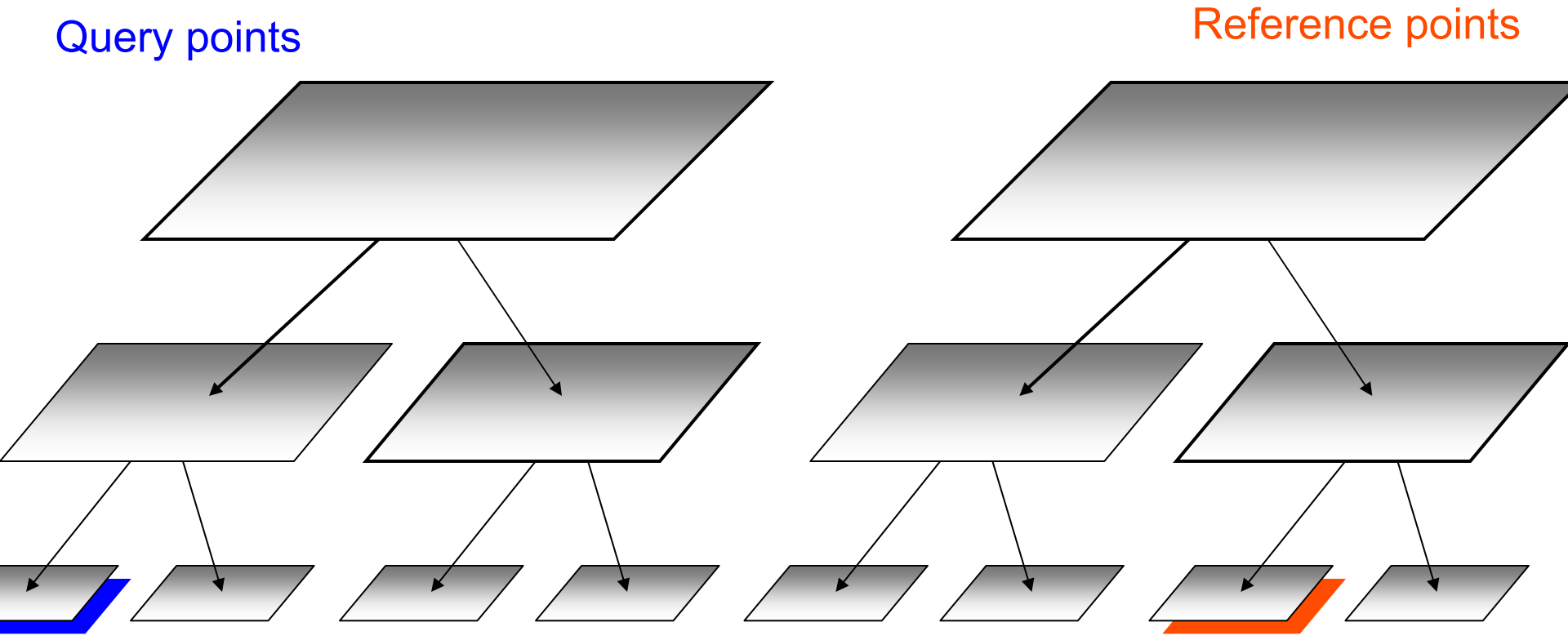
Dual-tree traversal



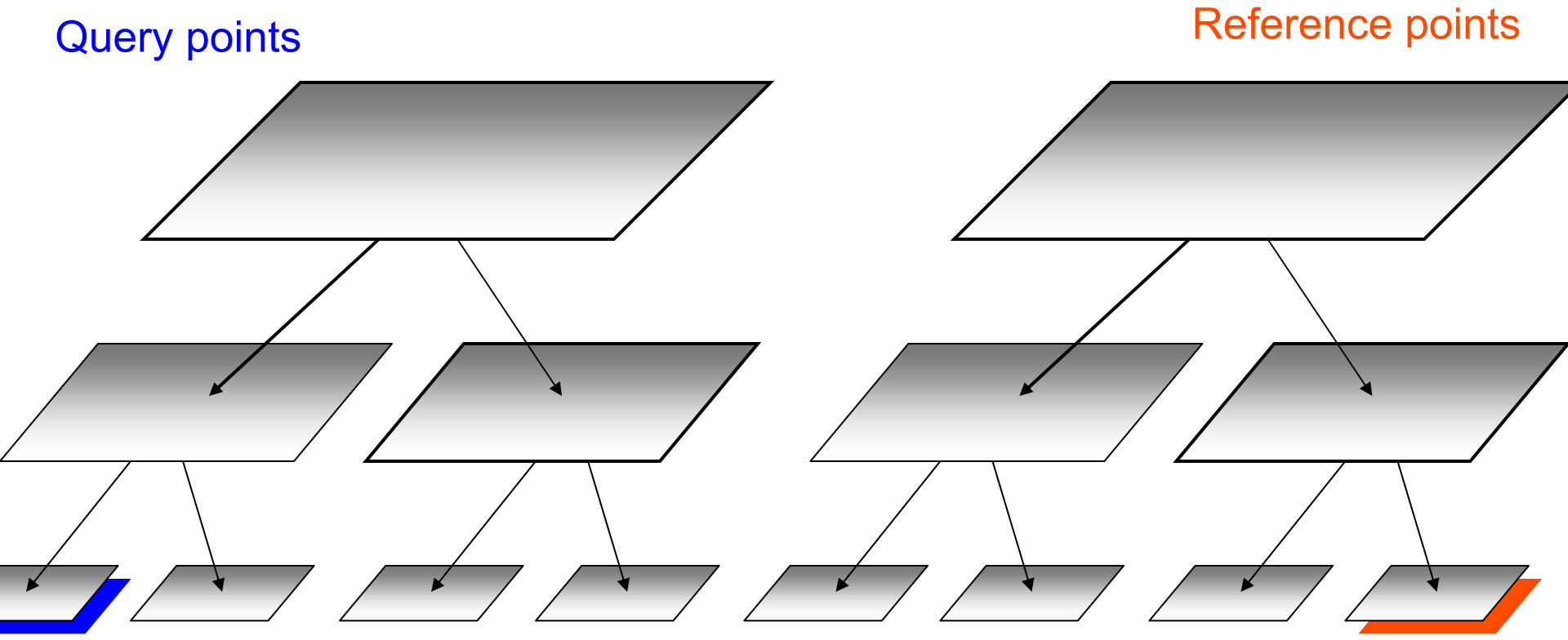
Dual-tree traversal



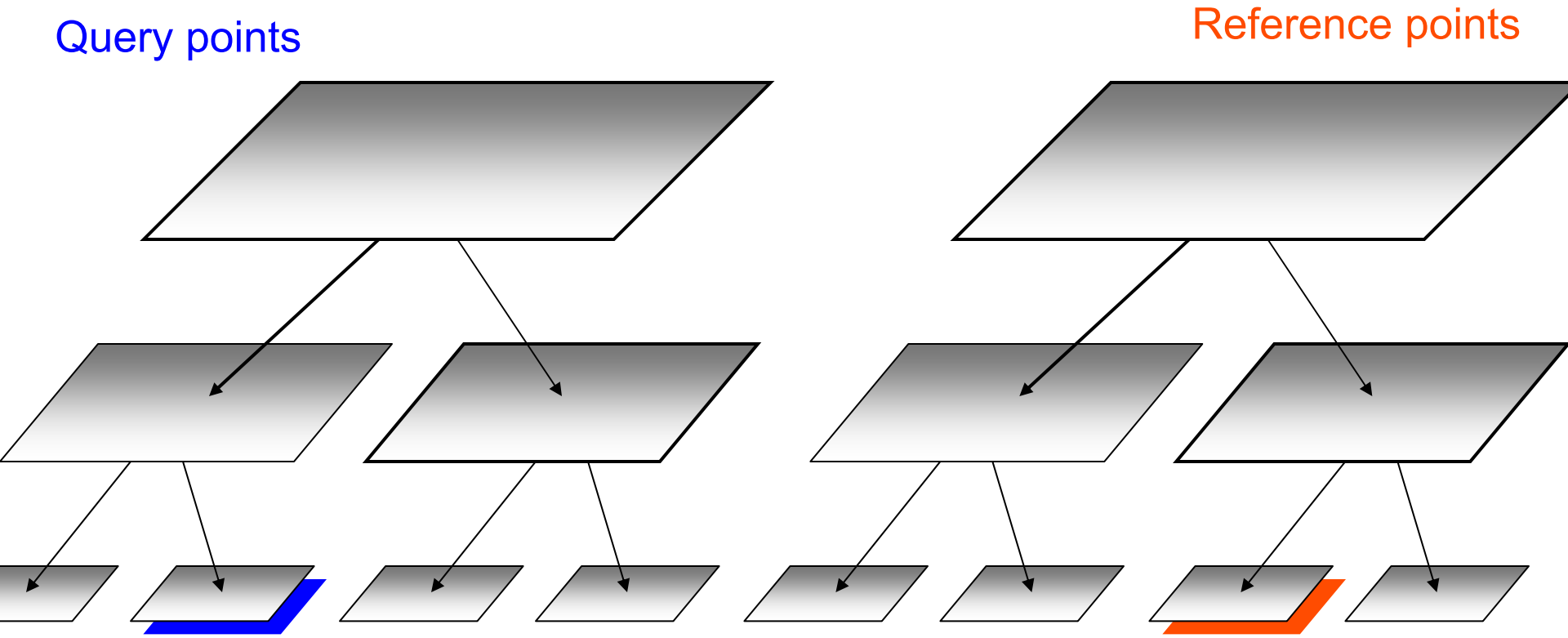
