MAIT 627 Fast Multipole Methods

Lecture 11

Outline

- Diagonal forms of translation operators for 2D and 3D Laplace equations
- Exponential (“Plane wave”) expansions
- Signature function
- Signature

Exponential form for the S|R-translation (“Plane wave expansion”).

L. Greengard and V. Rokhlin, A new version of the fast multipole method for the Laplace equation in three dimensions, Acta Numerica, 6, 1997, 229-269.

H. Cheng, L. Greengard, and V. Rokhlin, A fast adaptive multipole algorithm in three dimensions, J. Comput. Phys., 155, 1999, 468-498.

Expansions of the Greens function and arbitrary harmonic function

$$G(\mathbf{r},\mathbf{r}_0) = \frac{1}{8\pi^2}\int_0^\infty e^{-\lambda(z-z_0)}\int_0^{2\pi} e^{i\lambda[(x-x_0)\cos\alpha+(y-y_0)\sin\alpha]}d\alpha d\lambda,$$

$$\mathbf{r} = (x,y,z), \quad \mathbf{r}_0 = (x_0,y_0,z_0), \quad z > z_0.$$

For

$$a \leqslant z - z_0 \leqslant b, \sqrt{(x-x_0)^2+(y-y_0)^2} \leqslant c, \quad (a = 1, b = 4, c = 4\sqrt{2}) :$$

$$G(\mathbf{r},\mathbf{r}_0) = \frac{1}{4\pi}\sum_{k=1}^{S(\epsilon)}\frac{w_k}{M_k}e^{-\lambda_k(z-z_0)}\sum_{j=1}^{M_k} e^{i\lambda_k[(x-x_0)\cos\alpha_{jk}+(y-y_0)\sin\alpha_{jk}]},$$

$$\phi(\mathbf{r}) = \sum_{k=1}^{S(\epsilon)}\sum_{j=1}^{M_k} W_{kj}e^{-\lambda_k z}e^{i\lambda_k(x\cos\alpha_{jk}+y\sin\alpha_{jk})},$$

$$S_{\exp} = \sum_{k=1}^{S(\epsilon)} M_k = \sigma p^2, \quad S(\epsilon) = \kappa p.$$

S|R-translation

$$\phi(\mathbf{r}+\mathbf{t}) = \sum_{k=1}^{S(\epsilon)} \sum_{j=1}^{M_k} W_{kj} e^{-\lambda_k t_z} e^{i\lambda_k (t_x \cos\alpha_{jk} + t_y \sin\alpha_{jk})} e^{-\lambda_k z} e^{i\lambda_k (x\cos\alpha_{jk} + y\sin\alpha_{jk})}$$

$$= \sum_{k=1}^{S(\epsilon)} \sum_{j=1}^{M_k} \widehat{W}_{kj} e^{-\lambda_k z} e^{i\lambda_k (x\cos\alpha_{jk} + y\sin\alpha_{jk})} = \hat{\phi}(\mathbf{r}),$$

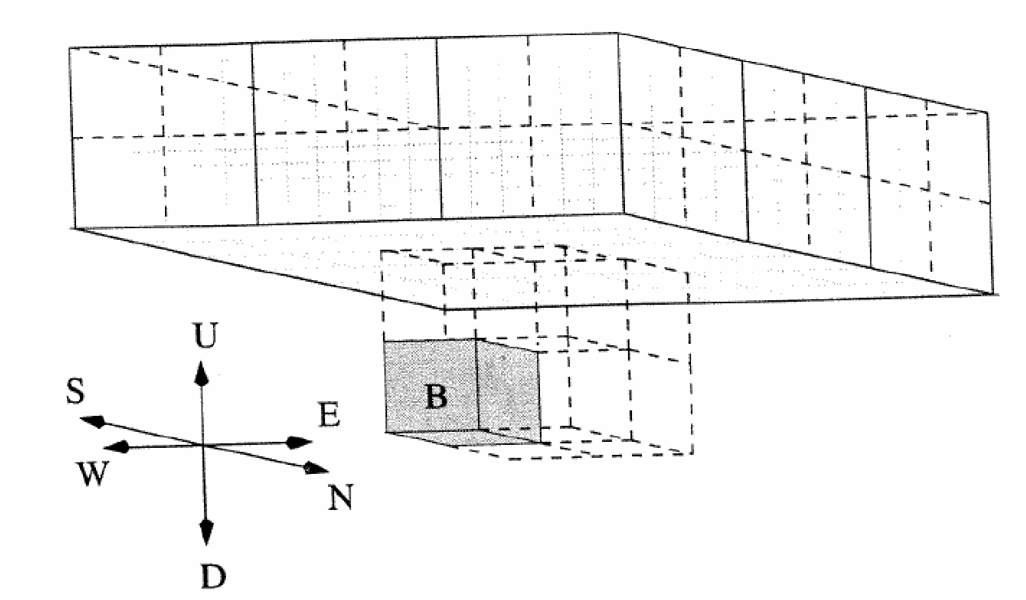
$$\widehat{W}_{kj} = E_{kj} W_{kj}, \quad E_{kj} = e^{-\lambda_k t_z} e^{i\lambda_k (t_x \cos\alpha_{jk} + t_y \sin\alpha_{jk})}, \quad \mathbf{t} = (t_x, t_y, t_z).$$

