Fréchet derivatives under various parameterizations using chain rule for LEGO module m_parameterization.f90

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Overview

Physical meaning of symbols uniformly used in this code:

 $\begin{array}{lll} \text{vp} & & \text{P-wave velocity} \\ \text{vs} & & \text{S-wave velocity} \\ \text{sp} = 1/\text{vp} & & \text{P-wave slowness} \\ \text{sps} = \text{vs/vp} & & \text{inv Vp-Vs ratio} \\ \end{array}$

ip =vp*rho P-wave (acoustic) impedance

rho density

kpa=rho*vp^2 bulk modulus

 $lda = rho*(vp^2-2vs^2) \quad 1st \ Lam\'e \ parameter$

 $mu = rho*vs^2$ 2nd Lamé parameter, shear modulus

Overview

Considered parameterizations

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SITUATION	PARAMETERIZATION	ALLOWED PARAMETERS
WaveEquation	moduli-density	kpa (or lda mu) rho
canonical models	velocities-density	vp vs rho
seismic	velocities-impedance	vp vs ip
tomography	slowness-density	sp sps rho
optimization	can be any of above	_

Source-Destination trilogy:

model m \xrightarrow{FWD} WaveEq Im	PARAMETERIZATION (optim x,g \xrightarrow{FWD}	model m
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- ▶ model m → WaveEq Im depending on field.
- WaveEq produces gkpa (or glda, gmu) and grho under moduli-density parameterization.
- ▶ then m_parameterization.f90 converts them to another parameterization for optim x,g, which can be any of parameterization

Overview

ACTIVE versus PASSIVE

- Active parameters will be converted to optim x via feature scaling (e.g. (par-par_min)/(par_max-par_min)), and will be updated by optimization methods.
 - ► Mono-parameter inversion: 1 active parameter.
 - Multi-parameter inversion: > 1 active parameters.
 - Scaling in m_linesearch.f90 depends only on the 1st active parameters (no matter of it's velocity or not).
 - Output of inversion results has same sequence of active parameters listed in setup.in
- Passive parameters will NOT be converted to optim x, and will NOT be updated by optimization methods.
- However, they may still be updated according to user-specified empirical law (e.g. Gardner), which serves as hard constraints between parameters.
 - User has to modified the code where necessary to insert such a law as symbolic computation is not straightforward in fortran
 - Such a law may change the optim g for active parameters.

velocities-density

velocities-impedance

slowness-density

$$\begin{cases} \kappa = \rho V_P^2 \\ \rho_0 = \rho \end{cases}$$

$$\nabla_{V_P} = \nabla_{\kappa} \frac{\partial \kappa}{\partial V_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_P}$$

$$= \nabla_{\kappa} 2\rho V_P$$

$$\nabla_{\rho} = \nabla_{\kappa} \frac{\partial \kappa}{\partial \rho} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial \rho}$$

$$= \nabla_{\kappa} V_P^2 + \nabla_{\rho_0}$$

$$\begin{cases}
\kappa = \rho V_{P}^{2} \\
\rho_{0} = \rho
\end{cases}$$

$$\begin{cases}
\kappa = \rho V_{P}^{2} \\
\rho_{0} = \rho
\end{cases}$$

$$\nabla_{\kappa} = \nabla_{\nu_{P}} \frac{\partial V_{P}}{\partial \kappa} + \nabla_{\rho} \frac{\partial \rho}{\partial \kappa}$$

$$= \nabla_{\nu_{P}} \frac{\partial V_{P}}{\partial \kappa} + \nabla_{\rho} \frac{\partial \rho}{\partial \kappa}$$

$$= \nabla_{\nu_{P}} \frac{1}{2\rho_{0}} \sqrt{\frac{\rho_{0}}{\kappa}}$$

$$= \nabla_{\nu_{P}} 0.5 \rho_{0}^{-0.5} \kappa^{-0.5}$$

$$\nabla_{\rho} = \nabla_{\kappa} \frac{\partial \kappa}{\partial \rho} + \nabla_{\rho_{0}} \frac{\partial \rho_{0}}{\partial \rho}$$

$$= \nabla_{\nu_{P}} \sqrt{\frac{\partial \nu_{P}}{\partial \rho}} + \nabla_{\rho} \frac{\partial \rho}{\partial \rho_{0}}$$

$$= \nabla_{\nu_{P}} \left(-\frac{\kappa}{2\rho_{0}^{2}} \sqrt{\frac{\rho_{0}}{\kappa}} \right) + \nabla_{\rho}$$

$$= \nabla_{\nu_{P}} \left(-0.5 \rho_{0}^{-1.5} \kappa^{0.5} \right) + \nabla_{\rho}$$