Dual-tree traversal



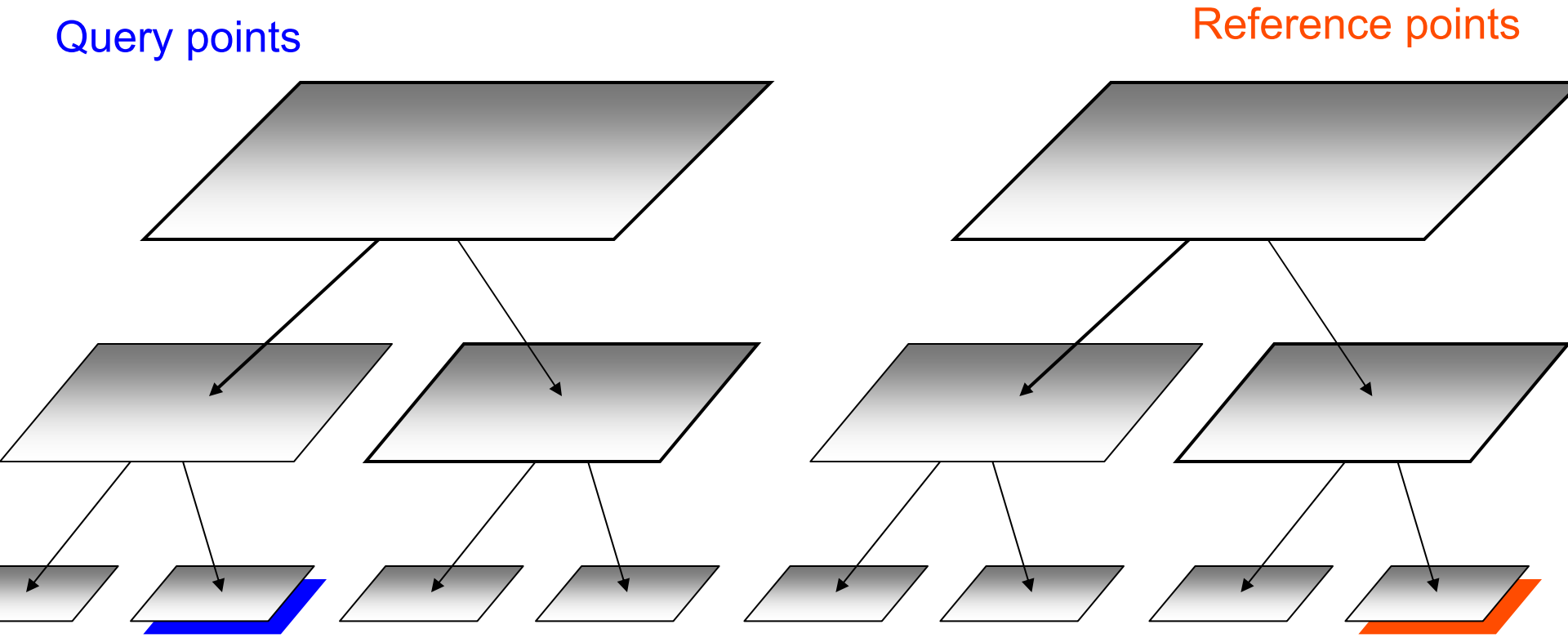
Dual-tree traversal



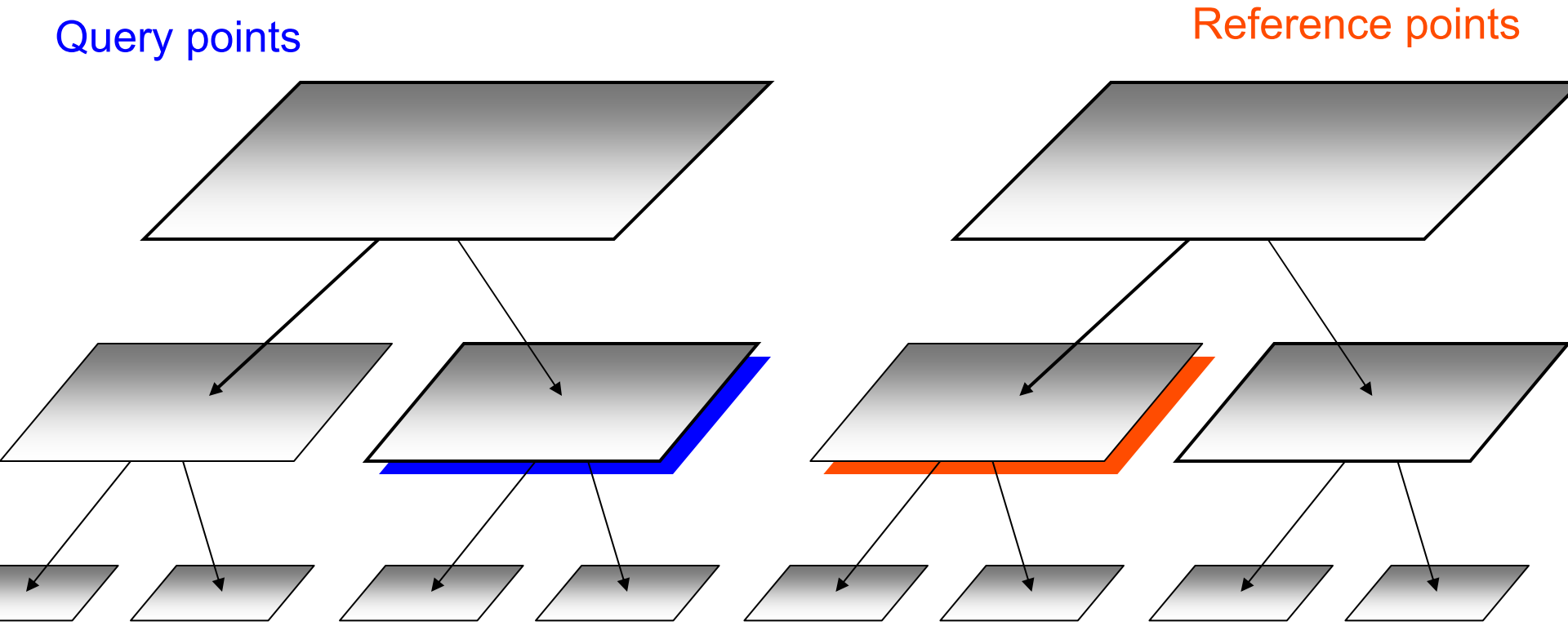
Dual-tree traversal



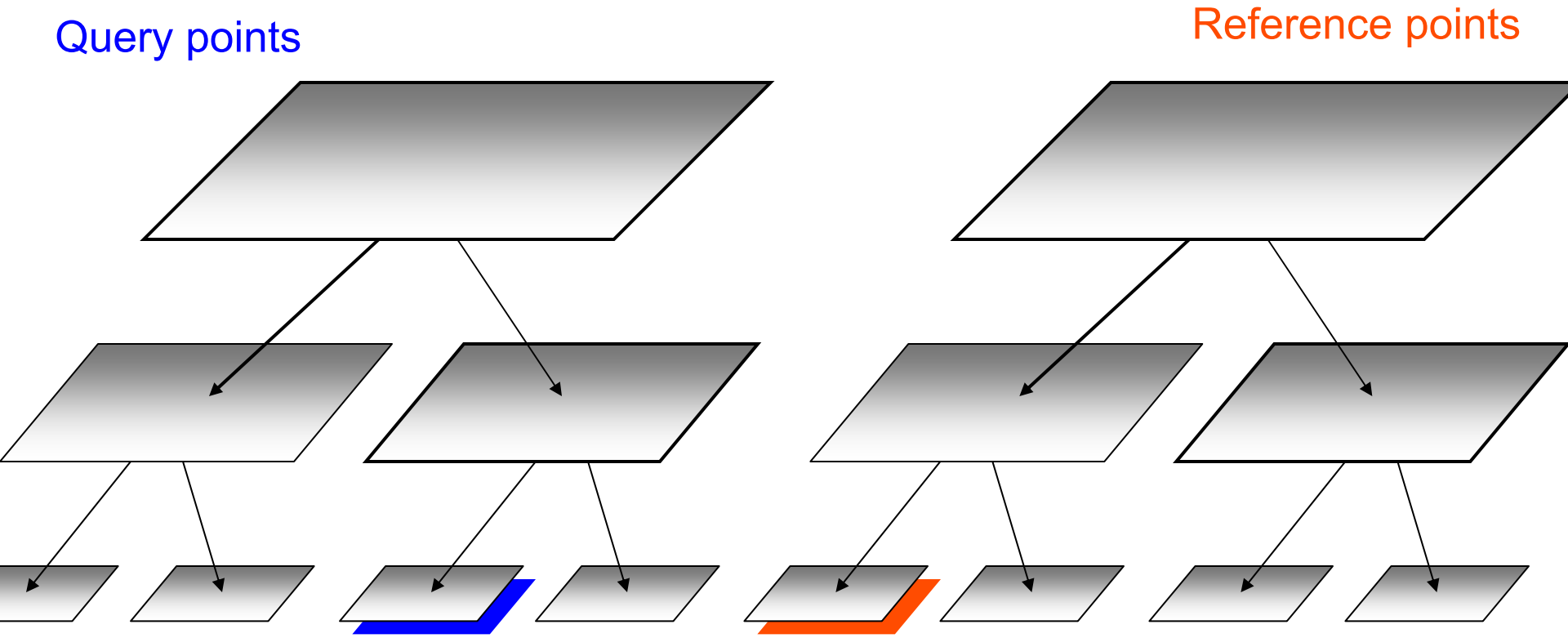