$$W_{kj} = \frac{w_k}{M_k d} \sum_{m=-(p-1)}^{p-1} e^{im\alpha_{jk}} \sum_{n=|m|}^{p-1} \frac{1}{\beta_n^m \beta_{(1)n}^m} \left(\frac{\lambda_k}{d}\right)^n \phi_n^m, \quad k = 1,\ldots,s(\epsilon), \quad j = 1,\ldots,M_k,$$

$$\phi_n^m = \alpha_n^m \alpha_{(1)n}^m \sum_{k=1}^{S(\epsilon)} \left(\frac{\lambda_k}{d}\right)^n \sum_{j=1}^{M_k} W_{kj} e^{-im\alpha_{jk}},$$

$$N^{(E|R)} = N^{(S|E)} \approx (\kappa + 4\sigma) p^3.$$

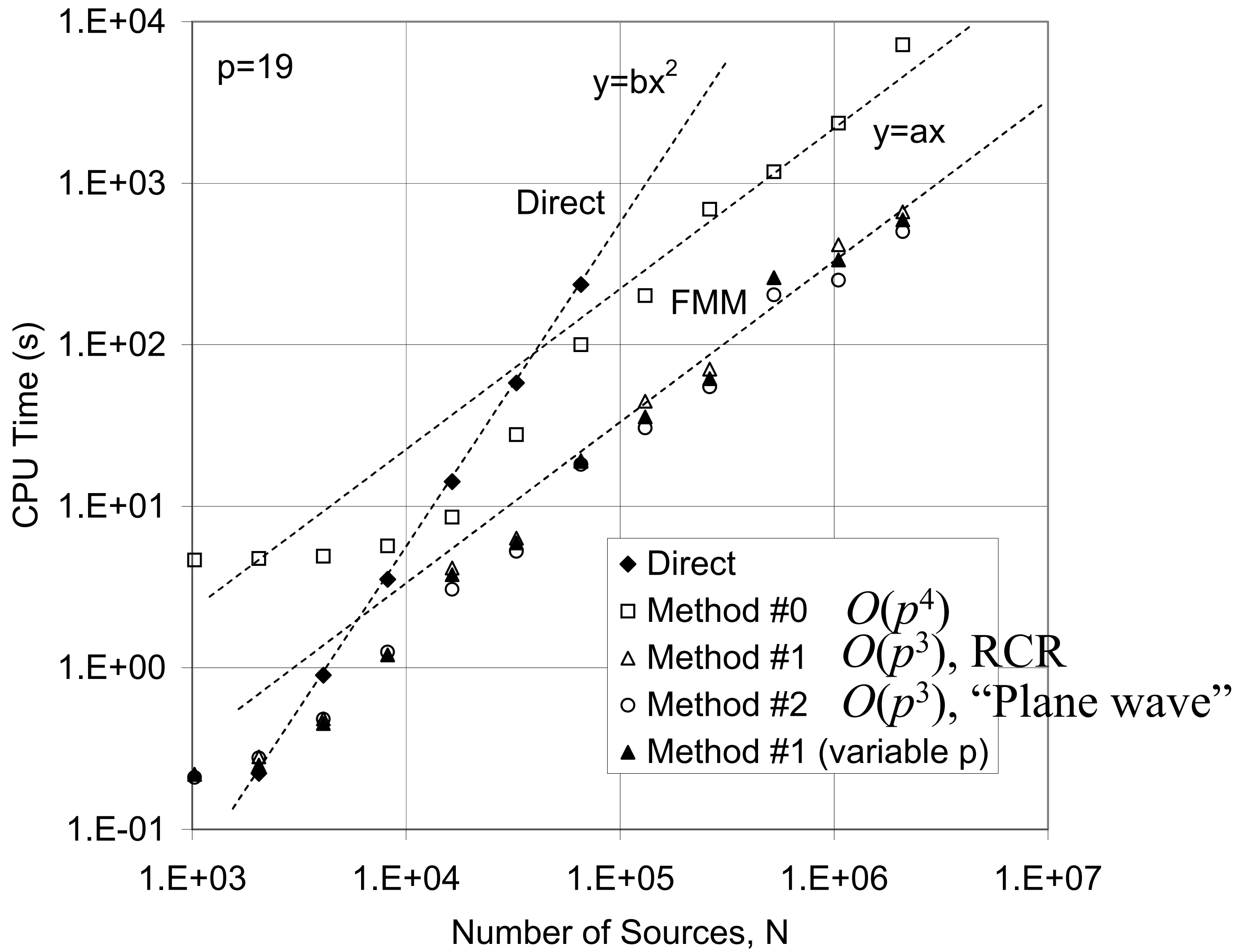
Translation scheme



Needs also 6 translation directions;
Performed by rotation transforms (axis flips);
$O(p^3)$ complexity;

(From Greengard & Rokhlin, 1997)

Comparison of translation methods (for the same accuracy)



Exponential form for the S|R-translation
(“Plane wave expansion”), 2D case

Tomasz Hrycak and Vladimir Rokhlin.
An improved fast multipole algorithm for potential fields.
SIAM Journal of Scientific Computing, 19(6):1804-1826, 1998.