PARAMETERIZATION velocities-density + PASSIVE gardner

isotropic ACoustic

$$\begin{bmatrix}
\rho = aV_P^b \\
\\
\rho_0 = \rho = aV_P^b
\end{bmatrix}$$

$$\begin{cases}
\kappa = \rho V_P^2 = aV_P^{b+2} \\
\rho_0 = \rho = aV_P^b
\end{cases}$$

$$V_P = \left(\frac{\kappa}{a}\right)^{\frac{1}{b+2}}$$

$$\nabla_{V_P} = \nabla_{\kappa} \frac{\partial \kappa}{\partial V_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_P} \\
= \nabla_{\kappa} a(b+2)V_P^{b+1} + \nabla_{\rho_0} abV_P^{b-1}$$

$$= \left(\nabla_{\kappa} \frac{b+2}{b} V_P^2 + \nabla_{\rho_0}\right) abV_P^{b-1}$$

$$= \nabla_{V_P} \frac{1}{a(b+2)} \left(\frac{\kappa}{a}\right)^{-\frac{b+1}{b+2}}$$

$$\begin{cases} \lambda = \rho(V_P^2 - 2V_S^2) \\ \mu = \rho V_S^2 \\ \rho_0 = \rho \end{cases} \qquad \begin{cases} V_P = \sqrt{\frac{\lambda + 2\mu}{\rho_0}} \\ V_S = \sqrt{\frac{\mu}{\rho_0}} \\ V_S = \sqrt{\frac{\mu}{\rho_0}} \end{cases} \\ \nabla_{V_P} = \nabla_{\lambda} \frac{\partial \lambda}{\partial V_P} + \nabla_{\mu} \frac{\partial \mu}{\partial V_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_P} \end{cases} \qquad \begin{cases} V_P = \sqrt{\frac{\lambda + 2\mu}{\rho_0}} \\ V_S = \sqrt{\frac{\mu}{\rho_0}} \\ \rho = \rho_0 \end{cases} \\ = \nabla_{\lambda} 2\rho V_P \\ \nabla_{V_S} = \nabla_{\lambda} \frac{\partial \lambda}{\partial V_S} + \nabla_{\mu} \frac{\partial \mu}{\partial V_S} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_S} = \dots \\ = \nabla_{\lambda} (-4)\rho V_S + \nabla_{\mu} 2\rho V_S \\ = (-2\nabla_{\lambda} + \nabla_{\mu}) 2\rho V_S \end{cases} \qquad = \dots \\ \nabla_{\rho} = \nabla_{\lambda} \frac{\partial \lambda}{\partial \rho} + \nabla_{\mu} \frac{\partial \mu}{\partial \rho} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial \rho} \qquad \nabla_{\rho_0} = \nabla_{V_P} \frac{\partial V_P}{\partial \rho} + \nabla_{V_S} \frac{\partial V_S}{\partial \rho} + \nabla_{\rho} \frac{\partial \rho}{\partial \rho_0} \\ = \nabla_{\lambda} (V_P^2 - 2V_S^2) + \nabla_{\mu} V_S^2 + \nabla_{\rho_0} = \dots \\ = \nabla_{\lambda} V_P^2 + (-2\nabla_{\lambda} + \nabla_{\mu}) V_S^2 + \nabla_{\rho_0} \end{cases} = \dots$$

$$\rho = aV_P^b$$

$$\left\{ \begin{array}{l} \lambda = \rho(V_P^2 - 2V_S^2) = aV_P^{b+2} - 2aV_P^bV_S^2 \\ \mu = \rho V_S^2 = aV_P^bV_S^2 \\ \rho_0 = \rho = aV_P^b \end{array} \right.$$