Dual-tree traversal



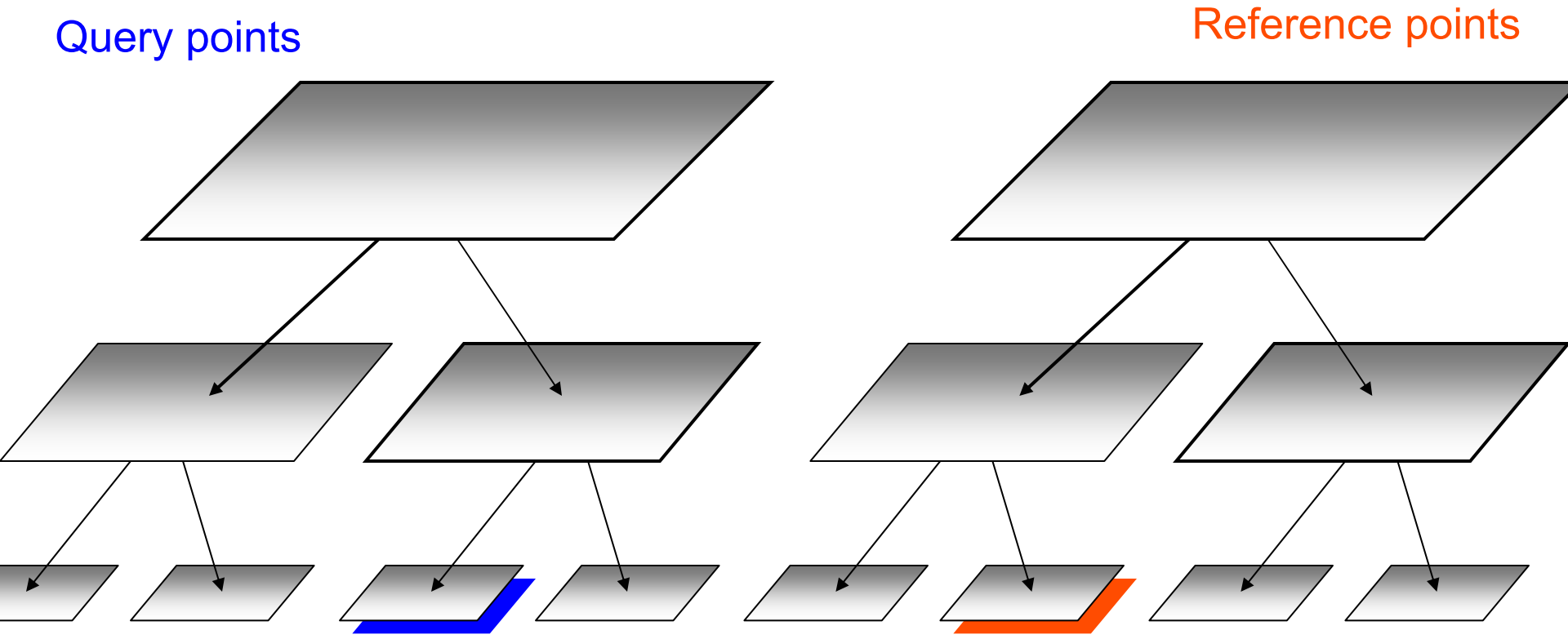
Dual-tree traversal



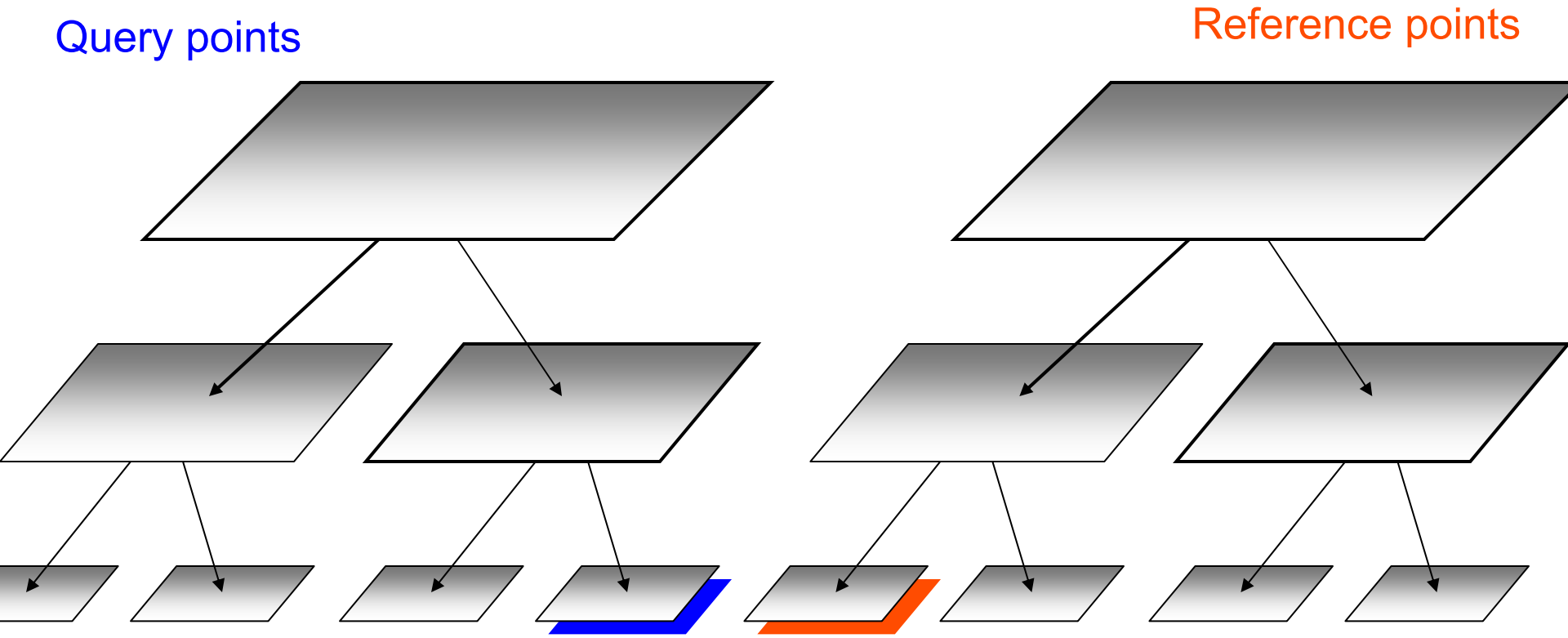
Dual-tree traversal