Exponential expansions

$$\frac{1}{z-z_0} = \int_0^\infty e^{-x(z-z_0)}dx \approx \sum_{j=1}^{S(\epsilon)} w_j e^{-x_j(z-z_0)}, \quad \mathrm{Re}(z-z_0) > 0.$$

$$\phi(z) = \sum_{k=1}^{M} \frac{q_k}{z-z_k} \approx \sum_{j=1}^{S(\epsilon)} \sum_{k=1}^{M} w_j q_k e^{-x_j(z-z_k)} = \sum_{j=1}^{S(\epsilon)} W_j e^{-x_j z},$$

$$W_j = w_j \sum_{k=1}^{M} q_k e^{x_j z_k}.$$

$$\phi(z+t) = \sum_{j=1}^{S(\epsilon)} W_j e^{-x_j(z+t)} = \sum_{j=1}^{S(\epsilon)} E_j W_j e^{-x_j z} = \sum_{j=1}^{S(\epsilon)} \widehat{E}_j e^{-x_j z} = \hat{\phi}(z),$$

$$\widehat{E}_j = E_j W_j, \quad E_j = e^{-x_j t}.$$

Conversion of expansions

$$\phi(z) = \sum_{n=0}^{p-1} c_n S_n(z) = \sum_{j=1}^{S(\epsilon)} W_j e^{-x_j z}, \quad W_j = \sum_{n=0}^{p-1} (S|E)_{jn} c_n.$$

$$\phi(z) = \sum_{j=1}^{S(\epsilon)} W_j e^{-x_j z} = \sum_{n=0}^{p-1} d_n R_n(z), \quad d_n = \sum_{j=1}^{S(\epsilon)} (E|R)_{nj} W_j.$$