$$\begin{array}{lll} \nabla_{V_{P}} & = & \nabla_{\lambda} \frac{\partial \lambda}{\partial V_{P}} + \nabla_{\mu} \frac{\partial \mu}{\partial V_{P}} + \nabla_{\rho_{0}} \frac{\partial \rho_{0}}{\partial V_{P}} \\ & = & \nabla_{\lambda} \left(a(b+2)V_{P}^{b+1} - 2abV_{P}^{b-1}V_{S}^{2} \right) + \nabla_{\mu}abV_{P}^{b-1}V_{S}^{2} + \nabla_{\rho_{0}}abV_{P}^{b-1} \\ & = & \left(\nabla_{\lambda} \left(\frac{b+2}{b}V_{P}^{2} - 2V_{S}^{2} \right) + \nabla_{\mu}V_{S}^{2} + \nabla_{\rho_{0}} \right) abV_{P}^{b-1} \\ & = & \left(\nabla_{\lambda} \frac{b+2}{b}V_{P}^{2} + \left(-2\nabla_{\lambda} + \nabla_{\mu} \right)V_{S}^{2} + \nabla_{\rho_{0}} \right) abV_{P}^{b-1} \\ \nabla_{V_{S}} & = & \nabla_{\lambda} \frac{\partial \lambda}{\partial V_{S}} + \nabla_{\mu} \frac{\partial \mu}{\partial V_{S}} + \nabla_{\rho_{0}} \frac{\partial \rho_{0}}{\partial V_{S}} \\ & = & \nabla_{\lambda} (-4aV_{P}^{b}V_{S}) + \nabla_{\mu}2aV_{P}^{b}V_{S} \\ & = & \left(-2\nabla_{\lambda} + \nabla_{\mu} \right) 2aV_{P}^{b}V_{S} \end{array}$$

velocities-density

velocities-impedance

slowness-density

PARAMETERIZATION velocities-impedance

isotropic ACoustic

$$\begin{cases}
\kappa = \rho V_{P}^{2} = V_{P}I_{P} \\
\rho_{0} = \rho = \frac{I_{P}}{V_{P}}
\end{cases}$$

$$\nabla_{V_{P}} = \nabla_{\kappa} \frac{\partial \kappa}{\partial V_{P}} + \nabla_{\rho_{0}} \frac{\partial \rho_{0}}{\partial V_{P}}$$

$$= \nabla_{\kappa} I_{P} + \nabla_{\rho_{0}} (-I_{P}V_{P}^{-2})$$

$$= (\nabla_{\kappa} - \nabla_{\rho_{0}} V_{P}^{-2}) V_{P}\rho$$

$$\nabla_{I_{P}} = \nabla_{\kappa} \frac{\partial \kappa}{\partial I_{P}} + \nabla_{\rho_{0}} \frac{\partial \rho_{0}}{\partial I_{P}}$$

$$= \nabla_{\kappa} V_{P} + \nabla_{\rho_{0}} V_{P}^{-1}$$

$$\nabla_{\rho_{0}} = \nabla_{\rho_{0}} V_{P}^{-1}$$

$$\nabla_{\rho_{0}} = \nabla_{\rho_{0}} \frac{\partial V_{P}}{\partial \rho_{0}} + \nabla_{\rho_{0}} \frac{\partial I_{P}}{\partial \rho_{0}}$$

$$= \nabla_{\rho_{0}} \frac{\partial V_{P}}{\partial \rho_{0}} + \nabla_{I_{P}} \frac{\partial I_{P}}{\partial \rho_{0}}$$

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$$= \nabla_{\rho_{0}} \frac{\partial V_{P}}{\partial \rho_{0}} + \nabla_{\rho_{0}} \frac{\kappa}{\partial \rho_{0}}$$

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$$= \nabla_{\rho_{0}} \frac{\partial V_{P}}{\partial \rho_{0}} + \nabla_{\rho_{0}} \frac{\kappa}{\partial \rho_{0}}$$