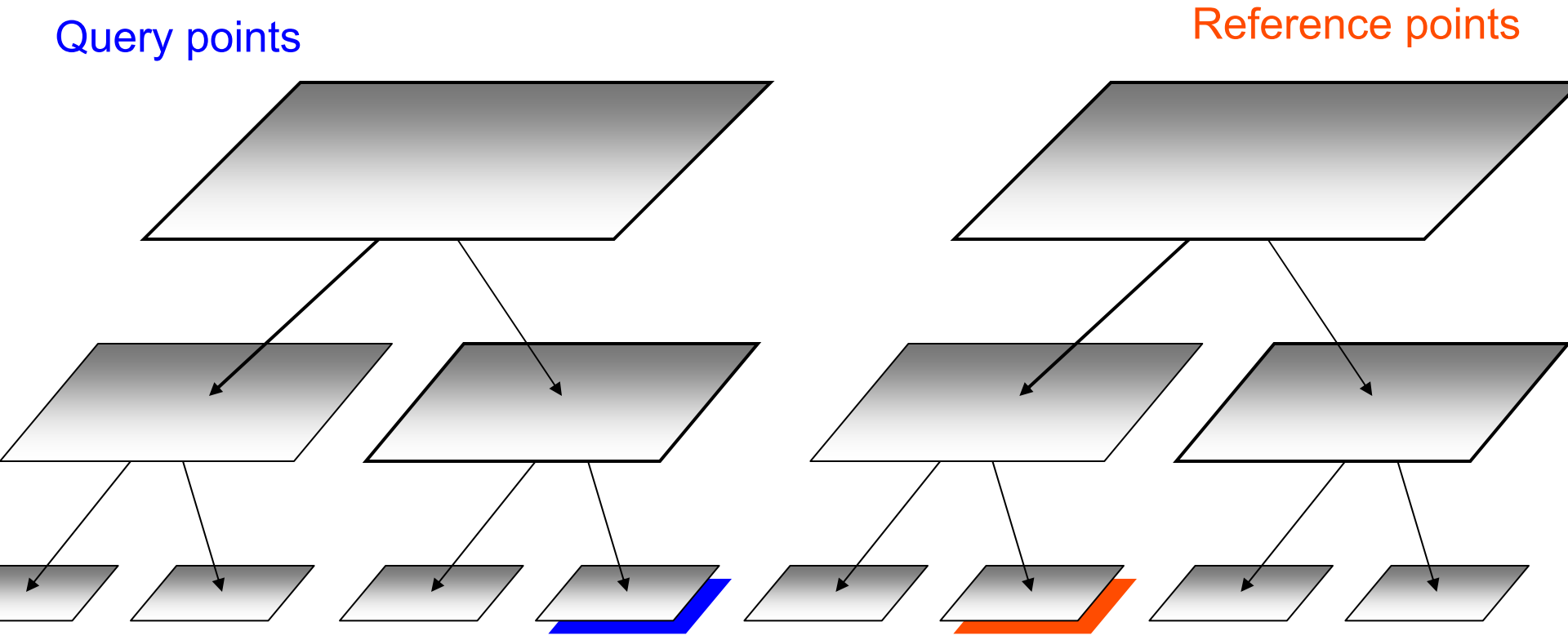
Dual-tree traversal



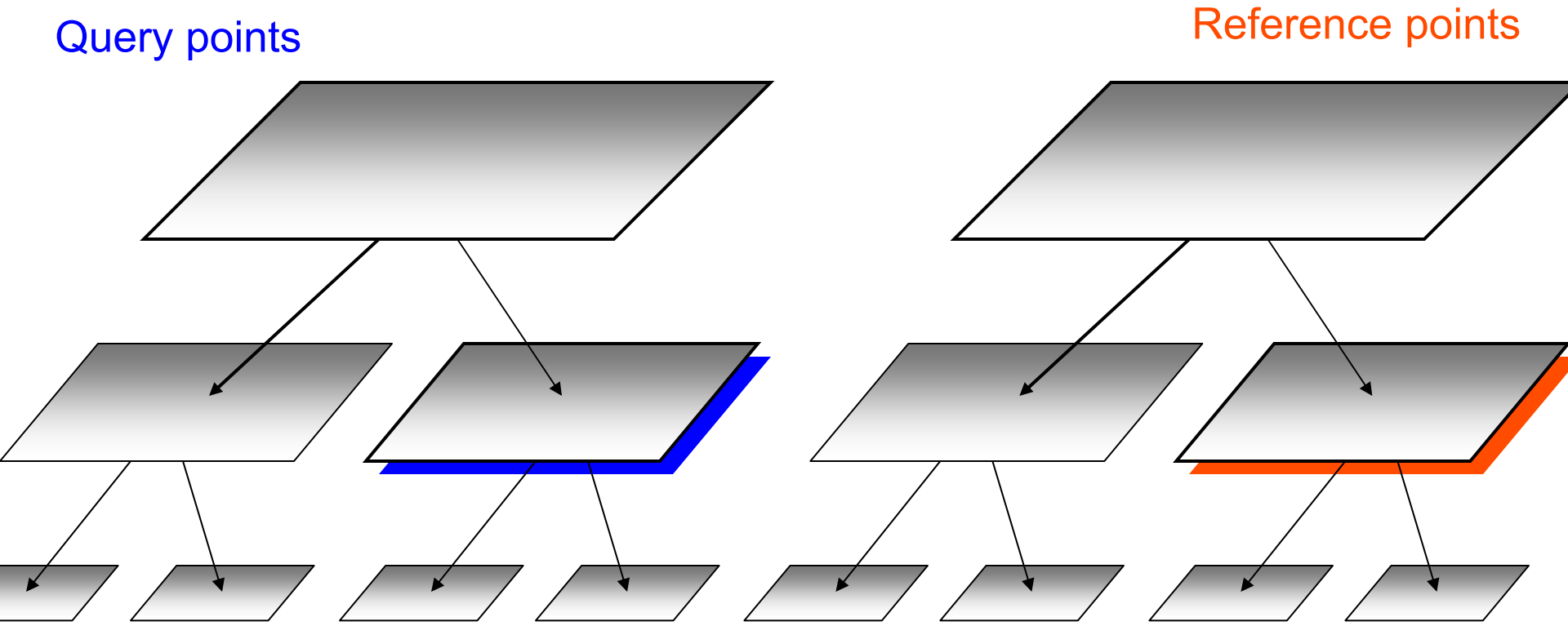
Dual-tree traversal



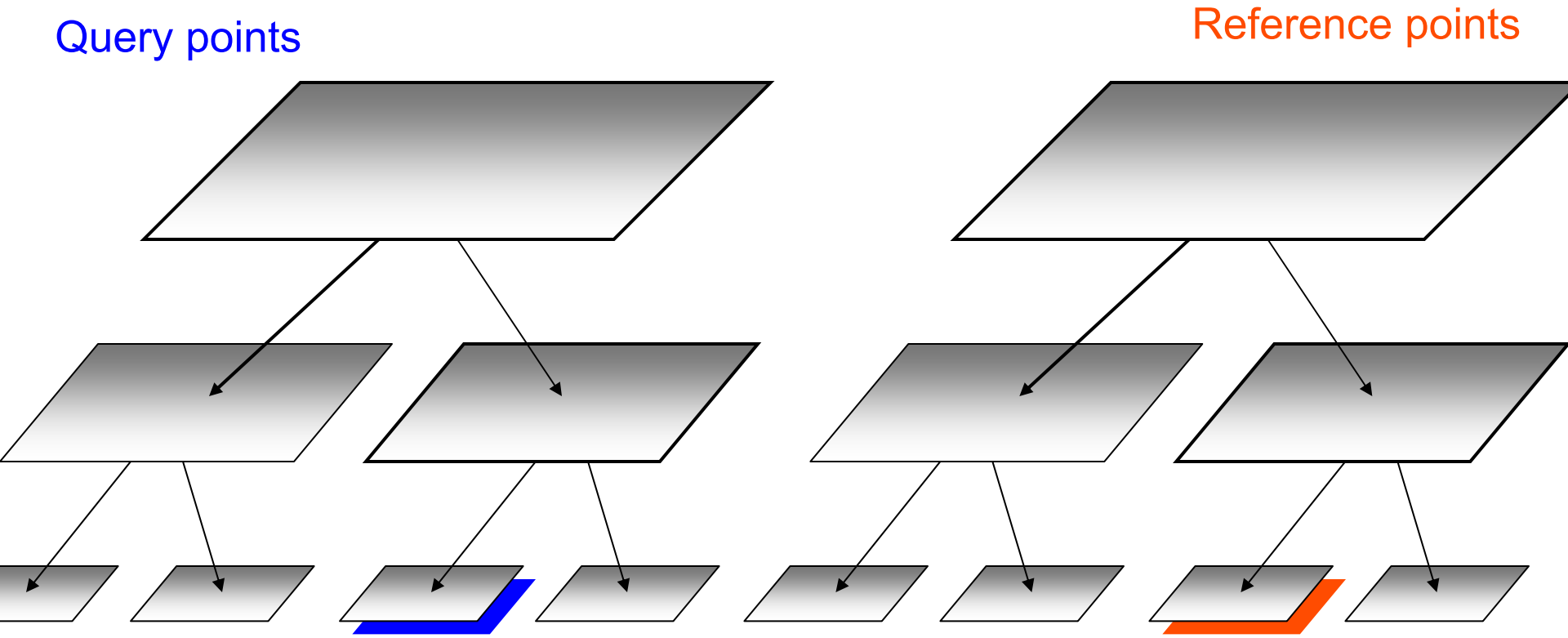