S|R-translation scheme

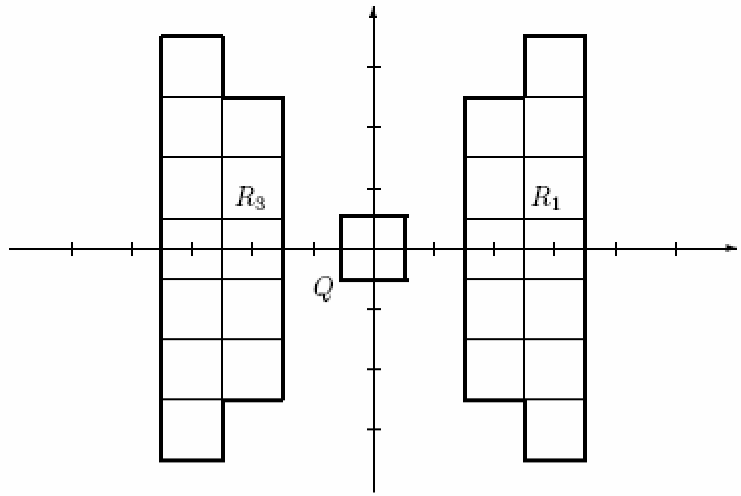


FIG. 1. *The domains R_1 and R_3.*

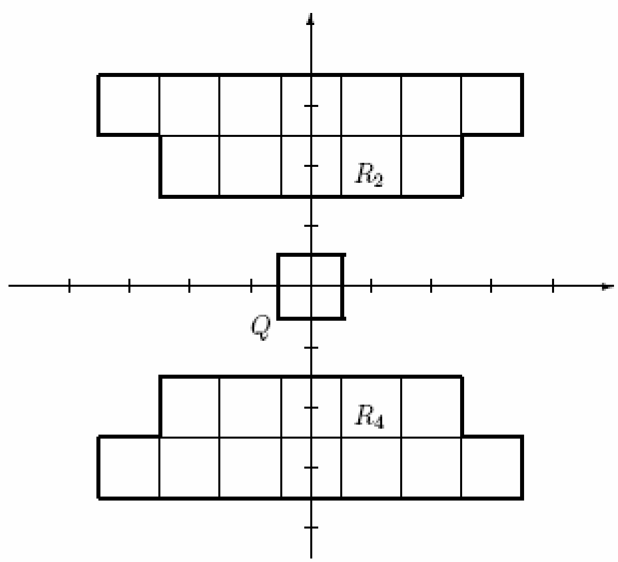


FIG. 2. *The domains R_2 and R_4.*

Theory of Signature Function 2D case

Translation kernels

$$\Lambda_r(z;\alpha) = \sum_{n=0}^{\infty} e^{in\alpha} R_n(z),$$

$$\Lambda_s^{(p)}(z;\alpha) = \sum_{n=0}^{p-1} e^{-in\alpha} S_n(z).$$

$$\Lambda_r(z;\alpha) = \sum_{n=0}^{\infty} e^{in\alpha} R_n(z) = \sum_{n=0}^{\infty} \frac{(-ze^{i\alpha})^n}{n!} = e^{-ze^{i\alpha}}.$$

Integral representation of basis functions(1)

$$R_n(z) = \frac{1}{2\pi}\int_0^{2\pi} e^{-in\alpha}\Lambda_r(z;\alpha)d\alpha, \quad n = 0,1,\ldots, \quad 0 \leqslant |z| < \infty.$$

Indeed:

$$\begin{aligned}\frac{1}{2\pi}\int_0^{2\pi} e^{-in\alpha}\Lambda_r(z;\alpha)d\alpha &= \frac{1}{2\pi}\int_0^{2\pi} e^{-in\alpha}\sum_{m=0}^{\infty} e^{im\alpha}R_m(z)d\alpha \\ &= \sum_{m=0}^{\infty} R_m(z)\frac{1}{2\pi}\int_0^{2\pi} e^{i(m-n)\alpha}d\alpha \\ &= \sum_{m=0}^{\infty} R_m(z)\delta_{mn} = R_n(z).\end{aligned}$$

Integral representation of basis functions(2)

$$S_n(z) = \frac{1}{2\pi}\int_0^{2\pi} e^{in\alpha}\Lambda_s^{(p)}(z;\alpha)\,d\alpha, \quad n = 0, 1, \ldots, p-1, \quad 0 < |z| < \infty.$$