 $I_P = V_P \rho$

PARAMETERIZATION velocities-impedance

$$\begin{cases} \lambda = \rho(V_P^2 - 2V_S^2) = V_P I_P - \frac{2V_S^2 I_P}{V_P} \\ \mu = \rho V_S^2 = \frac{V_S^2 I_P}{V_P} \\ \rho_0 = \rho = \frac{I_P}{V_P} \end{cases}$$

$$\nabla_{V_{P}} = \nabla_{\lambda} \frac{\partial \lambda}{\partial V_{P}} + \nabla_{\mu} \frac{\partial \mu}{\partial V_{P}} + \nabla_{\rho_{0}} \frac{\partial \rho_{0}}{\partial V_{P}}$$

$$= \nabla_{\lambda} \left(I_{P} + \frac{2V_{S}^{2}I_{P}}{V_{P}^{2}} \right) + \nabla_{\mu} \left(-\frac{V_{S}^{2}I_{P}}{V_{P}^{2}} \right) + \nabla_{\rho_{0}} \left(-\frac{I_{P}}{V_{P}^{2}} \right)$$

$$= \left(\nabla_{\lambda} (V_{P}^{2} + 2V_{S}^{2}) - \nabla_{\mu} V_{S}^{2} - \nabla_{\rho_{0}} \right) \frac{I_{P}}{V_{P}^{2}}$$

$$= \left(\nabla_{\lambda} V_{P}^{2} + (2\nabla_{\lambda} - \nabla_{\mu}) V_{S}^{2} - \nabla_{\rho_{0}} \right) \frac{\rho}{V_{P}}$$

$$\nabla_{V_{S}} = \nabla_{\lambda} \frac{\partial \lambda}{\partial V_{S}} + \nabla_{\mu} \frac{\partial \mu}{\partial V_{S}} + \nabla_{\rho_{0}} \frac{\partial \rho_{0}}{\partial V_{S}}$$

$$= \nabla_{\lambda} \frac{-4V_{S}I_{P}}{V_{P}} + \nabla_{\mu} \frac{2V_{S}I_{P}}{V_{P}}$$

$$= \left(-2\nabla_{\lambda} + \nabla_{\mu} \right) \frac{2V_{S}I_{P}}{V_{P}}$$

$$= \left(-2\nabla_{\lambda} + \nabla_{\mu} \right) 2V_{S}\rho$$

PARAMETERIZATION velocities-impedance

isotropic P-SV continued

$$\begin{cases} \lambda = \rho(V_P^2 - 2V_S^2) = V_P I_P - \frac{2V_S^2 I_P}{V_P} \\ \mu = \rho V_S^2 = \frac{V_S^2 I_P}{V_P} \\ \rho_0 = \rho = \frac{I_P}{V_P} \end{cases}$$

$$\begin{split} \nabla_{I_P} &= \nabla_{\lambda} \frac{\partial \lambda}{\partial I_P} + \nabla_{\mu} \frac{\partial \mu}{\partial I_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial I_P} \\ &= \nabla_{\lambda} \left(V_P - \frac{2V_S^2}{V_P} \right) + \nabla_{\mu} \frac{V_S^2}{V_P} + \nabla_{\rho_0} \frac{1}{V_P} \\ &= \left(\nabla_{\lambda} (V_P^2 - 2V_S^2) + \nabla_{\mu} V_S^2 + \nabla_{\rho_0} \right) \frac{1}{V_P} \\ &= \left(\nabla_{\lambda} V_P^2 + (-2\nabla_{\lambda} + \nabla_{\mu}) V_S^2 + \nabla_{\rho_0} \right) \frac{1}{V_P} \end{split}$$

velocities-density

velocities-impedance

slowness-density

isotropic ACoustic

$$S_P = 1/V_P$$

$$\begin{cases} \kappa = \rho V_P^2 = \rho S_P^{-2} \\ \rho_0 = \rho \end{cases}$$

$$\nabla_{S_P} = \nabla_{\kappa} \frac{\partial \kappa}{\partial S_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial S_P}$$

$$= \nabla_{\kappa} (-2\rho S_P^{-3})$$

$$= \nabla_{\kappa} (-2\rho V_P^3)$$

$$\nabla_{\rho} = \nabla_{\kappa} \frac{\partial \kappa}{\partial \rho} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial \rho}$$