Dual-tree traversal



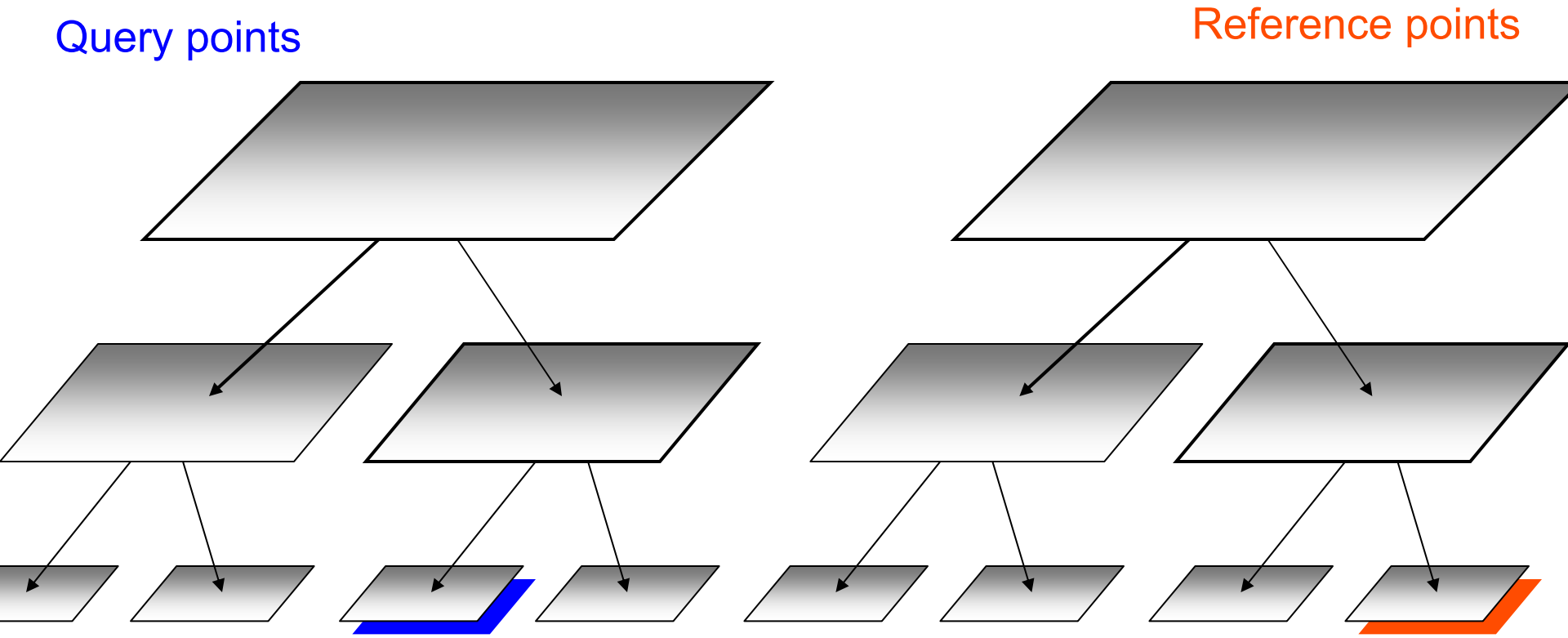
Dual-tree traversal



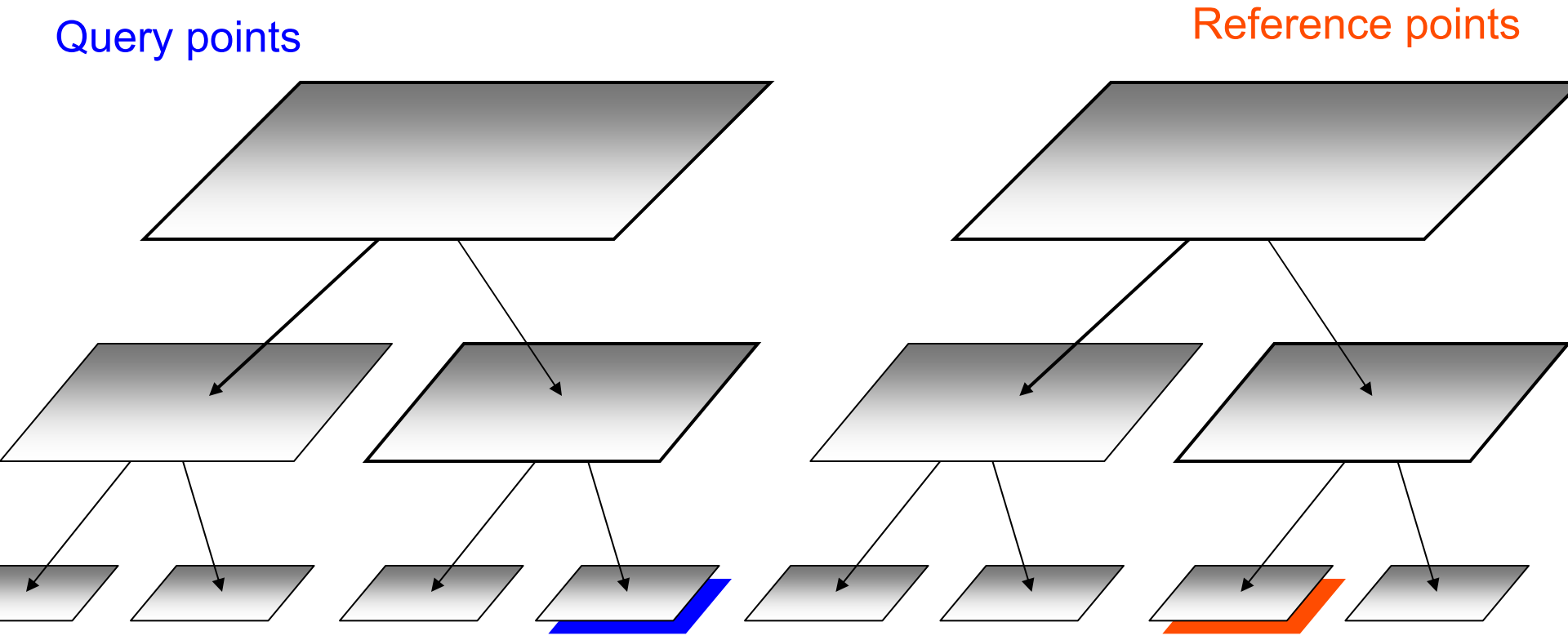
Dual-tree traversal



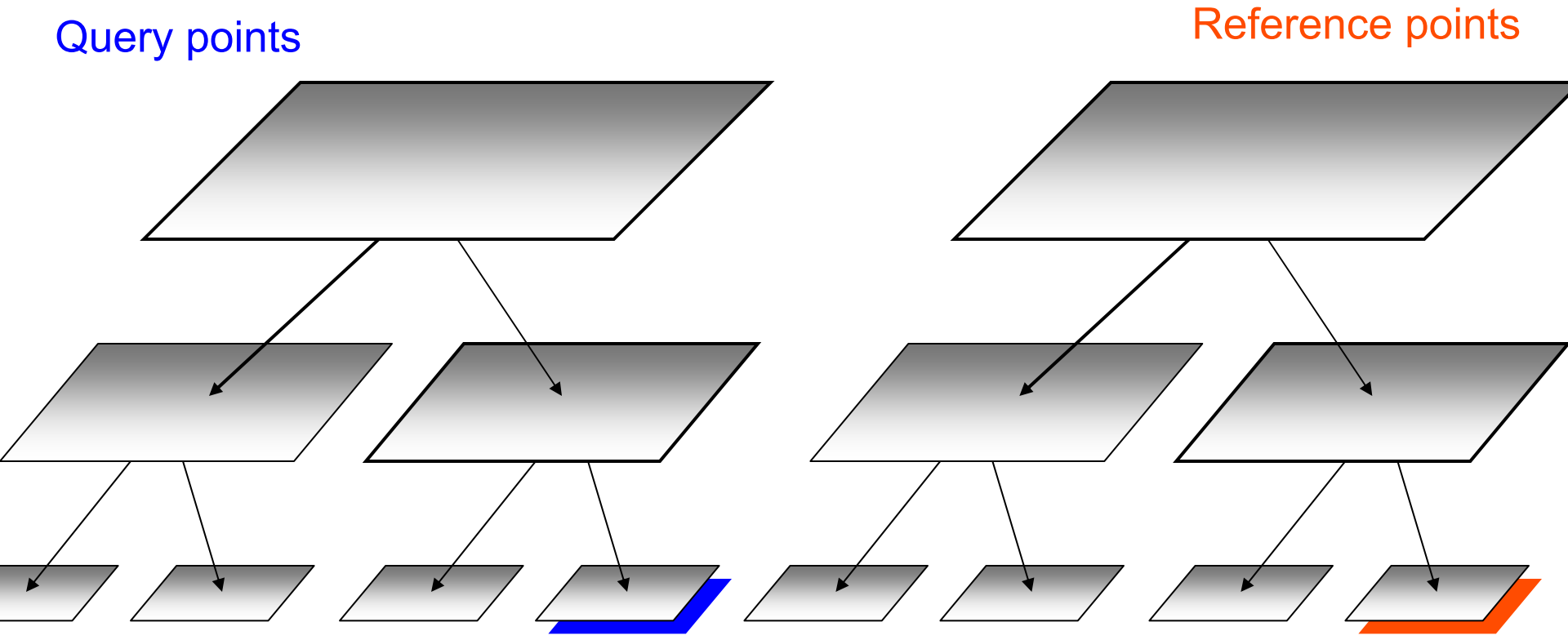
Dual-tree traversal



Dual-tree traversal



Dual-tree traversal



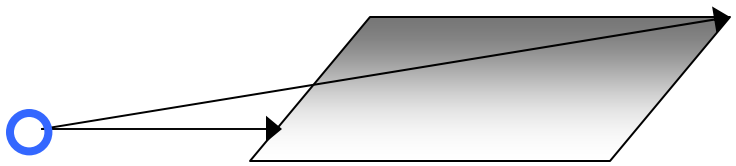
Finite-difference function approximation.