Indeed:

$$\frac{1}{2\pi}\int_0^{2\pi} e^{in\alpha}\Lambda_s^{(p)}(z;\alpha)\,d\alpha = \frac{1}{2\pi}\int_0^{2\pi} e^{in\alpha}\sum_{m=0}^{p-1} e^{-im\alpha}S_m(z)\,d\alpha$$

$$= \sum_{m=0}^{p-1} S_m(z)\frac{1}{2\pi}\int_0^{2\pi} e^{i(n-m)\alpha}\,d\alpha$$

$$= \sum_{m=0}^{p-1} S_m(z)\delta_{mn} = S_n(z).$$

R-signature function

$$\phi(z) = \sum_{n=0}^{\infty} \phi_n R_n(z) \rightarrow \quad \Phi_r(\alpha) = \sum_{n=0}^{\infty} \phi_n e^{-in\alpha}.$$

Arbitrary function

$$\phi(z) = \sum_{n=0}^{\infty} \phi_n R_n(z) = \sum_{n=0}^{\infty} \phi_n \frac{1}{2\pi} \int_0^{2\pi} e^{-in\alpha} \Lambda_r(z;\alpha) d\alpha$$

$$= \frac{1}{2\pi} \int_0^{2\pi} \left(\sum_{n=0}^{\infty} \phi_n e^{-in\alpha} \right) \Lambda_r(z;\alpha) d\alpha = \frac{1}{2\pi} \int_0^{2\pi} \Phi_r(\alpha) \Lambda_r(z;\alpha) d\alpha.$$

Green's function:

$$G(z - z_0) = \lim_{p\to\infty} \sum_{n=0}^{p-1} S_n(-z_0) R_n(z) =$$

$$= \lim_{p\to\infty} \sum_{n=0}^{p-1} S_n(-z_0) \frac{1}{2\pi} \int_0^{2\pi} e^{-in\alpha} \Lambda_r(z;\alpha) d\alpha$$

$$= \lim_{p\to\infty} \frac{1}{2\pi} \int_0^{2\pi} \Lambda_s^{(p)}(-z_0;\alpha) \Lambda_r(z;\alpha) d\alpha, \quad 0 \leqslant |z| < a < |z_0|.$$

S-signature function

$$\phi(z) = \sum_{n=0}^{\infty} \phi_n S_n(z) \rightarrow \quad \Phi_s(\alpha) = \sum_{n=0}^{\infty} \phi_n e^{in\alpha}.$$

Arbitrary function

$$\phi(z) = \sum_{n=0}^{\infty} \phi_n S_n(z) = \lim_{p\to\infty} \sum_{n=0}^{p-1} \phi_n \frac{1}{2\pi} \int_0^{2\pi} e^{in\alpha} \Lambda_s^{(p)}(z;\alpha) d\alpha$$

$$= \frac{1}{2\pi} \int_0^{2\pi} \left(\sum_{n=0}^{\infty} \phi_n e^{in\alpha} \right) \Lambda_s^{(p)}(z;\alpha) d\alpha = \frac{1}{2\pi} \int_0^{2\pi} \Phi_s(\alpha) \Lambda_s^{(p)}(z;\alpha) d\alpha.$$

$$\phi(z) = \lim_{p\to\infty} \phi^{(p)}(z), \quad \phi^{(p)}(z) = \frac{1}{2\pi} \int_0^{2\pi} \Phi_s(\alpha) \Lambda_s^{(p)}(z;\alpha) d\alpha, \quad 0 < a < |z|,$$

Green's function:

$$G(z - z_0) = \ln \frac{1}{z - z_0} = \sum_{n=0}^{\infty} R_n(-z_0) S_n(z), \quad |z| > |z_0|,$$

$$G(z - z_0) \rightarrow \Phi_s(\alpha) = \Lambda_r(-z_0;\alpha).$$

Translations of signature function

R|R-translation

$$\hat{\phi}(z) = \phi(z+t) = \frac{1}{2\pi}\int_0^{2\pi} \Phi_r(\alpha)\Lambda_r(z+t;\alpha)d\alpha$$

$$= \frac{1}{2\pi}\int_0^{2\pi} \Phi_r(\alpha)\Lambda_r(t;\alpha)\Lambda_r(z;\alpha)d\alpha = \frac{1}{2\pi}\int_0^{2\pi} \widehat{\Phi}_r(\alpha)\Lambda_r(z;\alpha)d\alpha,$$

since

$$\Lambda_r(z+t;\alpha) = e^{-(z+t)e^{i\alpha}} = e^{-te^{i\alpha}}e^{-ze^{i\alpha}} = \Lambda_r(t;\alpha)\Lambda_r(z;\alpha).$$