$$= \nabla_{\kappa} S_P^{-2} + \nabla_{\rho_0}$$

$$= \nabla_{\kappa} V_P^2 + \nabla_{\rho_0}$$

$$\nabla_{\kappa} = \nabla_{S_{P}} \frac{\partial S_{P}}{\partial \kappa} + \nabla_{\rho} \frac{\partial \rho}{\partial \kappa}$$
$$= \nabla_{S_{P}} \left(\frac{1}{2} \sqrt{\frac{\kappa}{\rho_{0}} \frac{-\rho_{0}}{\kappa^{2}}} \right)$$

$$= \nabla_{S_{P}} \left(\frac{1}{2} \sqrt{\frac{\kappa}{\rho_{0}}} \frac{-\rho_{0}}{\kappa^{2}} \right)$$

$$= \nabla_{S_{P}} (-0.5) \rho_{0}^{0.5} \kappa^{-1.5}$$

$$\nabla_{\rho_{0}} = \nabla_{S_{P}} \frac{\partial S_{P}}{\partial \rho_{0}} + \nabla_{\rho} \frac{\partial \rho}{\partial \rho_{0}}$$

$$= \nabla_{S_{P}} \left(\frac{1}{2} \sqrt{\frac{\kappa}{\rho_{0}}} \frac{1}{\kappa} \right) + \nabla_{\rho}$$

$$= \nabla_{S_{P}} 0.5 \rho_{0}^{-0.5} \kappa^{-0.5} + \nabla_{\rho}$$

isotropic ACoustic

$$\left[\begin{array}{ccc} \rho = aS_P^{-b} \\ \\ \rho = aS_P^{-b} \\ \end{array} \right]$$

$$\left\{ \begin{array}{ccc} \kappa = \rho V_P^2 = aS_P^{-b-2} \\ \rho_0 = \rho = aS_P^{-b} \\ \end{array} \right.$$

$$\nabla_{S_P} = \nabla_{\kappa} \frac{\partial \kappa}{\partial S_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial S_P}$$

$$= \nabla_{\kappa} a(-b-2)S_P^{-b-3} \\ + \nabla_{\rho_0} (-ab)S_P^{-b-1} \\ = \left(\nabla_{\kappa} \frac{b+2}{b} + \nabla_{\rho_0} S_P^2 \right) (-ab) S_P^{-b-3} = \nabla_{S_P} \frac{-1}{a(b+2)} \left(\frac{\kappa}{a} \right)^{-\frac{b+3}{b+2}}$$

$$= \left(\nabla_{\kappa} \frac{b+2}{b} + \nabla_{\rho_0} V_P^{-2} \right) (-ab) V_P^{b+3}$$

$$S_{PS} = V_S/V_P = V_S S_P$$

$$\left\{ \begin{array}{l} \lambda = \rho (V_P^2 - 2V_S^2) = \rho S_P^{-2} (1 - 2S_{PS}^2) \\ \mu = \rho V_S^2 = \rho (S_{PS}/S_P)^2 \\ \rho_0 = \rho \end{array} \right.$$

$$\nabla_{S_{P}} = \nabla_{\lambda} \frac{\partial \lambda}{\partial S_{P}} + \nabla_{\mu} \frac{\partial \mu}{\partial S_{P}} + \nabla_{\rho_{0}} \frac{\partial \rho_{0}}{\partial S_{P}}
= \nabla_{\lambda} \rho(-2) S_{P}^{-3} (1 - 2S_{PS}^{2}) + \nabla_{\mu} \rho S_{PS}^{2} (-2) S_{P}^{-3}
= \left(\nabla_{\lambda} (1 - 2S_{PS}^{2}) + \nabla_{\mu} S_{PS}^{2}\right) (-2) \rho S_{P}^{-3}
= \left(\nabla_{\lambda} + (-2\nabla_{\lambda} + \nabla_{\mu}) (V_{S}/V_{P})^{2}\right) (-2) \rho V_{P}^{3}
\nabla_{S_{PS}} = \nabla_{\lambda} \frac{\partial \lambda}{\partial S_{PS}} + \nabla_{\mu} \frac{\partial \mu}{\partial S_{PS}} + \nabla_{\rho_{0}} \frac{\partial \rho_{0}}{\partial S_{PS}}
= \nabla_{\lambda} \rho S_{P}^{-2} (-4) S_{PS} + \nabla_{\mu} 2 \rho S_{PS} / S_{P}^{2}
= (-2\nabla_{\lambda} + \nabla_{\mu}) 2 \rho S_{PS} S_{P}^{-2}
= (-2\nabla_{\lambda} + \nabla_{\mu}) 2 \rho V_{P} V_{S}$$