Taylor expansion:

$$f(x) \approx f(a) + f'(a)(x-a)$$

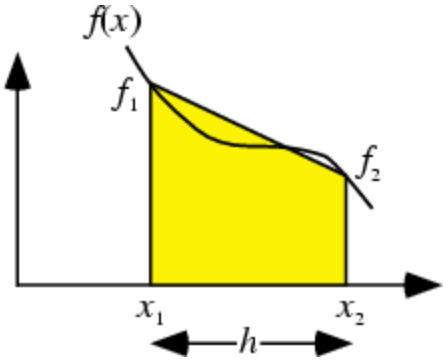
Gregory-Newton finite form:

$$f(x) \approx f(x_i) + \frac{1}{2}\left(\frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}\right)(x - x_i)$$



$$K(\delta) \approx K(\delta^{\min}) + \frac{1}{2}\left(\frac{K(\delta^{\max}) - K(\delta^{\min})}{\delta^{\max} - \delta^{\min}}\right)(\delta - \delta^{\min})$$

Finite-difference function approximation.

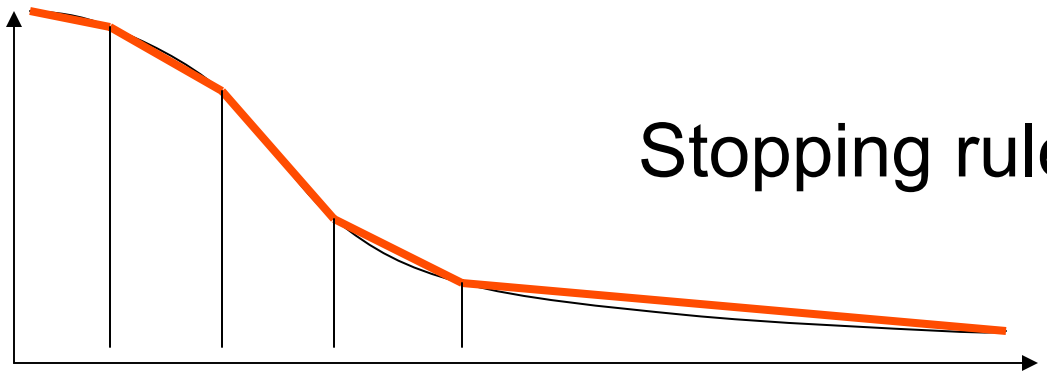


assumes monotonic decreasing kernel

$$\overline{K} = \tfrac{1}{2}\left[K(\delta_{QR}^{\min}) + K(\delta_{QR}^{\max})\right]$$

$$err_q = \sum_{r}^{N_R} \left| K(\delta_{qr}) - \overline{K} \right| \le \frac{N_R}{2}\left[K(\delta_{QR}^{\min}) - K(\delta_{QR}^{\max})\right]$$

could also use center of mass



Stopping rule: approximate if *s* > *r*

Simple approximation method

approximate(Q,R)
{

$$dl = N_R K(\delta_{\max}), du = N_R K(\delta_{\min}).$$

if $\delta_{\min} \geq s_{\min} \cdot \max(diam(Q), diam(R))$

incorporate(*dl*, *du*).
}

→trivial to change kernel
→hard error bounds

Runtime analysis

THEOREM: Dual-tree algorithm is ***O(N)***
in worst case (linear-depth trees)

NOTE: Faster algorithm using different approximation rule: O(N) expected case

ASSUMPTION: *N* points from density *f*

$$0 < c \leq f \leq C$$

Recurrence for self-finding

single-tree (point-node)

$$T(N) = T(N/2) + O(1)$$

$$T(1) = O(1)$$

$$\Rightarrow N \cdot O(\log N)$$

dual-tree (node-node)

$$T(N) = 2T(N/2) + O(1)$$

$$T(1) = O(1)$$

$$\Rightarrow O(N)$$

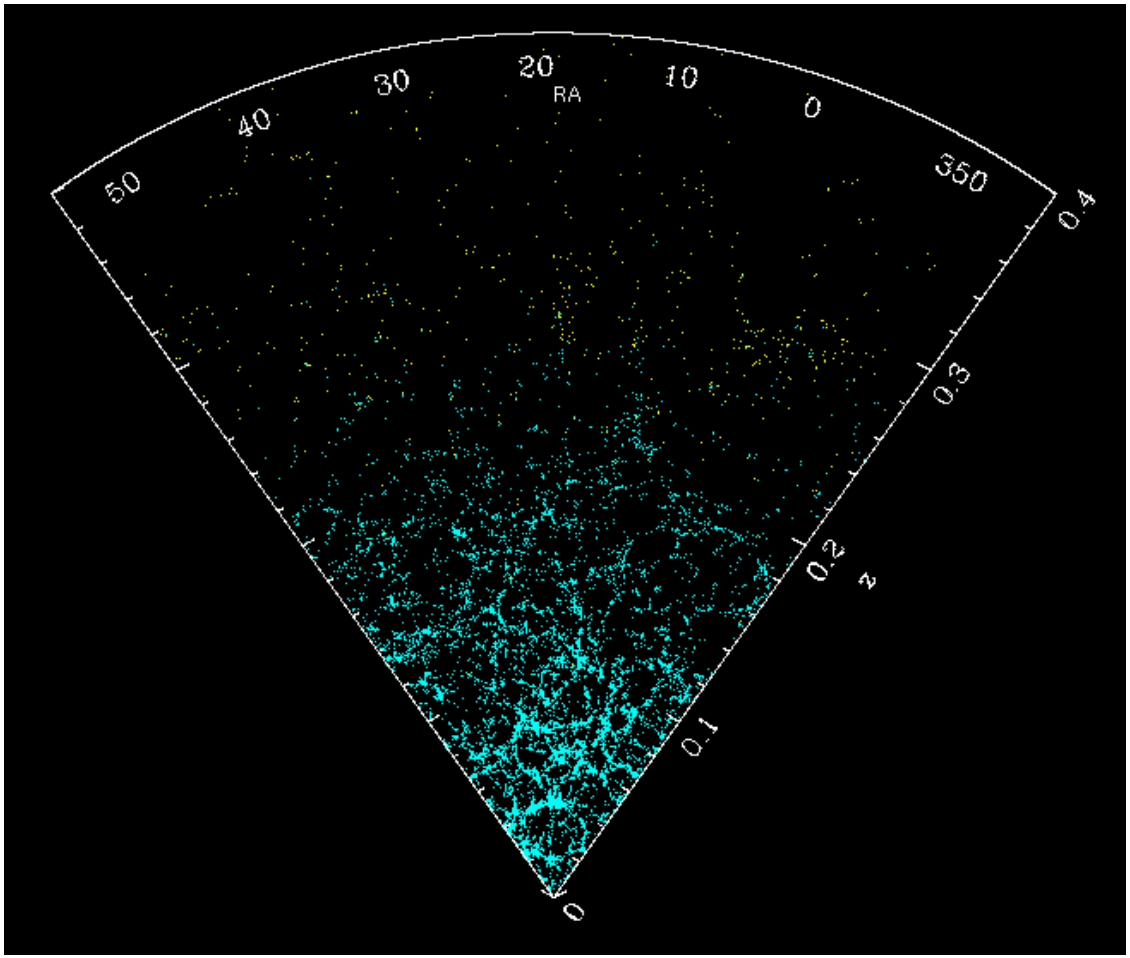
Packing bound

LEMMA: Number of nodes that are *well-separated* from a query node Q is bounded by a constant $\lceil 1 + g(s, c, C) \rceil^D$

Thus the recurrence yields the entire runtime. Done.

CONJECTURE: should actually be *D'* (the intrinsic dimension).