So

$$\widehat{\Phi}_r(\alpha) = (\mathcal{R}|\mathcal{R})(t)[\Phi_r(\alpha)] = \Lambda_r(t;\alpha)\Phi_r(\alpha).$$

Translations of signature function

S|S-translation

$$\hat{\phi}_n = \sum_{n'=0}^{\infty} (S|S)_{nn'} \phi_{n'} = \sum_{n'=0}^{\infty} R_{n-n'}(t) \phi_{n'}.$$

$$\hat{\Phi}_s(\alpha) = \sum_{n=0}^{\infty} \hat{\phi}_n e^{in\alpha} = \sum_{n'=0}^{\infty} \left[\sum_{n=0}^{\infty} e^{i(n-n')\alpha} R_{n-n'}(t) \right] e^{in'\alpha} \phi_{n'}$$

$$= \Lambda_r(t;\alpha) \sum_{n'=0}^{\infty} e^{in'\alpha} \phi_{n'} = \Lambda_r(t;\alpha) \Phi_s(\beta, \alpha).$$

$$\hat{\Phi}_s(\alpha) = (\mathcal{S}|\mathcal{S})(\mathbf{t})[\Phi_s(\alpha)] = \Lambda_r(t;\alpha)\Phi_s(\alpha).$$

Translations of signature function

S|S-translation / Corollary

$$\breve{\phi}(z) = \phi(z+t) = \lim_{p\to\infty} \frac{1}{2\pi} \int_0^{2\pi} \Phi_s(\alpha)\Lambda_s^{(p)}(z+t;\alpha)\,d\alpha$$

$$= \lim_{p\to\infty} \frac{1}{2\pi} \int_0^{2\pi} \Phi_s(\alpha)\Lambda_s^{(p)}(z;\alpha)\Lambda_r(t;\alpha)\,d\alpha, \quad |z| > |t|.$$

Translations of signature function

S|R-translation

Corollary from S|S:

$$\hat{\phi}(z) = \phi(z+t) = \lim_{p\to\infty} \frac{1}{2\pi}\int_0^{2\pi} \Phi_s(\alpha)\Lambda_s^{(p)}(z+t;\alpha)d\alpha$$
$$= \lim_{p\to\infty} \frac{1}{2\pi}\int_0^{2\pi} \Phi_s(\alpha)\Lambda_s^{(p)}(z;\alpha)\Lambda_r(t;\alpha)d\alpha, \quad |z| > |t|.$$

Exchange *z* and *t*:

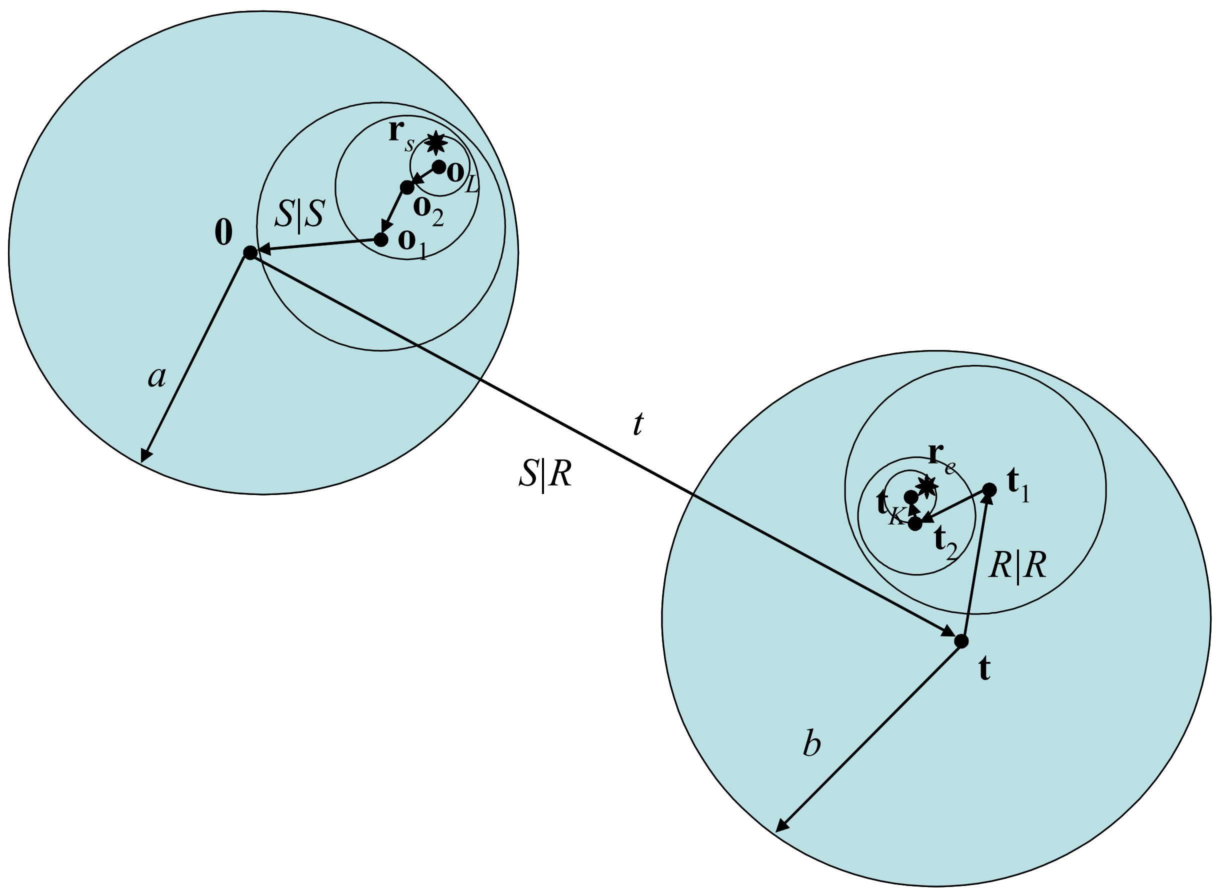
$$\hat{\phi}(z) = \phi(z+t) = \lim_{p\to\infty} \frac{1}{2\pi}\int_0^{2\pi} \Phi_s(\alpha)\Lambda_s^{(p)}(z+t;\alpha)d\alpha$$
$$= \lim_{p\to\infty} \frac{1}{2\pi}\int_0^{2\pi} \Phi_s(\alpha)\Lambda_s^{(p)}(t;\alpha)\Lambda_r(z;\alpha)d\alpha, \quad |t| > |z|.$$

S|R:

$$\widehat{\Phi}_r^{(p)}(\alpha) = (\mathcal{S}|\mathcal{R})^{(p)}(t)[\Phi_s(\alpha)] = \Lambda_s^{(p)}(t;\alpha)\Phi_s(\alpha).$$

$$\phi(z) = \lim_{p\to\infty} \phi^{(p)}(z), \quad \hat{\phi}^{(p)}(z) = \frac{1}{2\pi}\int_0^{2\pi} \widehat{\Phi}_r^{(p)}(\alpha)\Lambda_r(z;\alpha)d\alpha.$$

Translation error



Translation error

$$\Phi_s(\alpha) = \Lambda_r(\mathbf{o}_L - \mathbf{r}_s;\alpha)$$

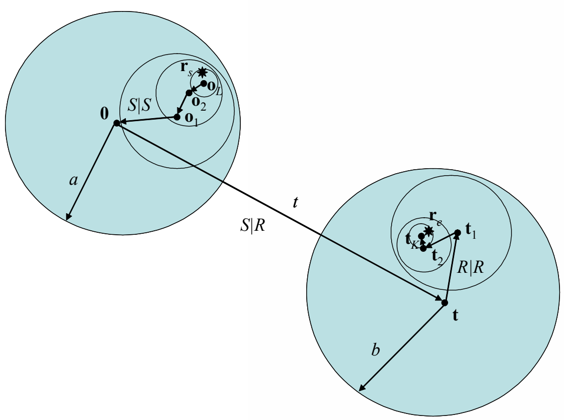
$$\Phi'_s(\alpha) = \Lambda_r(-\mathbf{o}_1;\alpha)\Lambda_r(\mathbf{o}_1 - \mathbf{o}_2;\alpha)\ldots\Lambda_r(\mathbf{o}_{L-1} - \mathbf{o}_L;\alpha)\Phi_s(\alpha),$$