isotropic P-SV continued

$$S_{PS} = V_S/V_P = V_S S_P$$

$$\begin{cases} \lambda = \rho(V_P^2 - 2V_S^2) = \rho S_P^{-2}(1 - 2S_{PS}^2) \\ \mu = \rho V_S^2 = \rho(S_{PS}/S_P)^2 \\ \rho_0 = \rho \end{cases}$$

$$\nabla_{\rho} = \nabla_{\lambda} \frac{\partial \lambda}{\partial \rho} + \nabla_{\mu} \frac{\partial \mu}{\partial \rho} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial \rho}$$

$$= \nabla_{\lambda} S_P^{-2} (1 - 2S_{PS}^2) + \nabla_{\mu} (S_{PS}/S_P)^2 + \nabla_{\rho_0}$$

$$= \left(\nabla_{\lambda} (1 - 2S_{PS}^2) + \nabla_{\mu} S_{PS} \right) S_P^{-2} + \nabla_{\rho_0}$$

$$= \nabla_{\lambda} V_P^2 + (-2\nabla_{\lambda} + \nabla_{\mu}) V_P V_S + \nabla_{\rho_0}$$

$$S_{PS} = V_S S_P; \rho = a S_P^{-b}$$

$$\begin{cases} \lambda = \rho S_P^{-2} (1 - 2S_{PS}^2) = a S_P^{-b-2} (1 - 2S_{PS}^2) \\ \mu = \rho (S_{PS}/S_P)^2 = a S_P^{-b-2} S_{PS}^2 \\ \rho_0 = a S_P^{-b} \end{cases}$$

$$\nabla_{S_{P}} = \nabla_{\lambda} \frac{\partial \lambda}{\partial S_{P}} + \nabla_{\mu} \frac{\partial \mu}{\partial S_{P}} + \nabla_{\rho_{0}} \frac{\partial \rho_{0}}{\partial S_{P}}$$

$$= \nabla_{\lambda} a(-b-2) S_{P}^{-b-3} (1-2S_{PS}^{2})$$

$$+ \nabla_{\mu} a(-b-2) S_{P}^{-b-3} S_{PS}^{2} + \nabla_{\rho_{0}} a(-b) S_{P}^{-b-1}$$

$$= \left(\nabla_{\lambda} (1-2S_{PS}^{2}) + \nabla_{\mu} S_{PS}^{2} + \nabla_{\rho_{0}} b(b+2) S_{P}^{2}\right) \frac{-a}{b+2} S_{P}^{-b-3}$$

$$= \left(\nabla_{\lambda} V_{P}^{2} + (-2\nabla_{\lambda} + \nabla_{\mu}) V_{S}^{2} + \nabla_{\rho_{0}} b(b+2)\right) \frac{-a}{b+2} V_{P}^{b+1}$$

$$\nabla_{S_{PS}} = \nabla_{\lambda} \frac{\partial \lambda}{\partial S_{PS}} + \nabla_{\mu} \frac{\partial \mu}{\partial S_{PS}} + \nabla_{\rho_{0}} \frac{\partial \rho_{0}}{\partial S_{PS}}$$

$$= \nabla_{\lambda} a S_{P}^{-b-2} (-4) S_{PS} + \nabla_{\mu} a S_{P}^{-b-2} 2 S_{PS}$$

$$= (-2\nabla_{\lambda} + \nabla_{\mu}) 2a S_{P}^{-b-2} S_{PS}$$

$$= (-2\nabla_{\lambda} + \nabla_{\mu}) 2a V_{P}^{b+1} V_{S}$$