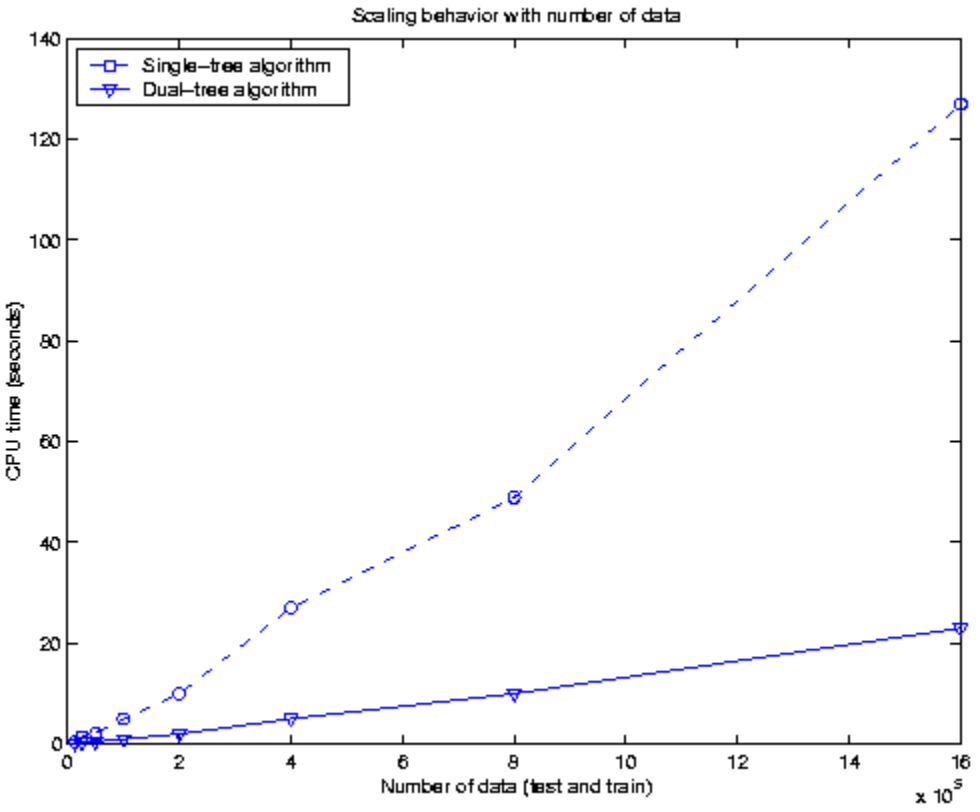
Real data: SDSS, 2-D



Speedup Results: Number of points

N	naïve	dual-tree
12.5K	7	.12
25K	31	.31
50K	123	.46
100K	494	1.0
200K	1976*	2
400K	7904*	5
800K	31616*	10
1.6M	35 hrs	23

5500x



One order-of-magnitude speedup over single-tree at ~2M points

Speedup Results: Different kernels

N	Epan.	Gauss.
12.5K	.12	.32
25K	.31	.70
50K	.46	1.1
100K	1.0	2
200K	2	5
400K	5	11
800K	10	22
1.6M	23	51

Epanechnikov:

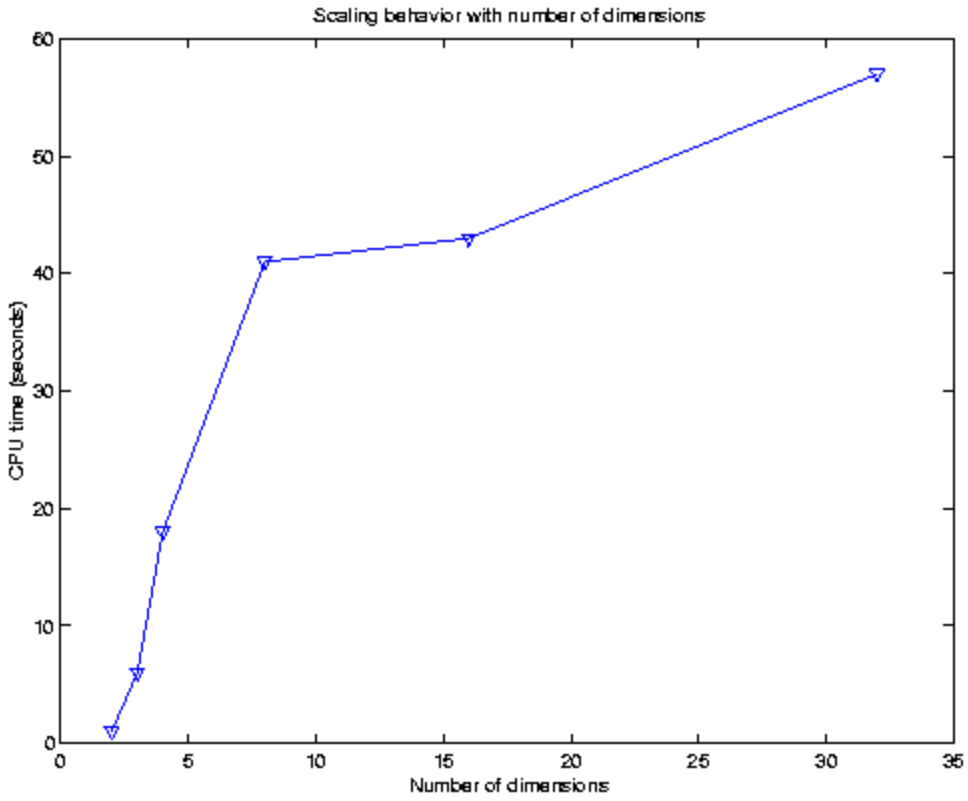
10^{-6} relative error

Gaussian:

10^{-3} relative error

Speedup Results: Dimensionality

N	Epan.	Gauss.
12.5K	.12	.32
25K	.31	.70
50K	.46	1.1
100K	1.0	2
200K	2	5
400K	5	11
800K	10	22
1.6M	23	51



Speedup Results: Different datasets

Name	N	D	Time (sec)
Bio5	103K	5	10
CovType	136K	38	8
MNIST	10K	784	24
PSF2d	3M	2	9

Meets desiderata?
Kernel density estimation

- Accuracy good enough? yes
- Separate query and reference datasets? yes
- Variable-scale kernels? yes
- Multiple scales simultaneously? yes
- Nonisotropic kernels? yes
- Arbitrary dimensionality? yes (depends on D'<<D)
- Allows all desired kernels? mostly
- Field-tested, compared to existing methods? yes

→ [Gray and Moore, 2003], [Gray and Moore 2005 in prep.]

Meets desiderata?
Smoothed particle hydrodynamics

- Accuracy good enough? yes
- Variable-scale kernels? yes
- Nonisotropic kernels? yes
- Allows all desired kernels? yes
- Edge-effect corrections (mixed kernels)? yes
- Highly non-uniform data? yes
- Fast tree-rebuilding? yes, soon perhaps faster
- Time stepping integrated? no
- Field-tested, compared to existing methods? no

Meets desiderata? Coulombic simulation

- Accuracy good enough? open question
- Allows multipole expansions? yes
- Allows all desired kernels? yes
- Fast tree-rebuilding? yes, soon perhaps faster
- Time stepping integrated? no
- Field-tested, compared to existing methods? no
- Parallelized? no

Which data structure is best in practice?

- consider nearest-neighbor as a proxy (and its variants: approximate, all-nearest-neighbor, bichromatic nearest-neighbor, point location)
- kd-trees? Uhlmann's metric trees? Fukunaga's metric trees? SR-trees? Miller et al.'s separator tree? WSPD? navigating nets? Locality-sensitive hashing?
- [Gray, Lee, Rotella, Moore] Coming soon to a journal near you

Side note: Many problems are easy for this framework

- Correlation dimension
- Hausdorff distance
- Euclidean minimum spanning tree
- more

Last step…

Now use q() to do importance sampling.

Compute $\hat{I}_q^{final} = \sum_i^M \frac{f(x_i)}{q(x_i)}, \quad x_i \sim q()$