$$\Phi'_r(\alpha) = \Lambda_s^{(p)}(\mathbf{t};\alpha)\Phi'_s(\alpha),$$

The only place for error!

$$\Phi_r(\alpha) = \Lambda_r(\mathbf{t}_K - \mathbf{t}_{K-1};\alpha)\Lambda_r(\mathbf{t}_2 - \mathbf{t}_1;\alpha)\ldots\Lambda_r(\mathbf{t}_1 - \mathbf{t};\alpha)\Phi'_r(\alpha),$$

$$\Psi(\alpha) = \Lambda_r(\mathbf{r}_e - \mathbf{t}_K;\alpha)\Phi_r(\alpha)$$



$$\Phi'_s(\alpha) = \Lambda_r(-\mathbf{o}_L;\alpha)\Phi_s(\alpha),$$

$$\Phi'_s(\alpha) = \Lambda_r(-\mathbf{r}_s;\alpha).$$

$$\Phi_r(\alpha) = \Lambda_r(\mathbf{t}_K - \mathbf{t};\alpha)\Phi'_r(\alpha).$$

$$\Psi(\alpha) = \Lambda_r(\mathbf{r}_e - \mathbf{t}_K;\alpha)\Phi_r(\alpha) = \Lambda_r(\mathbf{r}_e - \mathbf{t};\alpha)\Phi'_r(\alpha).$$

Sampling of signature function

The bandwidth of the singular kernel can differ from the number of samples!

$$\phi^{(p)}(z) = \frac{1}{2\pi}\int_0^{2\pi} \Psi(\alpha)d\alpha \approx \frac{1}{p'}\sum_{k=0}^{p'-1} \Lambda_r(z_e - z_s - t, \alpha_k)\Lambda_s^{(p)}(z_*, \alpha_k).$$

$$\alpha_k = k\gamma_{p'}, \quad k = 0, \ldots, p' - 1, \quad \gamma_{p'} = \frac{2\pi}{p'}.$$

Error bound

$$\left|\epsilon_1^{(p)}\right| = \left|\phi(z_e) - \phi_1^{(p)}(z_e)\right| \leqslant \sum_{n=p}^{\infty} \frac{(n-1)!}{t^n n!}\left(\frac{r}{t}\right)^n < \left(\frac{r}{t}\right)^p\left[\frac{1}{p} + \sum_{n=1}^{\infty}\frac{1}{n}\left(\frac{r}{t}\right)^n\right]$$

$$= \left(\frac{r}{t}\right)^p\left[\frac{1}{p} - \ln\left(1 - \frac{r}{t}\right)\right] \leqslant \left(\frac{2a}{t}\right)^p\left[\frac{1}{p} - \ln\left(1 - \frac{2a}{t}\right)\right].$$

$$|\epsilon^{(p)}| \leqslant \left(\frac{a}{t-a}\right)^p\left[\frac{1}{p} - \ln\left(1 - \frac{a}{t-a}\right)\right].$$

$$\frac{\frac{2a}{t}}{\frac{a}{t-a}} = \frac{2t-2a}{t} = 2 - \frac{2a}{t} > 1.$$

$$\left(\frac{2a}{t}\right)^{p_{eff}} = \left(\frac{a}{t-a}\right)^p,$$

$$p_{eff} = p\frac{\ln\left(\frac{a}{t-a}\right)}{\ln\left(\frac{2a}{t}\right)} = p\frac{\ln\left(\frac{\sqrt{2}/2}{2-\sqrt{2}/2}\right)}{\ln\left(\frac{2\left(\sqrt{2}/2\right)}{2}\right)} \approx 1.74p.$$